Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

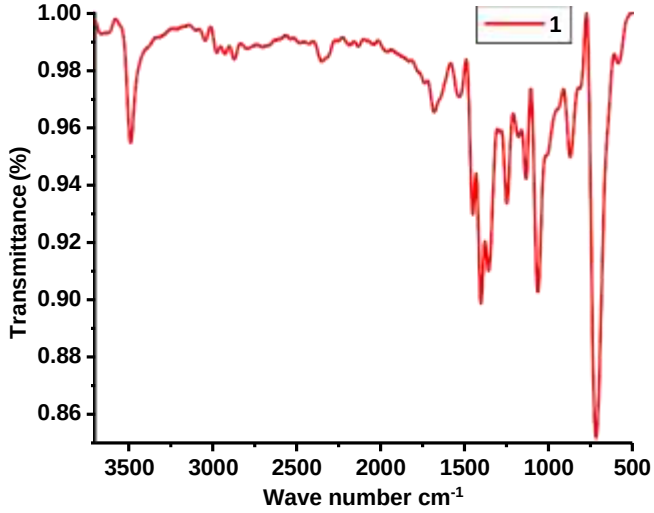


Figure S1. FT-IR spectrum of **1** (neat).

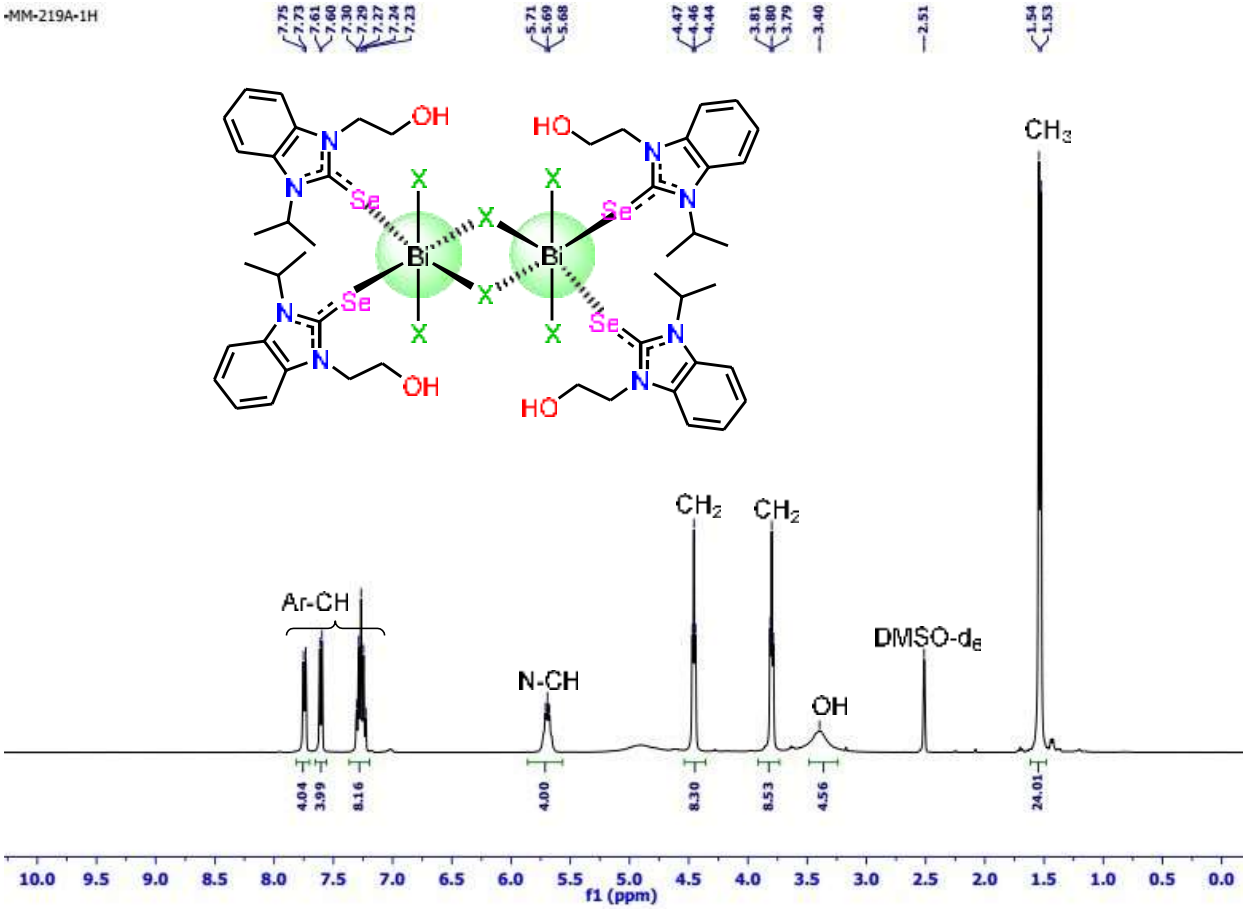


Figure S2. ^{1}H NMR spectrum of **1** in DMSO-d_6 at RT.

