Supporting Information.

Towards deep NIR emissive simple D-A-D dyes: A novel acceptor block providing Anti-Kasha's rule emission

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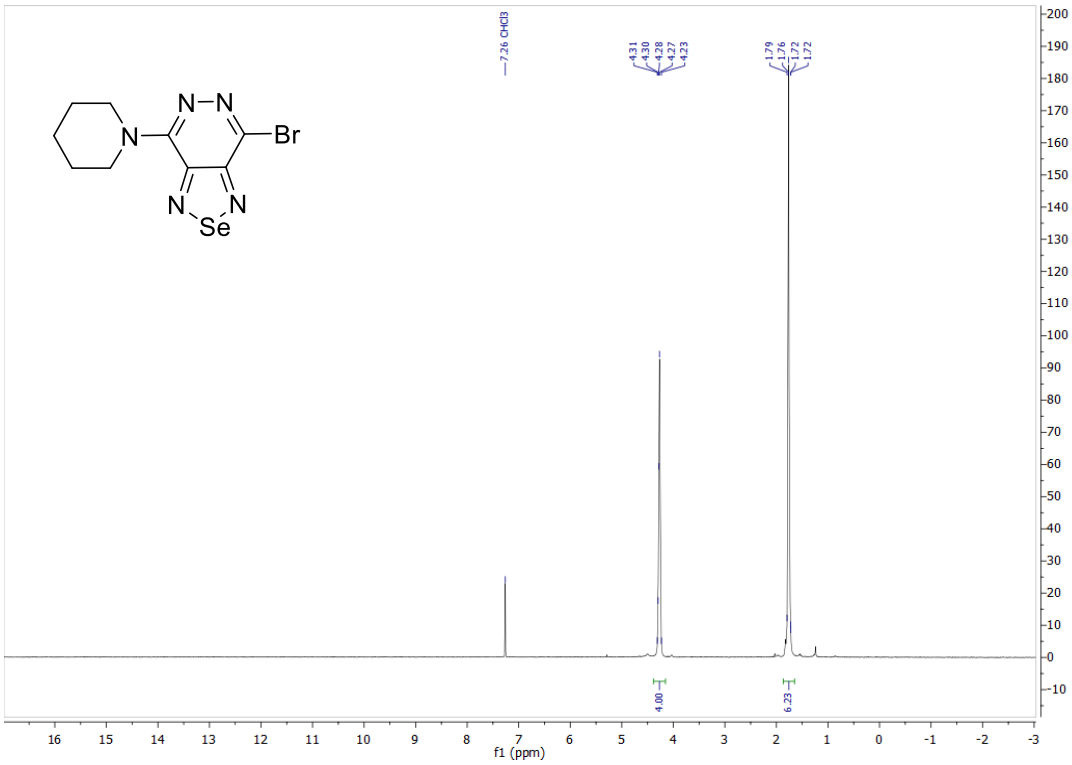
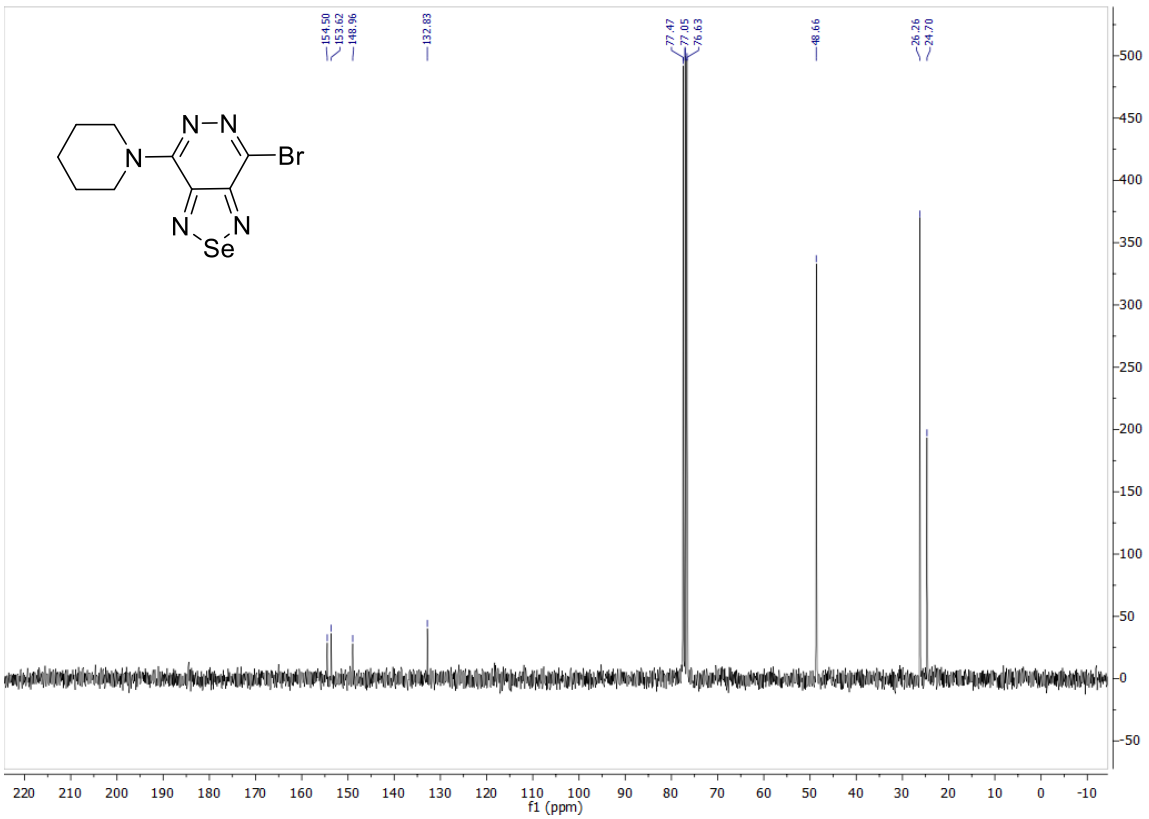
SI-1 NMR spectra ^{1}H, ^{13}C

4-Bromo-7-(piperidin-1-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (5a)

^{1}H NMR(300 MHz)