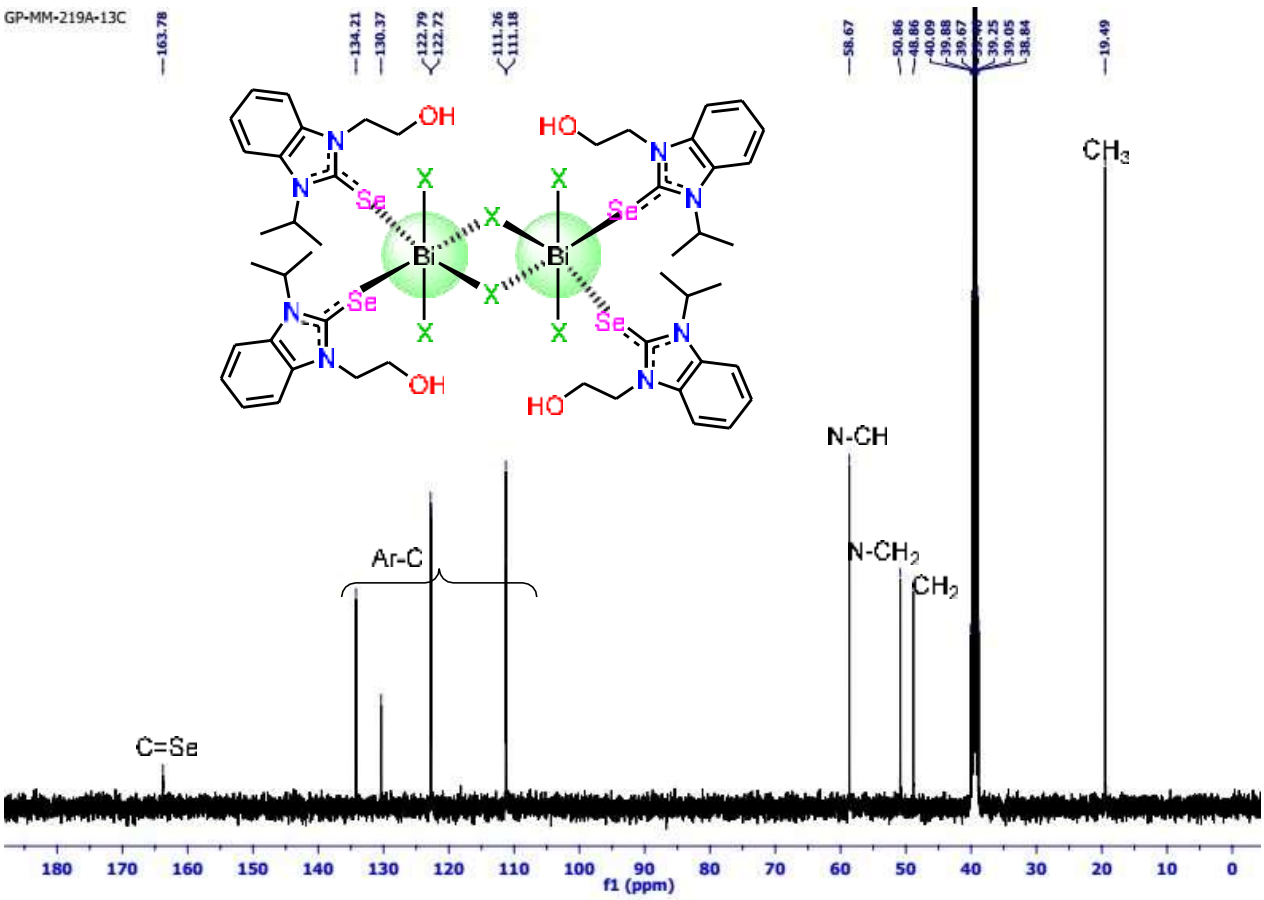


Figure S3. ^{13}C NMR spectrum of **1** in DMSO-d_6 at RT.

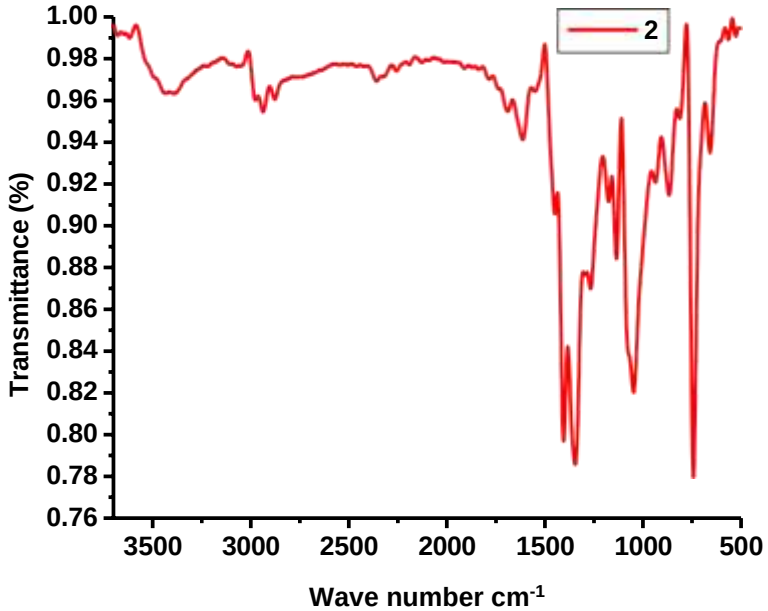


Figure S4. FT-IR spectrum of **2** (neat).

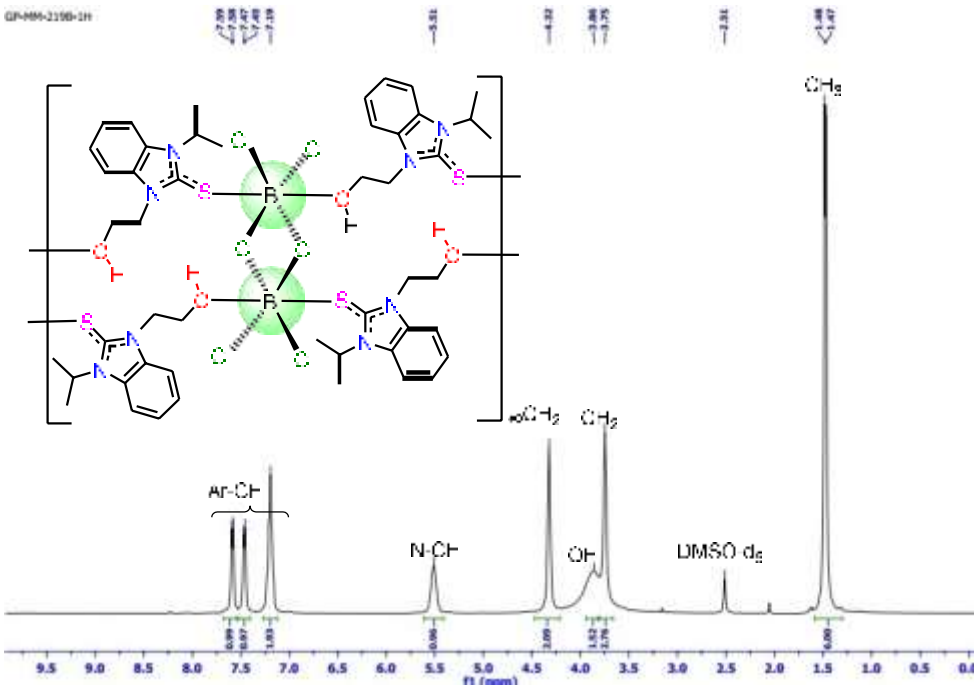


Figure S5. ^{1}H NMR spectrum of **2** in DMSO-d_6 at RT.