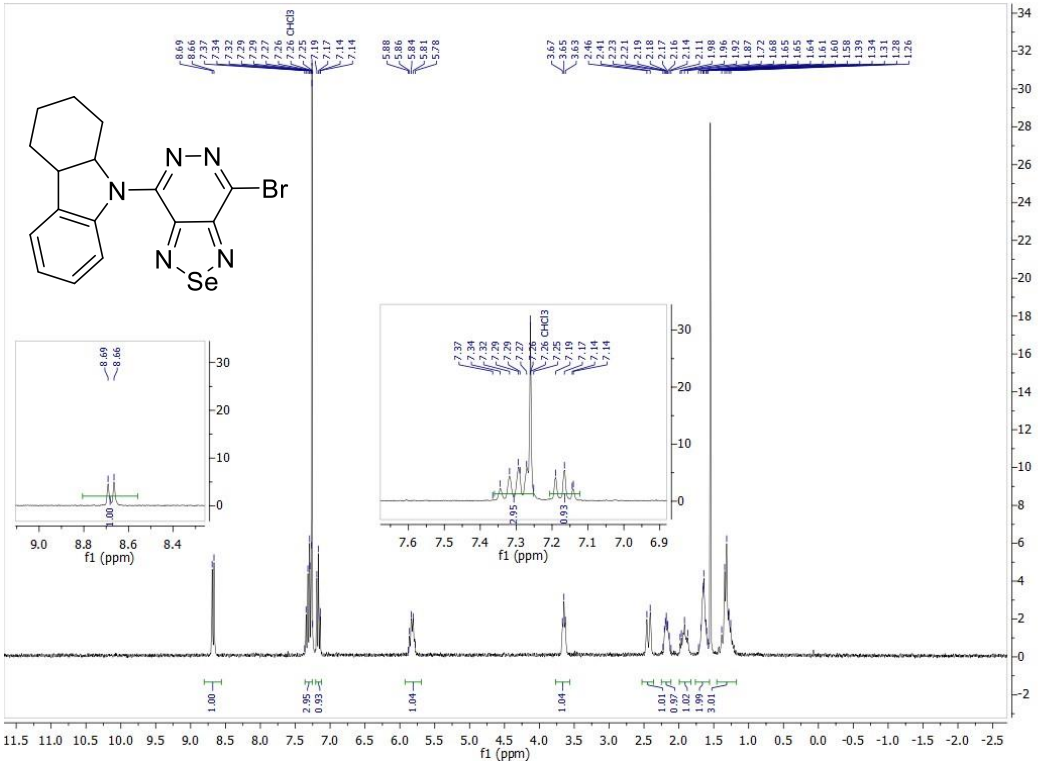


^{13}C NMR(75 MHz)

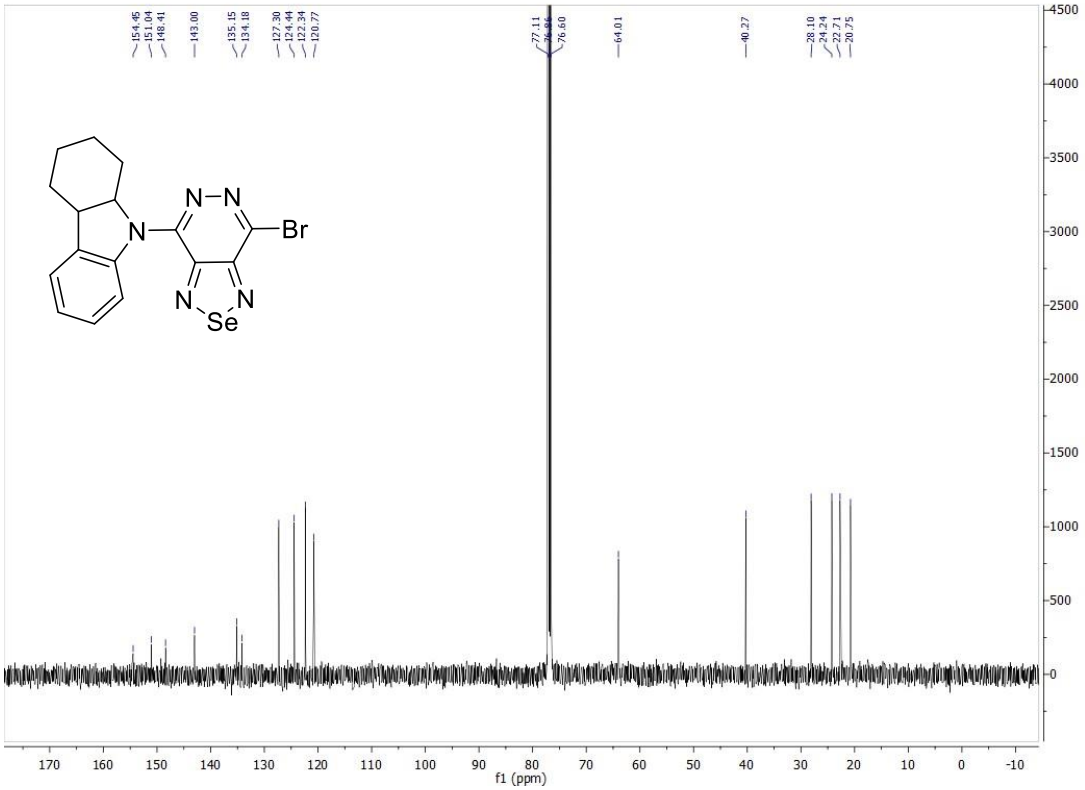


4-Bromo-7-(1,2,3,4,4a,9a-hexahydro-9H-carbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (5b)

^{1}H NMR(300 MHz)

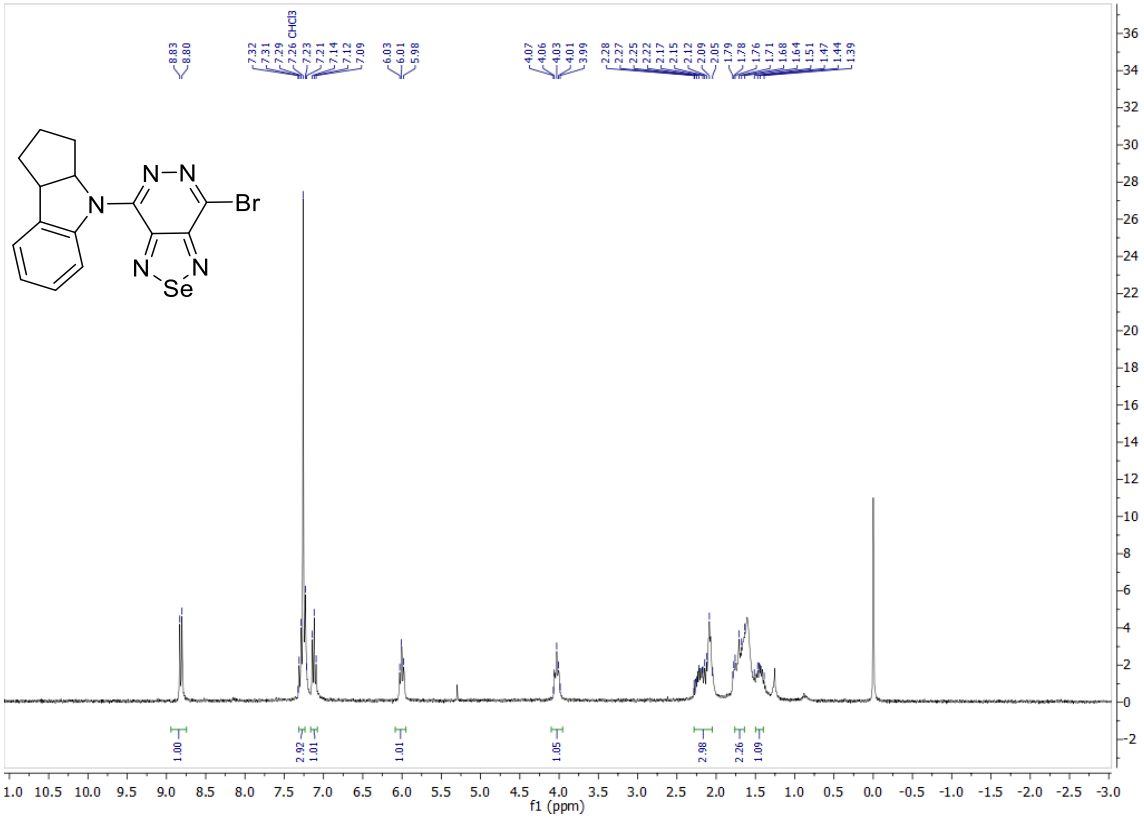


^{13}C NMR(75 MHz)



4-Bromo-7-(2,3,3a,8b-tetrahydrocyclopenta[b]indol-4(1H)-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (5c).

^{1}H NMR(300 MHz)



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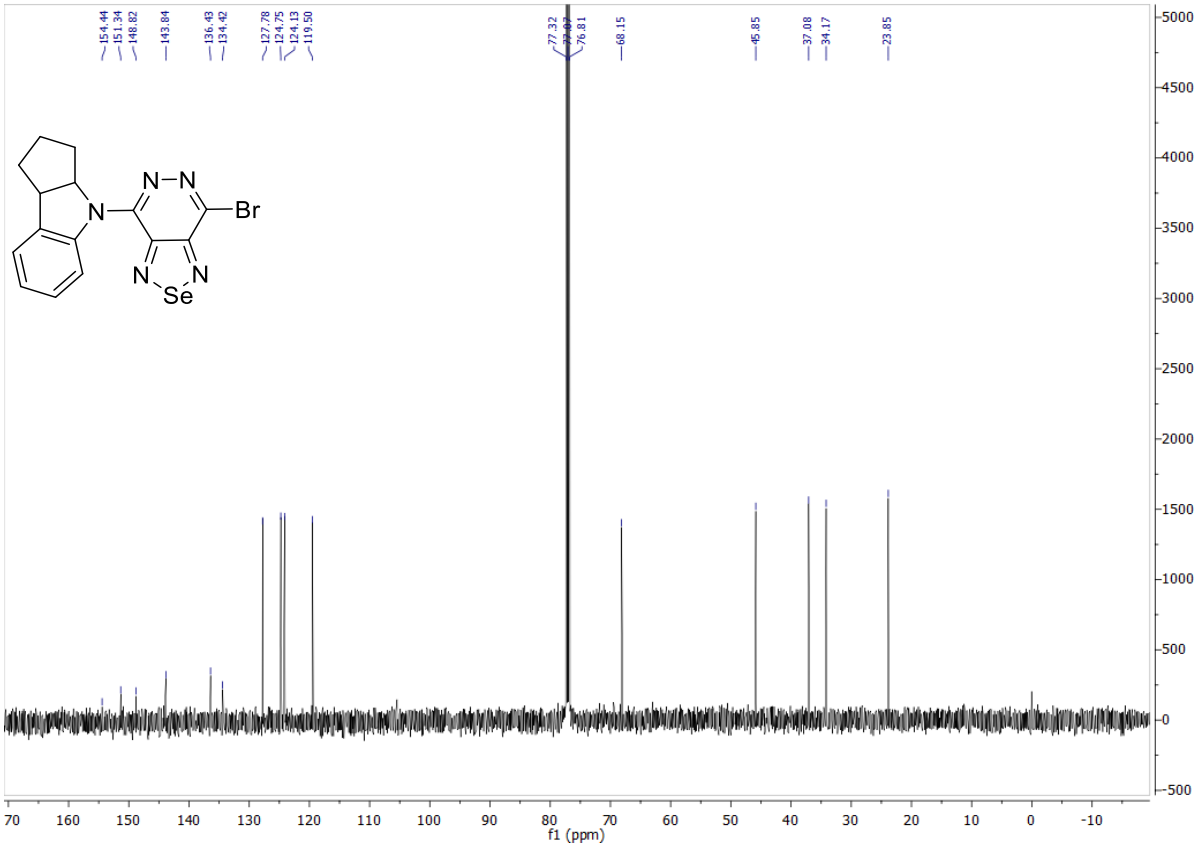
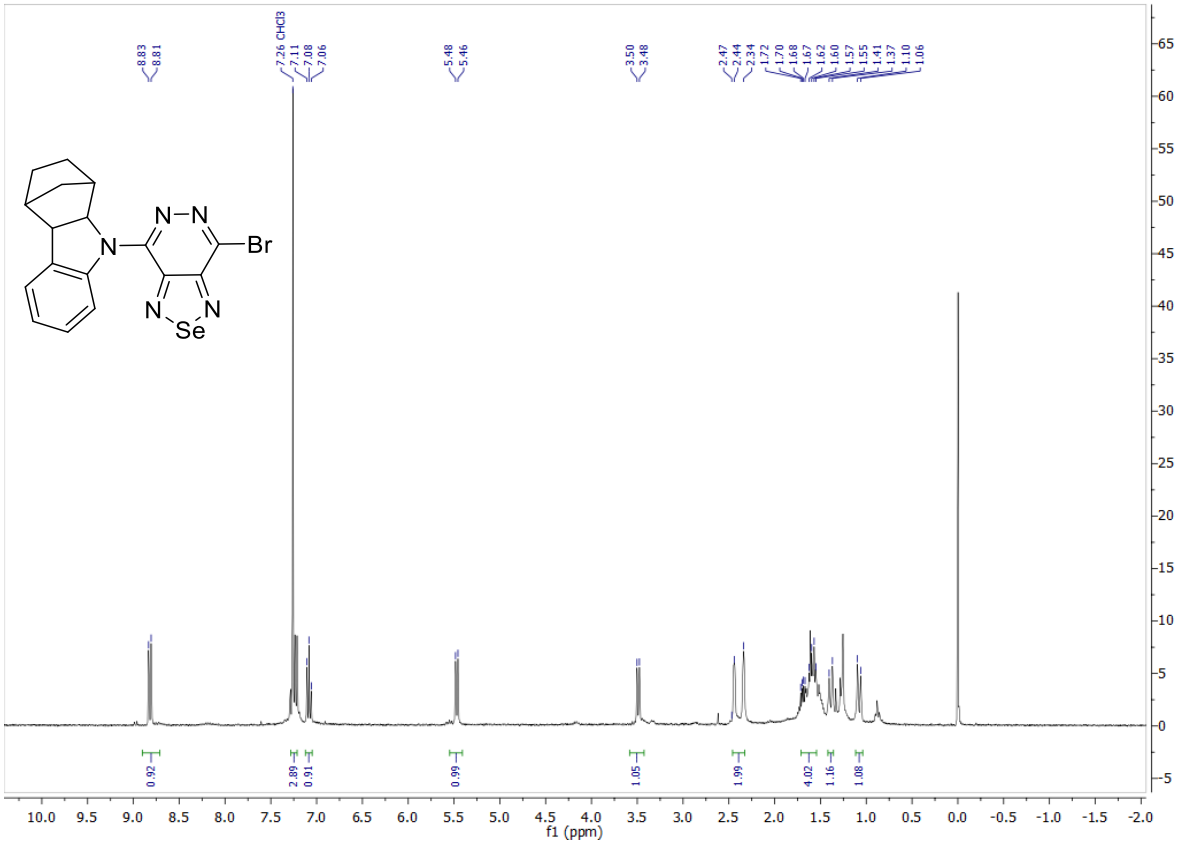


4-Bromo-7-(2,3,3a,8b-tetrahydrocyclopenta[b]indol-4(1H)-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (5d).