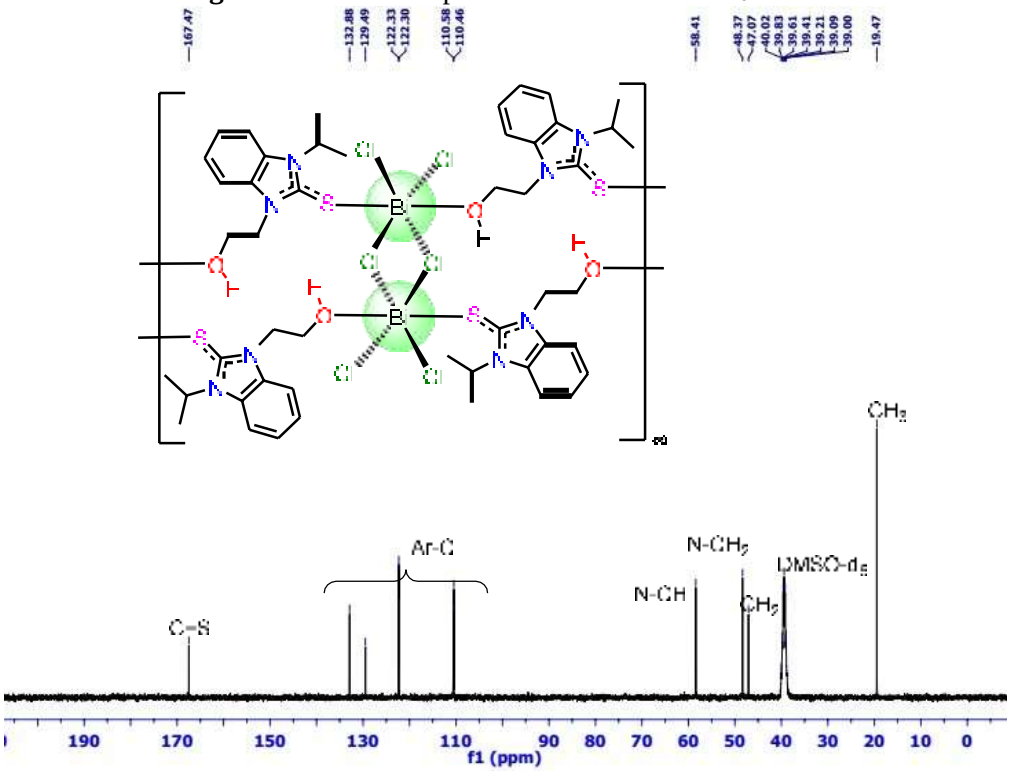


Figure S6. ^{13}C NMR spectrum of **2** in DMSO-d_6 at RT.

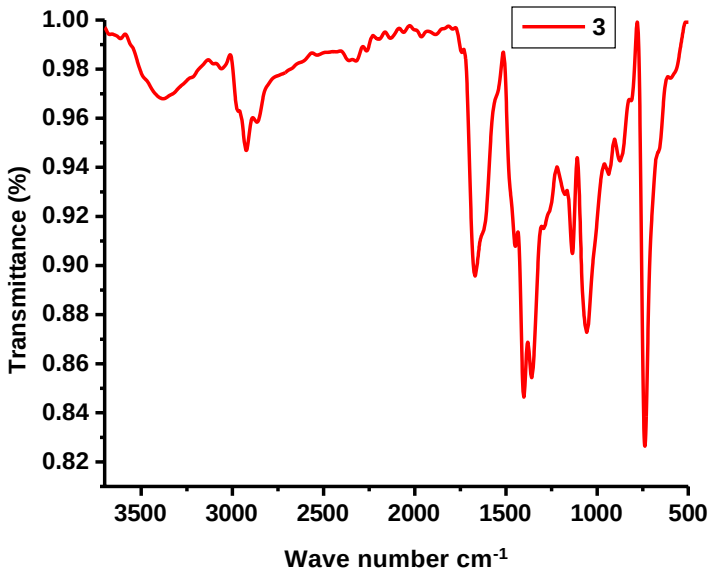


Figure S7. FT-IR spectrum of **3.**CH_3CN (neat).

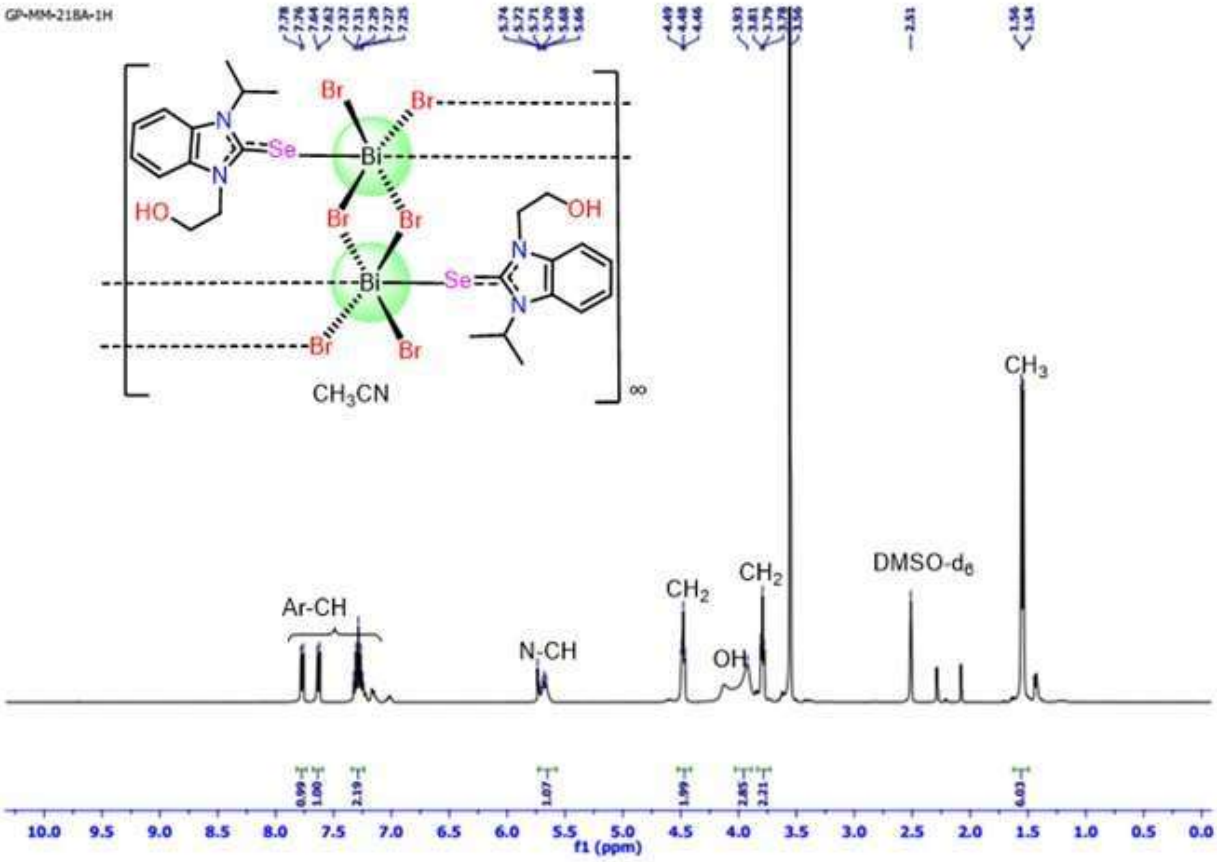


Figure S8. ^1H NMR spectrum of **3**.CH_3CN in DMSO-d_6 at RT.