^{1}H NMR(300 MHz)



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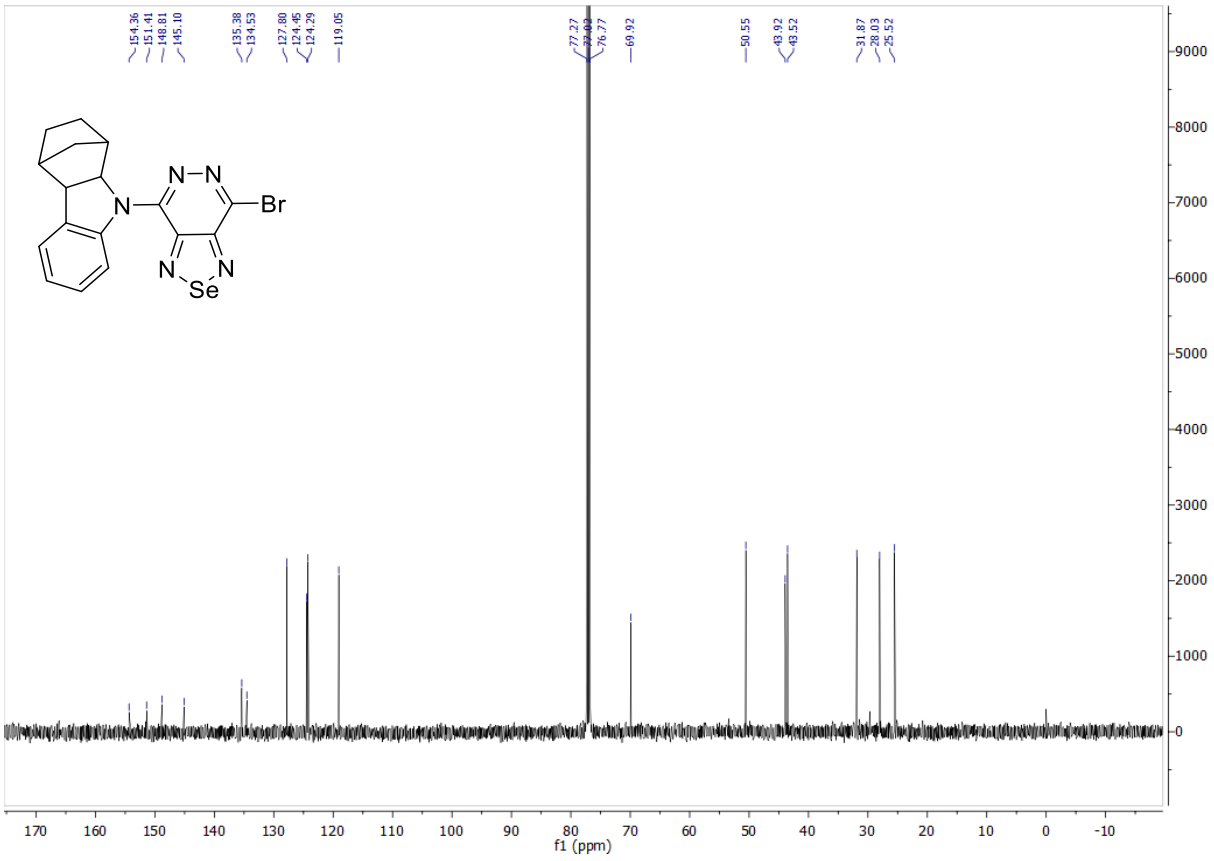
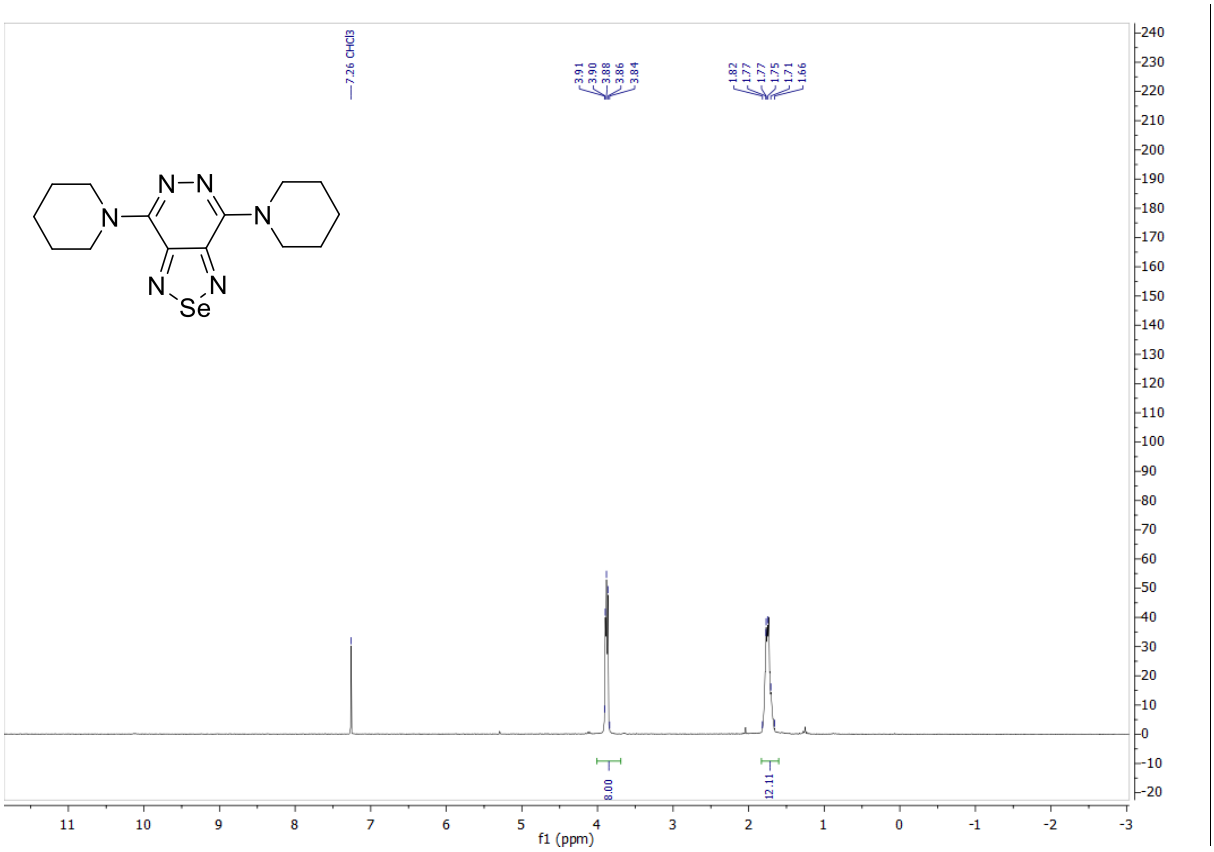


4,7-Di(piperidin-1-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (6a)

^{1}H NMR(300 MHz)



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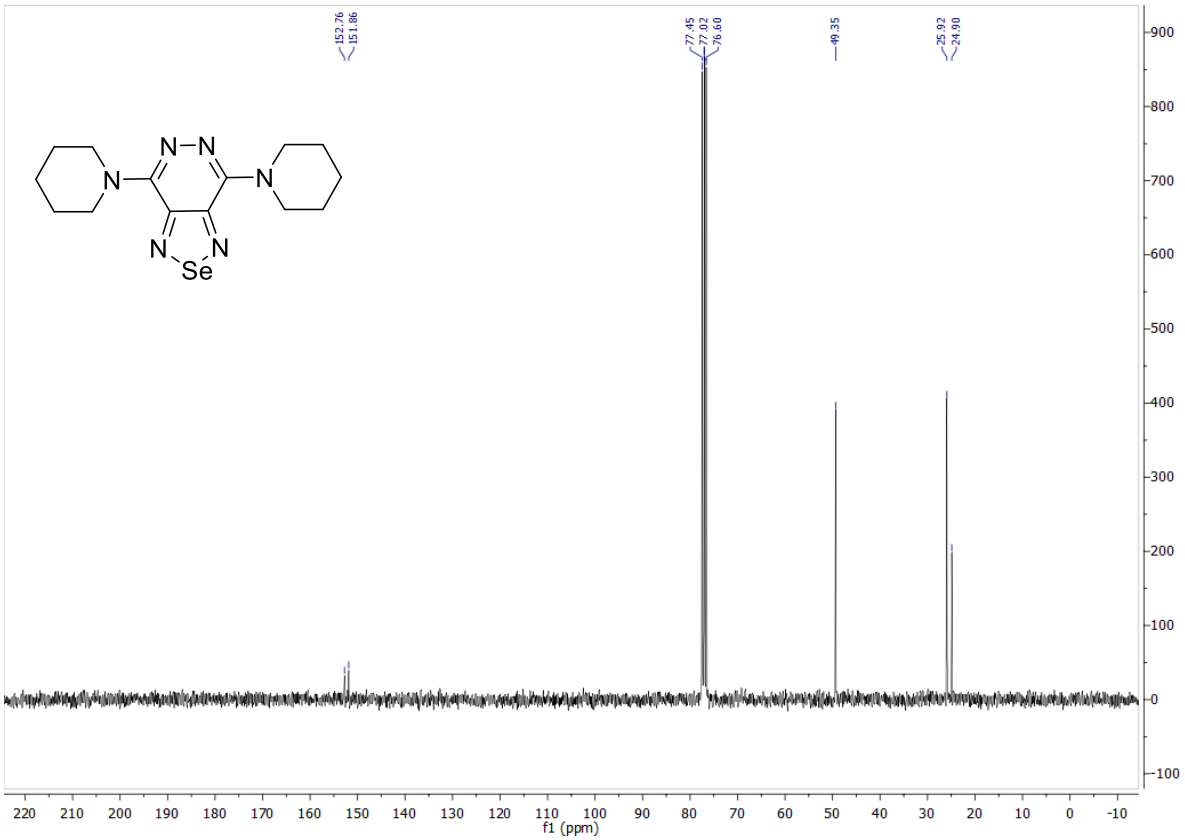
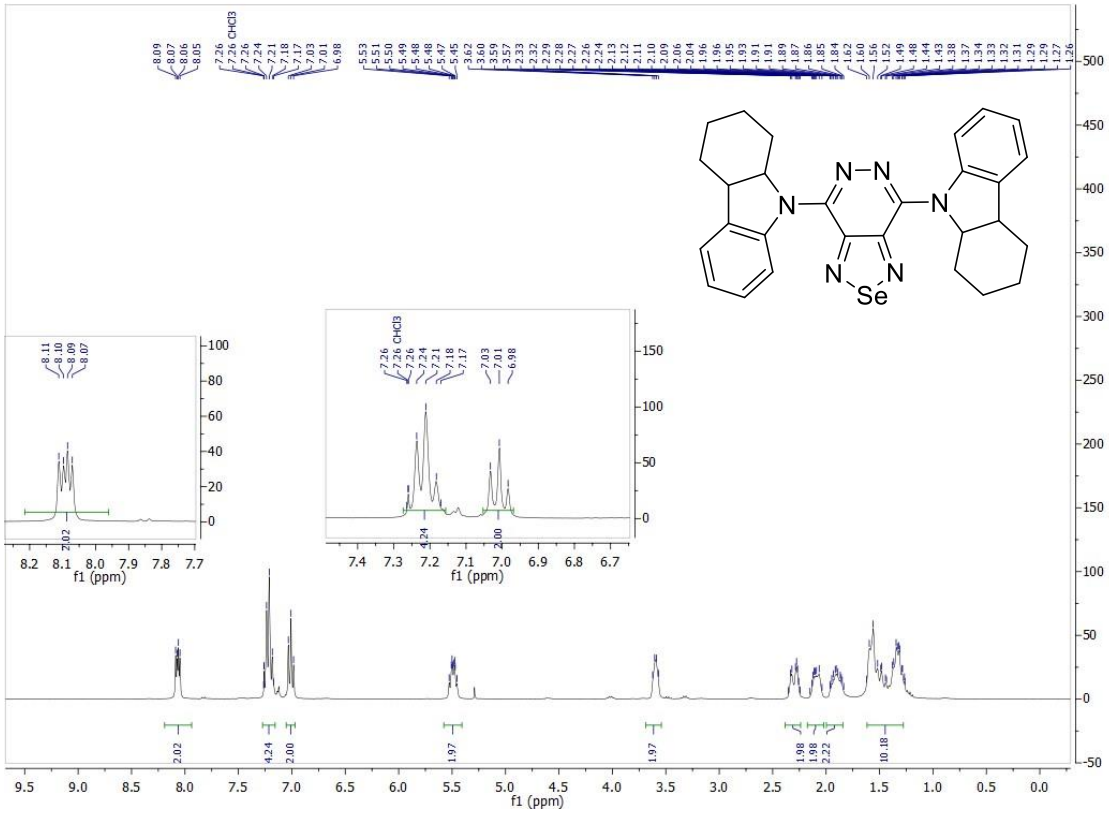
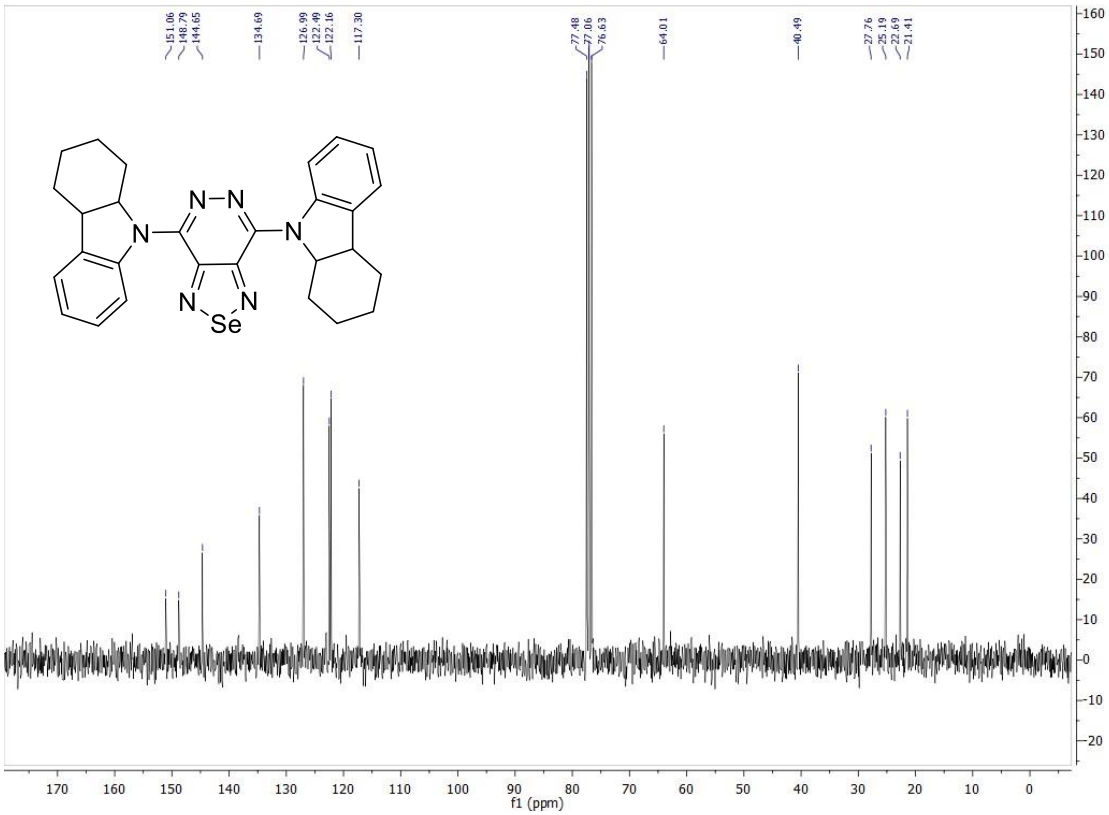