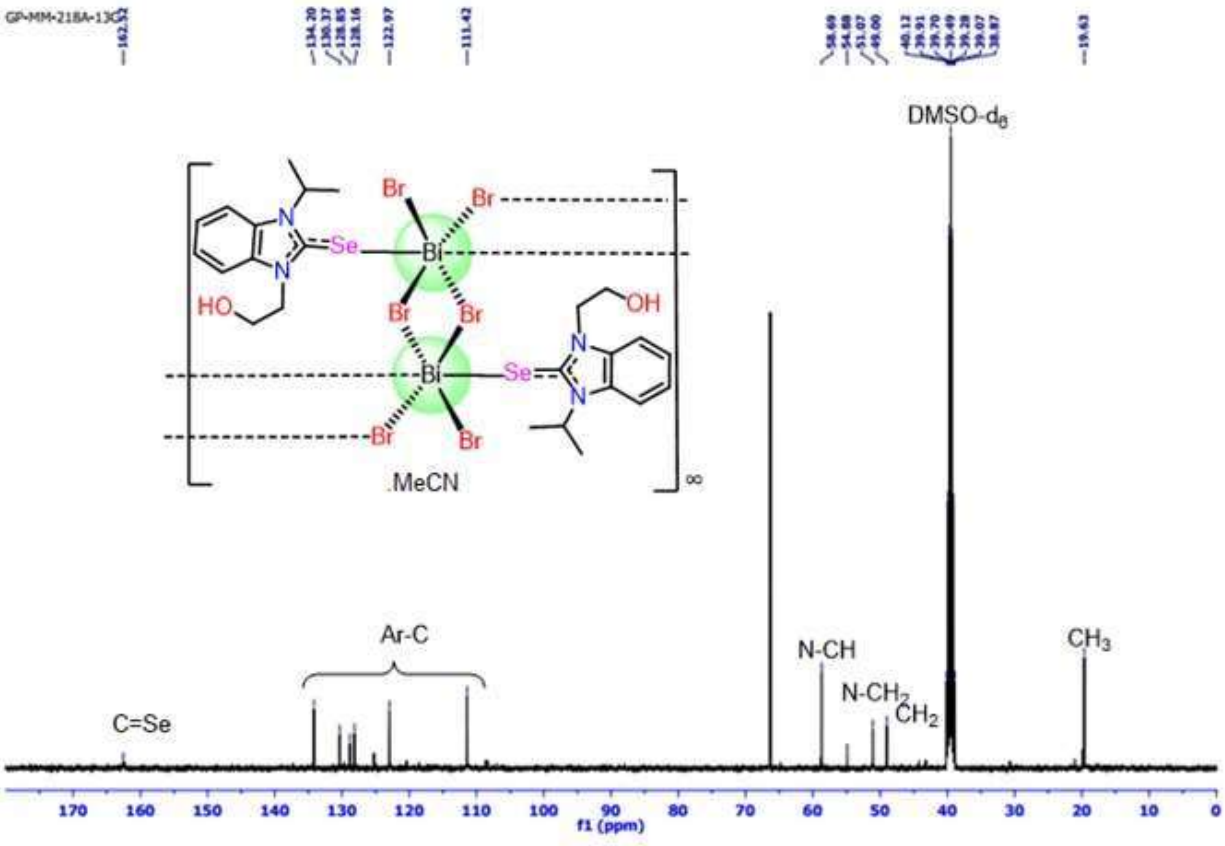


Figure S9. ^{13}C NMR spectrum of **3**.CH_3CN in DMSO-d_6 at RT.

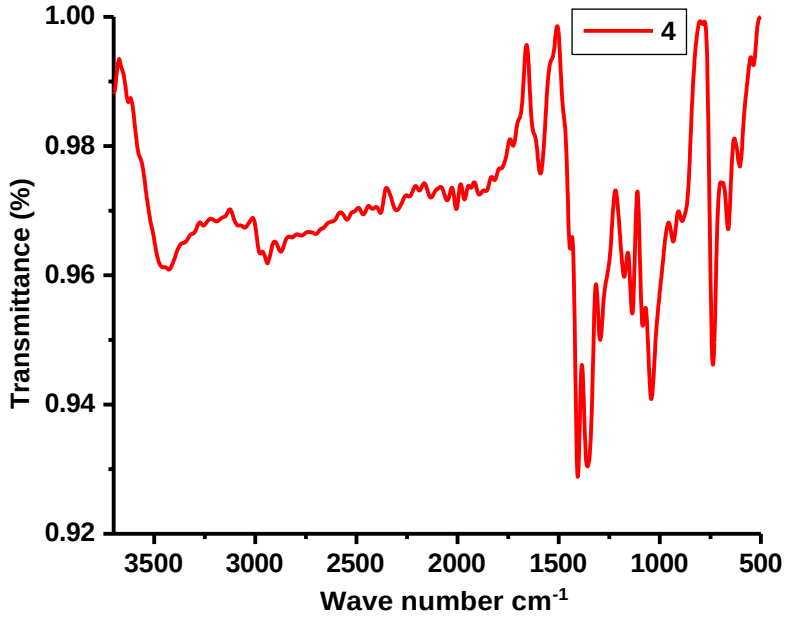


Figure S10. FT-IR spectrum of **4** (neat).

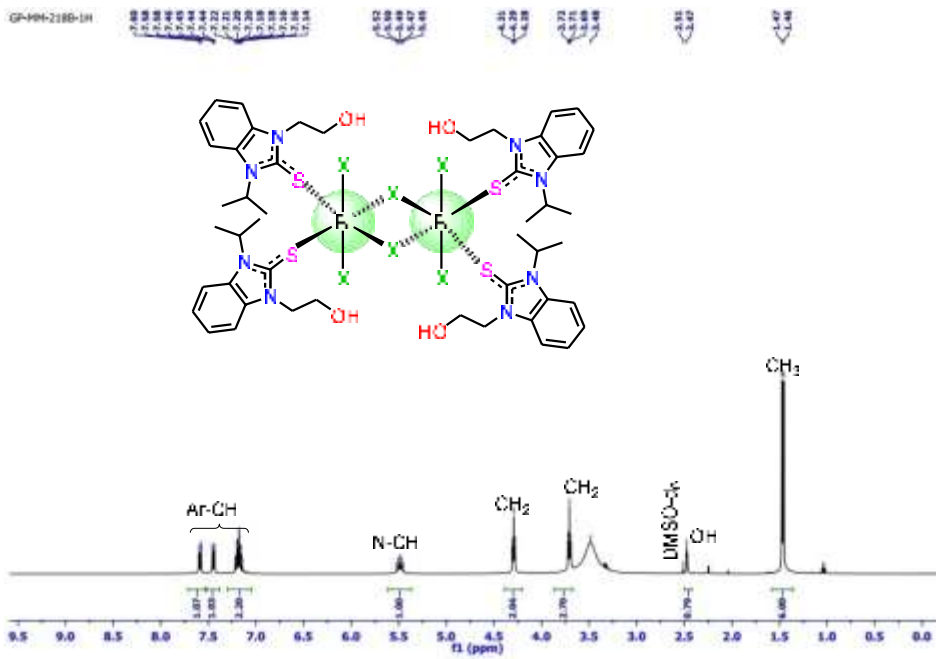


Figure S11. ^{1}H NMR spectrum of **4** in DMSO-d_6 at RT.

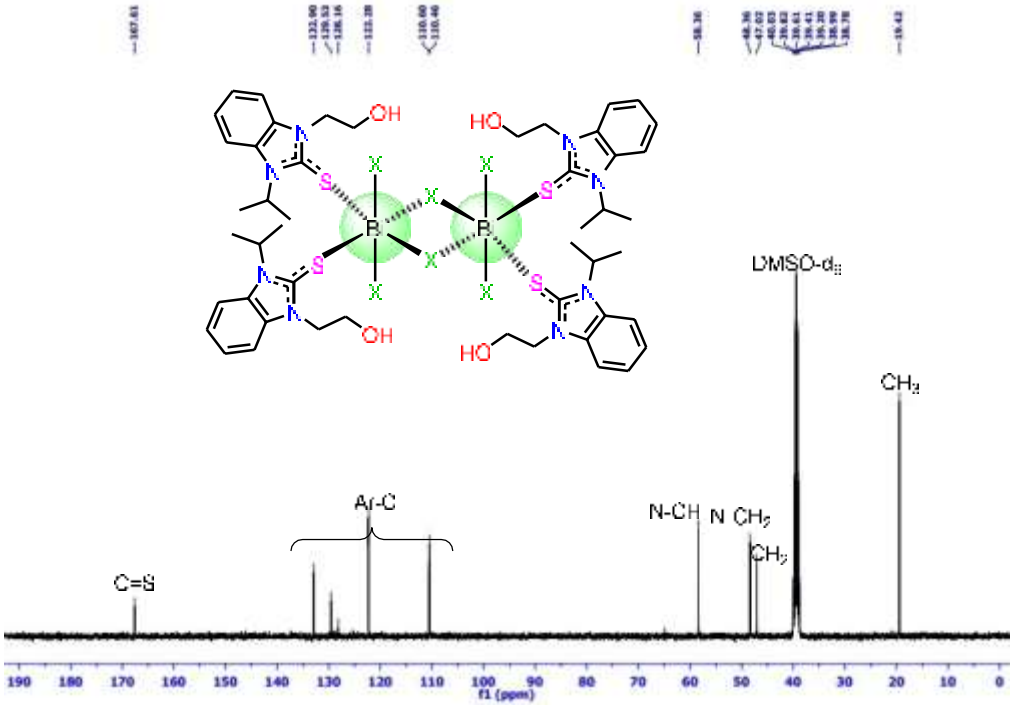
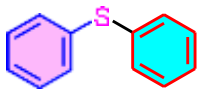


Figure S12. ^{13}C NMR spectrum of **4** in DMSO-d_6 at RT.

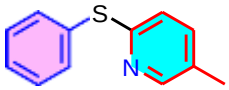
C-S cross coupling reaction

Entry **I**:



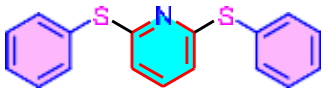
(Phenylsulfanyl)benzene. Chemical formula $C_{12}H_{10}S$; Colourless liquid. ^{1}H NMR ($CDCl_3$, 400.130 MHz): δ 7.40-7.29 (m, 10H).

Entry **II**:



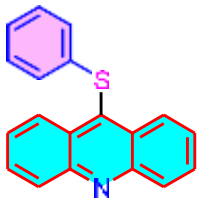
4-methyl-2-(phenylthio)pyridine. Chemical formula $C_{12}H_{11}NS$; Colourless liquid. ^{1}H NMR ($CDCl_3$, 400.130 MHz): 2.36 (s, 3 H), 6.81 (d, 1H), 6.92 (d, 1 H), 6.93 (d, 2 H), 7.19 (d, 2H), 7.36–7.46 (m, 1 H), 8.37 (d, 1 H).

Entry **III**:



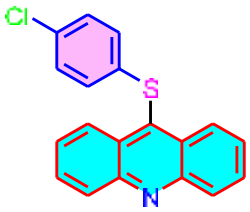
2,6-bis(phenylthio)pyridine. Chemical formula $C_{17}H_{13}NS_2$; White solid. ^{1}H NMR ($CDCl_3$, 400.130 MHz): δ 6.44 (d, 2H), 7.10 (t, 1H), 7.30-7.32 (m, 6H, including $CDCl_3$ peak as it is no well resolved), 7.48-7.50 (m, 4H).

Entry **IV**:



9-(phenylthio)acridine. Chemical formula $C_{19}H_{13}NS$; Yellow solid. ^{1}H NMR ($CDCl_3$, 400.130 MHz): δ 6.93-7.08 (m, 5H), 7.49-7.53 (t, 2H), 7.12-7.15 (t, 2H), 8.21-8.23(d, 2H), 8.63-8.65 (d, 2H). ^{13}C NMR ($CDCl_3$, 100.612 MHz): δ 158.73, 149.15, 146.42, 139.20, 130.34, 130.20, 129.20, 129.04, 127.46, 127.15, 126.77, 125.93.

Entry **V**:



9-((4-chlorophenyl)thio)acridine. Chemical formula $C_{19}H_{12}ClNS$; Yellow solid. ^{1}H NMR ($CDCl_3$, 400.130 MHz): δ 6.92 (d, 2H), 7.09 (d, 2H), 7.57-7.6 (t, 2H), 7.19-7.83 (m, 2H), 8.29 (d, 2H), 8.65 (d, 2H). ^{13}C NMR ($CDCl_3$, 100.612 MHz): δ 149.18, 138.45, 135.45, 131.90, 130.37, 129.33, 128.85, 128.67, 127.37, 126.48.

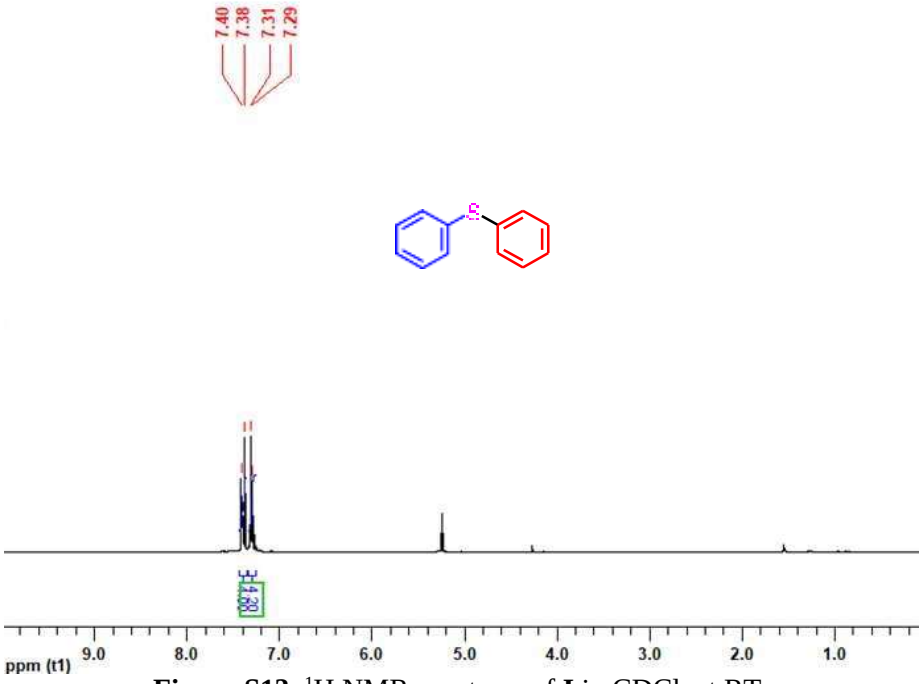


Figure S13. ^{1}H NMR spectrum of **I** in $CDCl_3$ at RT.