4,7-Bis(1,2,3,4,4a,9a-hexahydro-9H-carbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (6b)

^{1}H NMR(300 MHz)

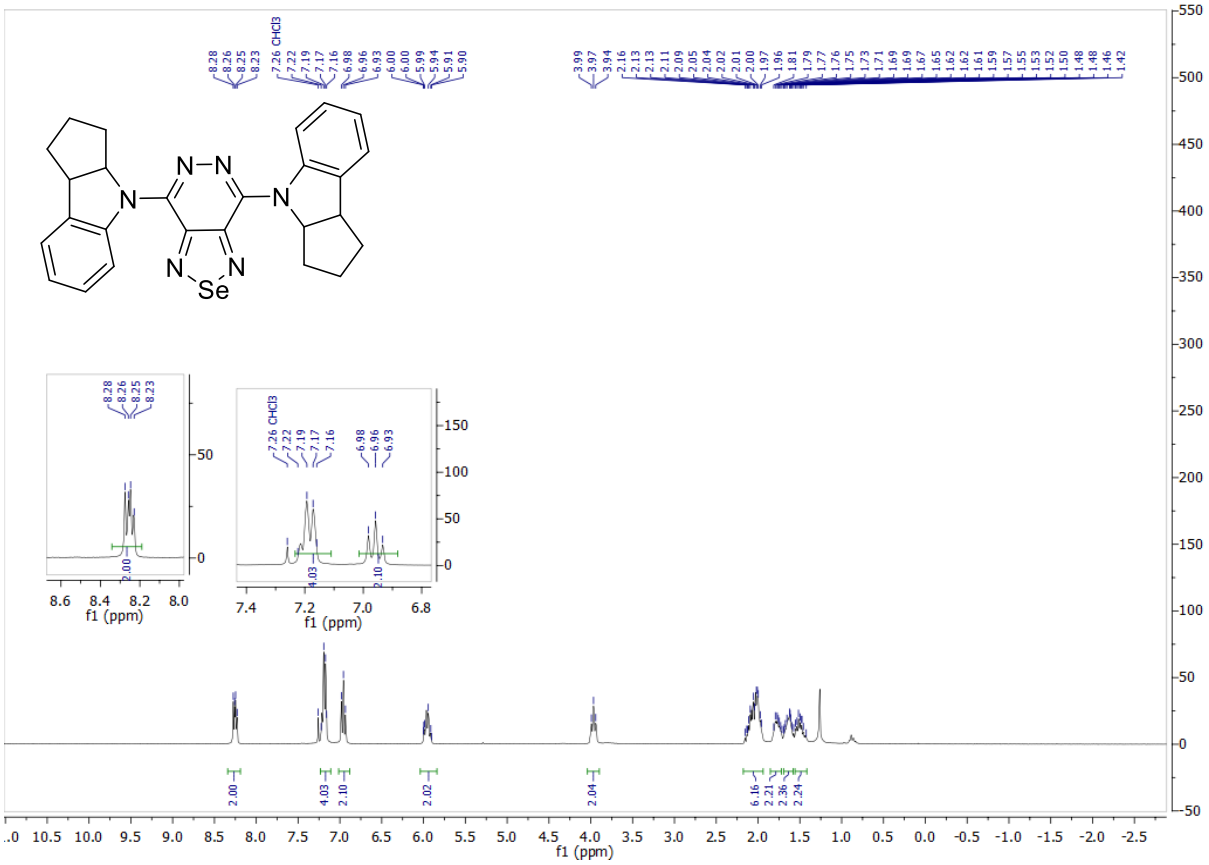


^{13}C NMR(75 MHz)

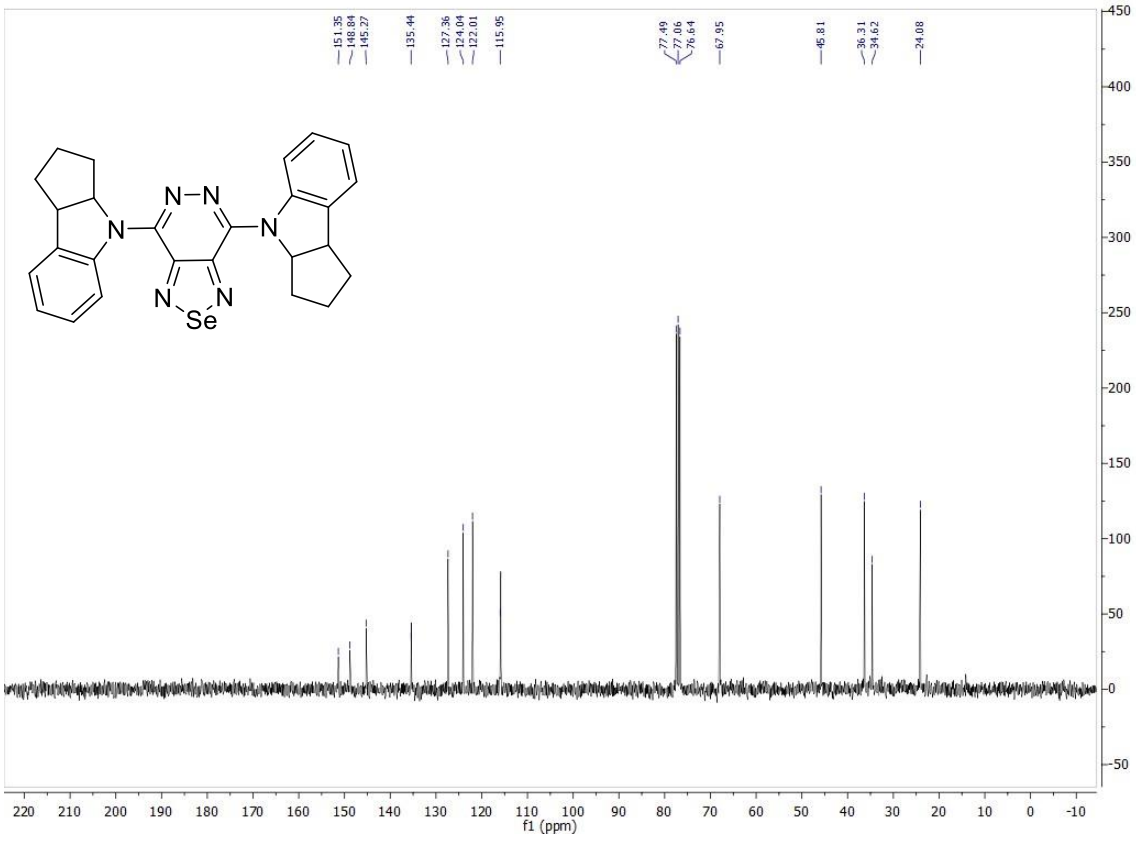


4,7-Bis(2,3,3a,8b-tetrahydrocyclopenta[b]indol-4(1H)-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (6c)

^{1}H NMR(300 MHz)

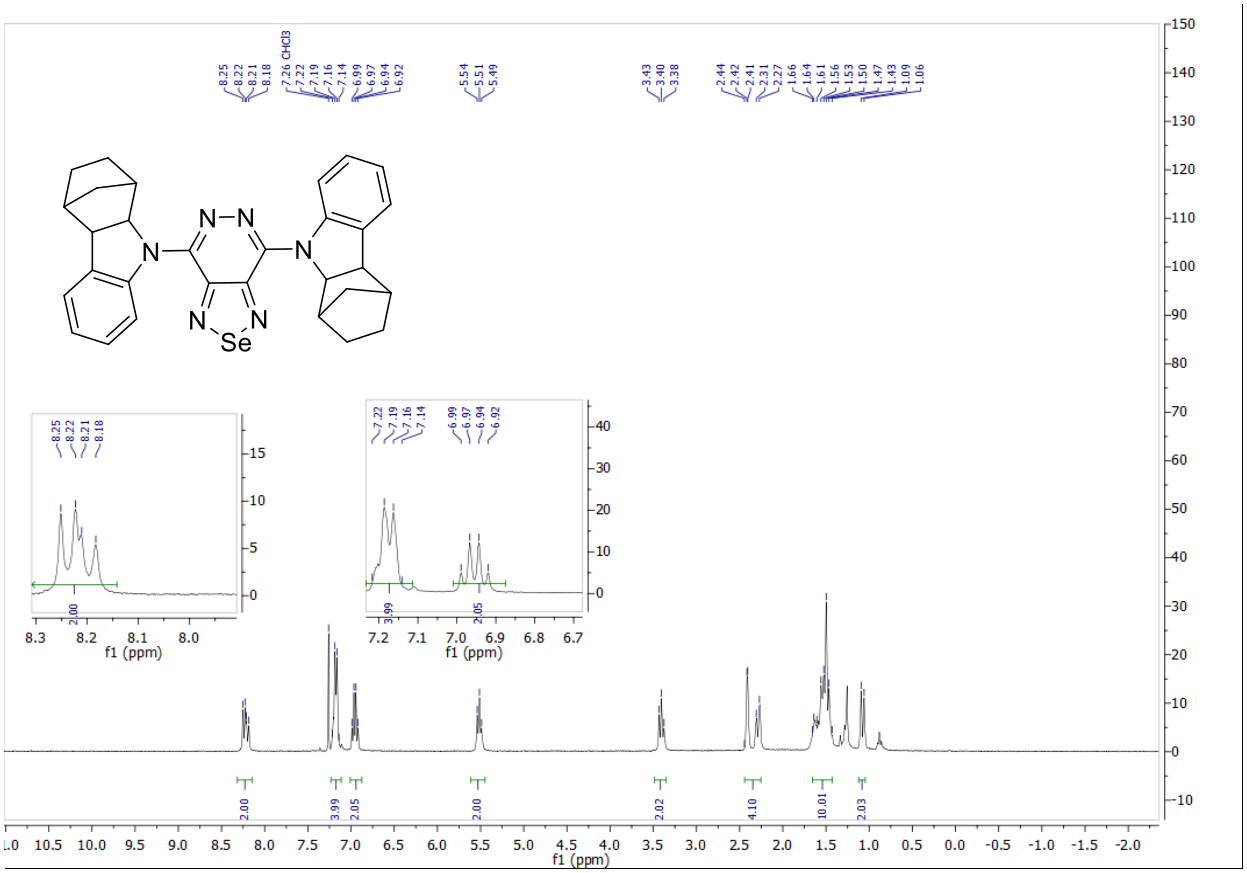


^{13}C NMR(75 MHz)