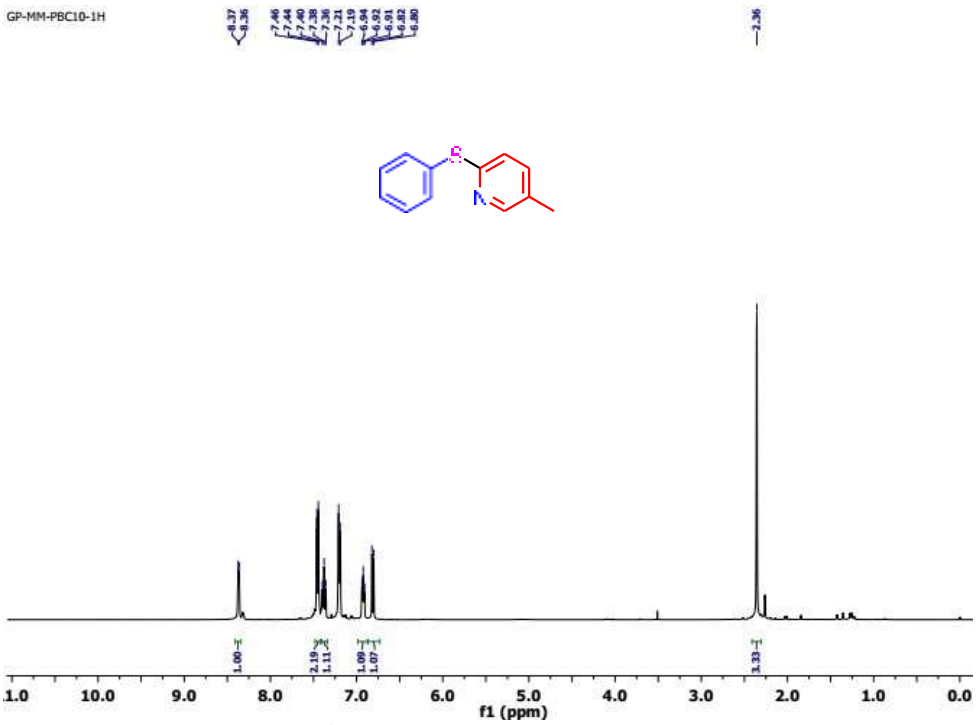


Figure S14. ^{1}H NMR spectrum of **II** in $CDCl_3$ at RT.

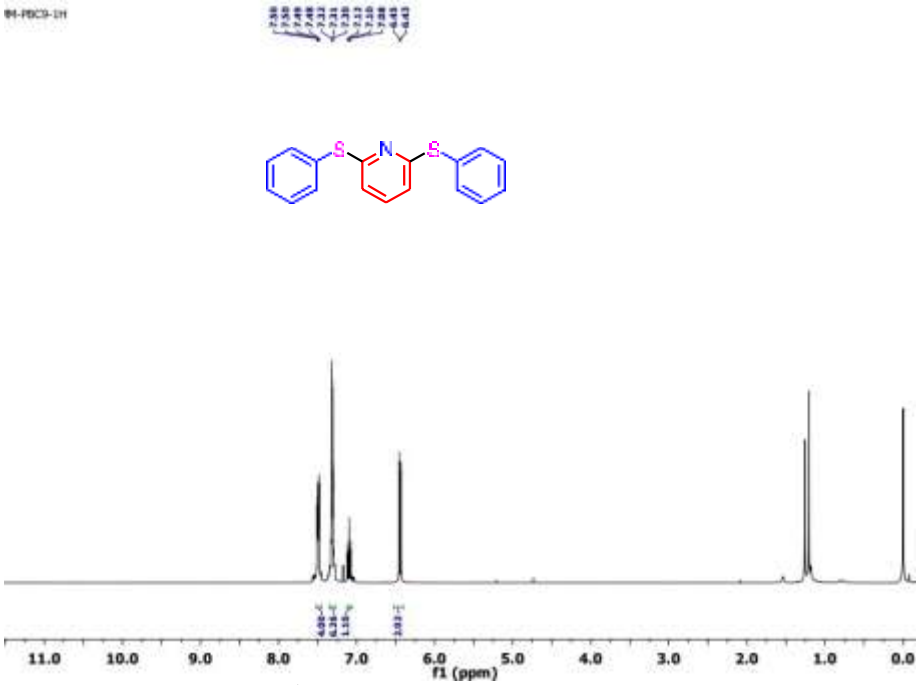


Figure S15. ^{1}H NMR spectrum of **III** in $CDCl_3$ at RT.

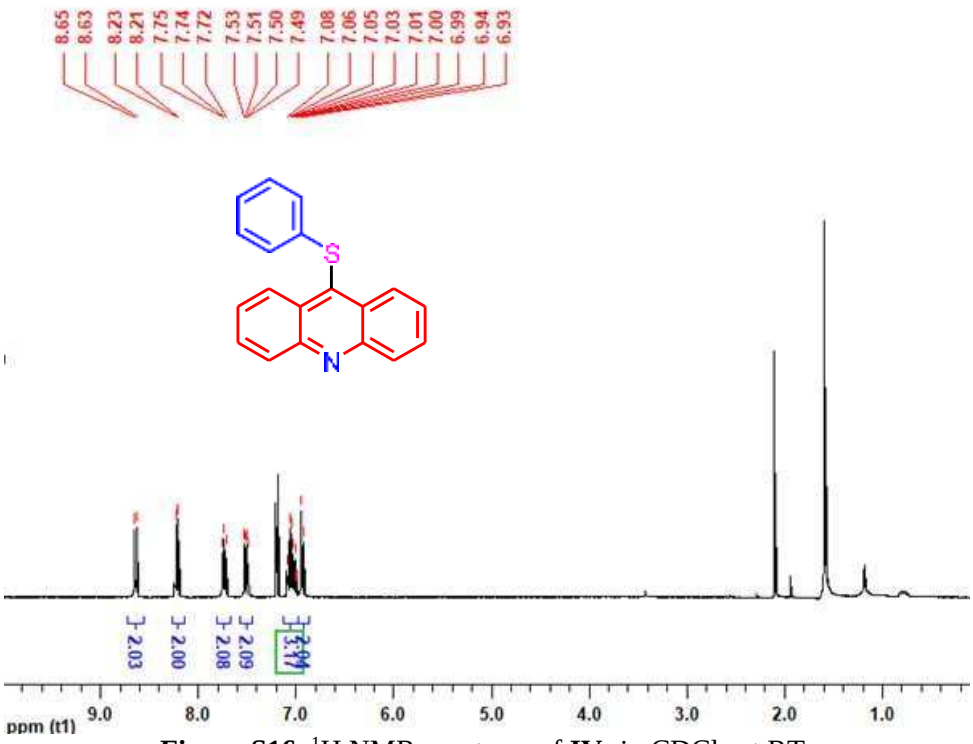


Figure S16. ^{1}H NMR spectrum of **IV** in $CDCl_3$ at RT.

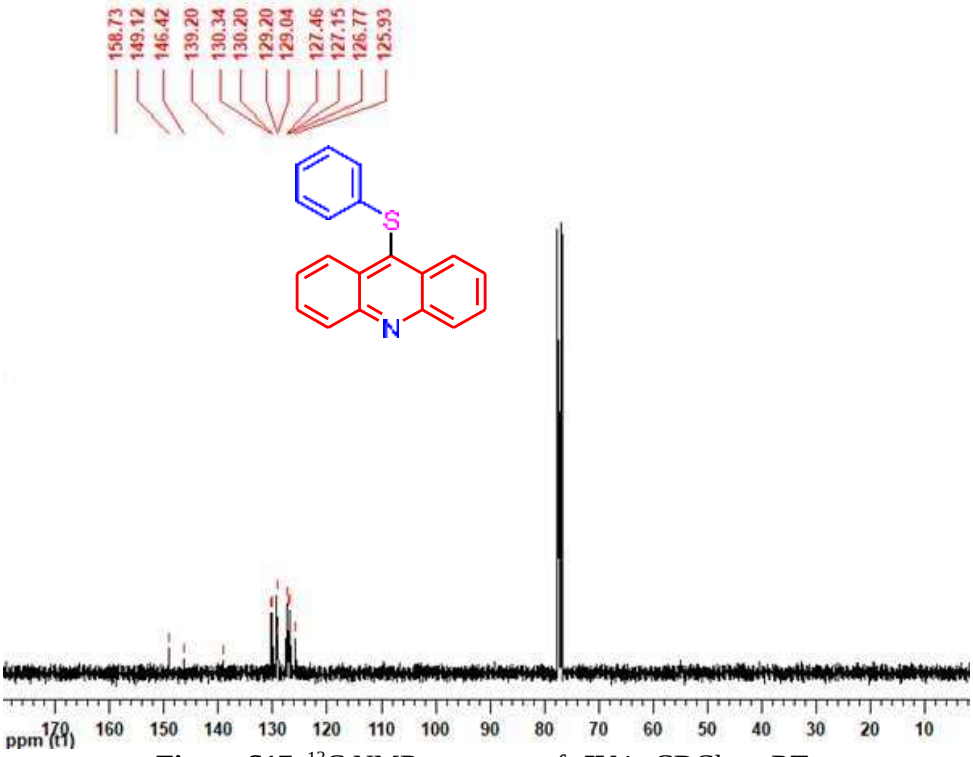


Figure S17. ^{13}C NMR spectrum of **IV** in $CDCl_3$ at RT.

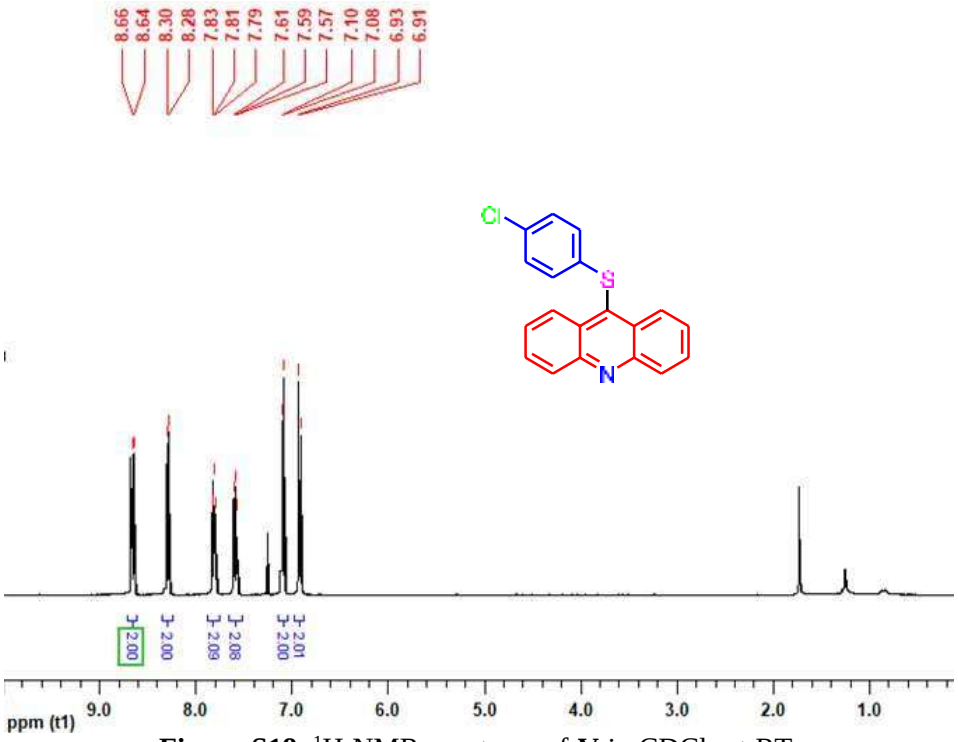


Figure S18. ^{1}H NMR spectrum of **V** in $CDCl_3$ at RT.

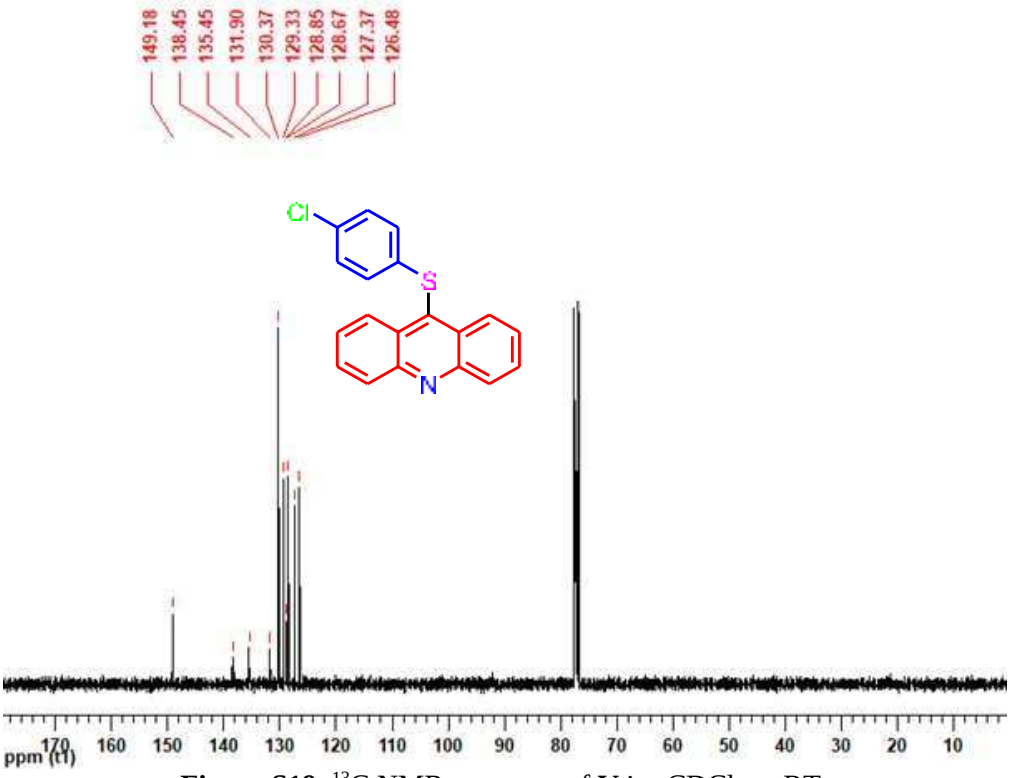


Figure S19. ^{13}C NMR spectrum of **V** in $CDCl_3$ at RT.

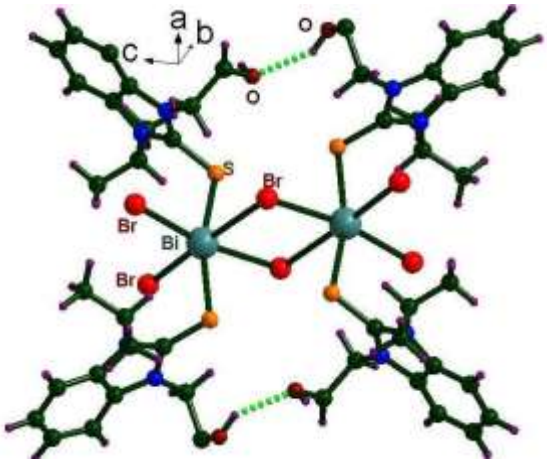


Figure S20. Molecular structure of **4** with intramolecular hydrogen bonding. Molecule **1** is isostructural to **4**.

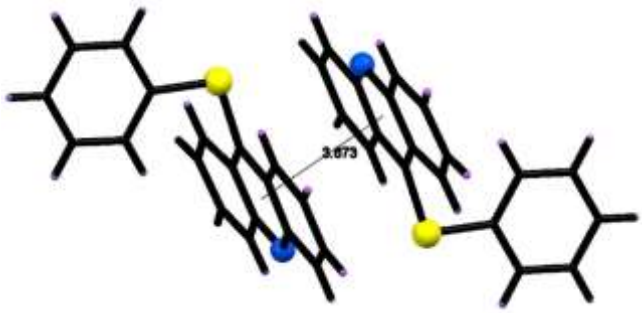


Figure S21. A weak π ⋯ π stacking interaction between acridine rings in **IV.**

Figure S22. A weak π⋯⋯π stacking interaction between acridine rings in **V.**

Table S1. Crystal data and structure refinement for **1-4**

	1	**2**	**3.**CH_3CN	**4**
CCDC	2129447	2129448	2129449	2129450
Empirical formula	$C_{48}H_{64}Bi_2Cl_6N_8O_4Se_4$	$C_{12}H_{16}BiCl_3N_2OS$	$C_{12}H_{16}BiBr_3N_2OSe$	$C_{48}H_{64}Bi_2Br_6N_8O_4S_4$
Formula weight	1763.61	551.68	730.92	1842.74
Temperature/K	293.15	293.0	293.0	293.0
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	P-1	$P2_1/n$
a/Å	9.148(2)	10.6327(2)	7.6380(4)	9.28018(15)
b/Å	23.974(5)	10.36708(17)	11.3080(4)	23.7009(3)
c/Å	14.150(3)	17.0092(3)	13.1866(7)	14.4183(3)
α/°	90.00(3)	90	77.900(4)	90
β/°	95.19(3)	105.4866(19)	78.288(4)	94.9584(15)
γ/°	90.00(3)	90	84.332(4)	90
Volume/$Å^3$	3090.5(12)	1806.84(6)	1088.56(9)	3159.41(9)
Z	2	4	2	2
$\rho_{calc}g/cm^3$	1.8951	2.0279	2.2298	1.9369
μ/mm^{-1}	8.347	24.290	15.271	16.853
F(000)	1674.5	1033.3	653.4	1743.2
Crystal size/mm^3	0.08 × 0.07 × 0.07	0.27 × 0.24 × 0.19	0.09 × 0.08 × 0.07	0.32 × 0.19 × 0.16
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.78 to 50	8.62 to 139.88	5.8 to 58.2	7.2 to 140.02
Index ranges	$-11 \le h \le 12$, $-32 \le k \le 31$, $-18 \le l \le 17$	$-11 \le h \le 12$, $-12 \le k \le 11$, $-20 \le l \le 11$	$-9 \le h \le 10$, $-10 \le k \le 14$, $-17 \le l \le 16$	$-10 \le h \le 11$, $-24 \le k \le 28$, $-15 \le l \le 17$
Reflections collected	30790	6672	8154	11869
Independent reflections	5434 [R_{int} = 0.0626, R_{sigma} = 0.0487]	3365 [R_{int} = 0.0325, R_{sigma} = 0.0446]	4770 [R_{int} = 0.0798, R_{sigma} = 0.1136]	5874 [R_{int} = 0.0597, R_{sigma} = 0.0776]
Data/restraints/parameters	5434/2/326	3365/0/185	4770/0/185	5874/0/332
Goodness-of-fit on F^2	1.002	1.024	0.927	0.980
Final R indexes [I>=2σ (I)]	R_1 = 0.0490, wR_2 = 0.1495	R_1 = 0.0346, wR_2 = 0.0872	R_1 = 0.0578, wR_2 = 0.1151	R_1 = 0.0544, wR_2 = 0.1286
Final R indexes [all data]	R_1 = 0.0568, wR_2 = 0.1756	R_1 = 0.0390, wR_2 = 0.0908	R_1 = 0.0910, wR_2 = 0.1321	R_1 = 0.0671, wR_2 = 0.1402
Largest diff. peak/hole / e $Å^{-3}$	2.74/-1.50	1.19/-2.04	3.49/-3.97	1.84/-2.83

Table S2. Crystal data and structure refinement for **IV,** and **V**

	IV	**V**
CCDC	2129451	2129452
Empirical formula	$C_{19}H_{13}NS$	$C_{1.19}H_{0.75}Cl_{0.06}N_{0.06}S_{0.06}$
Formula weight	287.39	321.83
Temperature/K	293.0	292
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	I2/c
a/Å	7.4635(8)	25.360(3)
b/Å	22.1889(13)	7.5833(5)
c/Å	9.3494(9)	33.138(3)
α/°	90	90
β/°	110.628(12)	110.162(11)
γ/°	90	90
Volume/Å^3	1449.1(3)	5982.3(10)
Z	4	16
ρ_{calc}g/cm^3	1.3172	1.4292
μ/mm^{-1}	1.894	0.389
F(000)	602.9	2661.2
Crystal size/mm^3	0.67 × 0.62 × 0.52	0.077 × 0.065 × 0.062
Radiation	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.96 to 139.34	4.98 to 58.18
Index ranges	$-6 \le h \le 6$, $-18 \le k \le 25$, $-8 \le l \le 8$	$-33 \le h \le 21$, $-9 \le k \le 9$, $-42 \le l \le 42$
Reflections collected	2122	12375
Independent reflections	1301 [R_{int} = 0.0148, R_{sigma} = 0.0210]	6817 [R_{int} = 0.1147, R_{sigma} = 0.3028]
Data/restraints/parameters	1301/0/191	6817/0/398
Goodness-of-fit on F^2	1.097	0.954
Final R indexes [I>=2σ (I)]	R_1 = 0.0339, wR_2 = 0.0889	R_1 = 0.0800, wR_2 = 0.0909
Final R indexes [all data]	R_1 = 0.0389, wR_2 = 0.0939	R_1 = 0.3443, wR_2 = 0.1791
Largest diff. peak/hole / e Å^{-3}	0.12/-0.17	2.02/-1.25