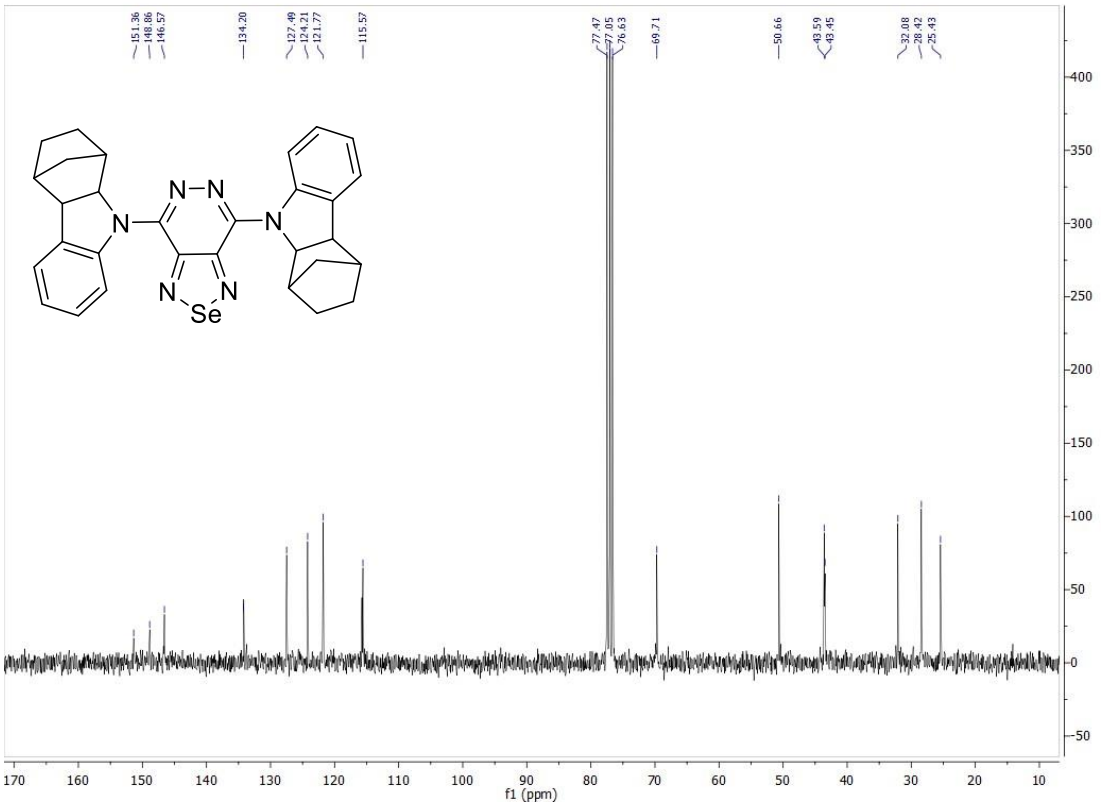


4,7-Bis(1,2,3,4,4a,9a-hexahydro-9H-1,4-methanocarbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (6d)

^{1}H NMR(300 MHz)

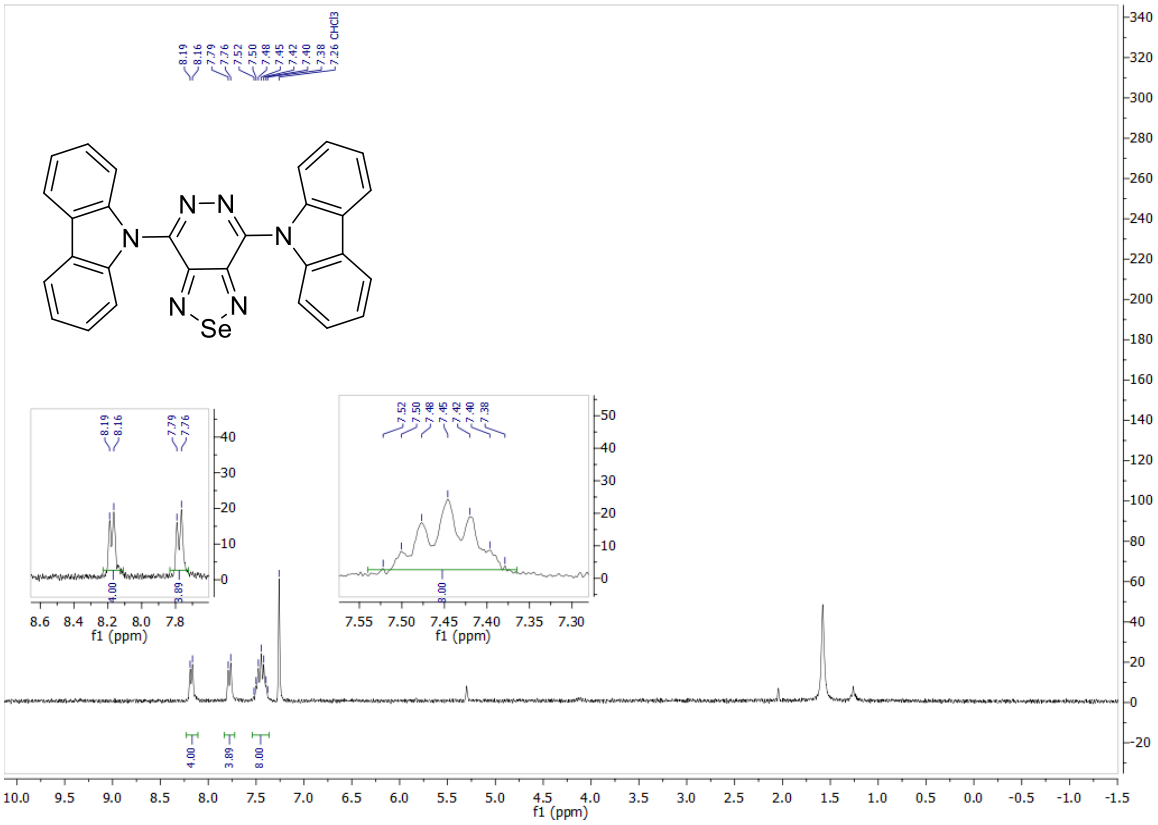


^{13}C NMR(75 MHz)

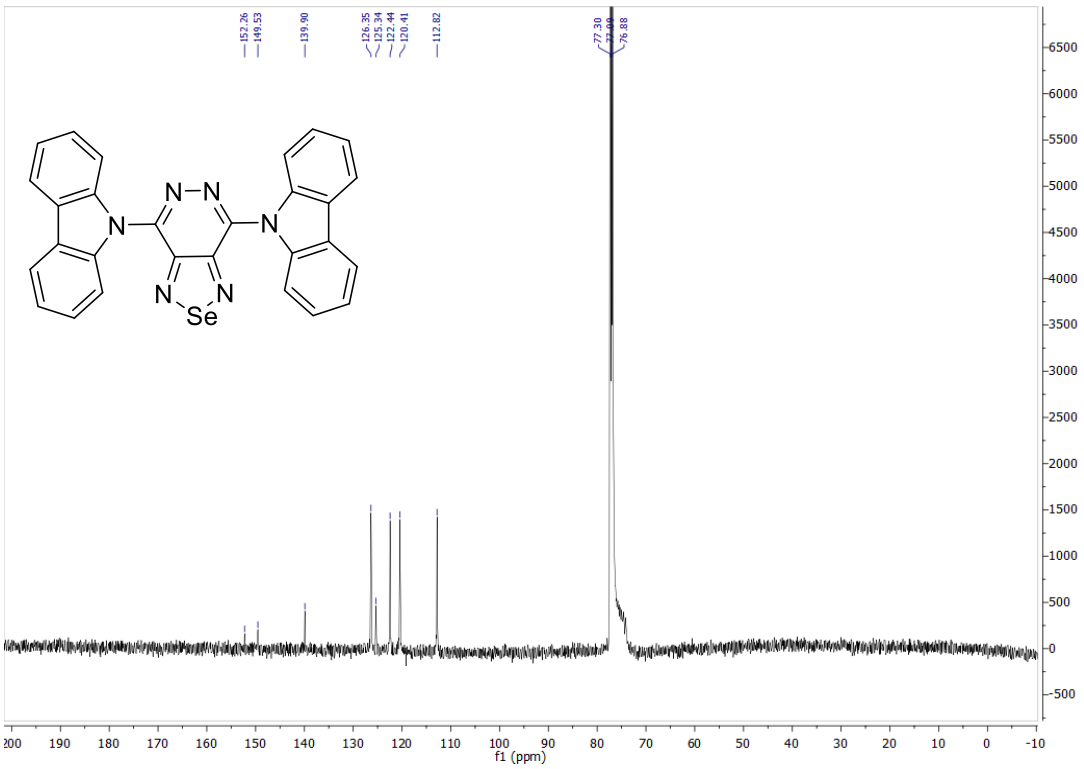


4,7-di(9H-carbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (6e)

^{1}H NMR(300 MHz)

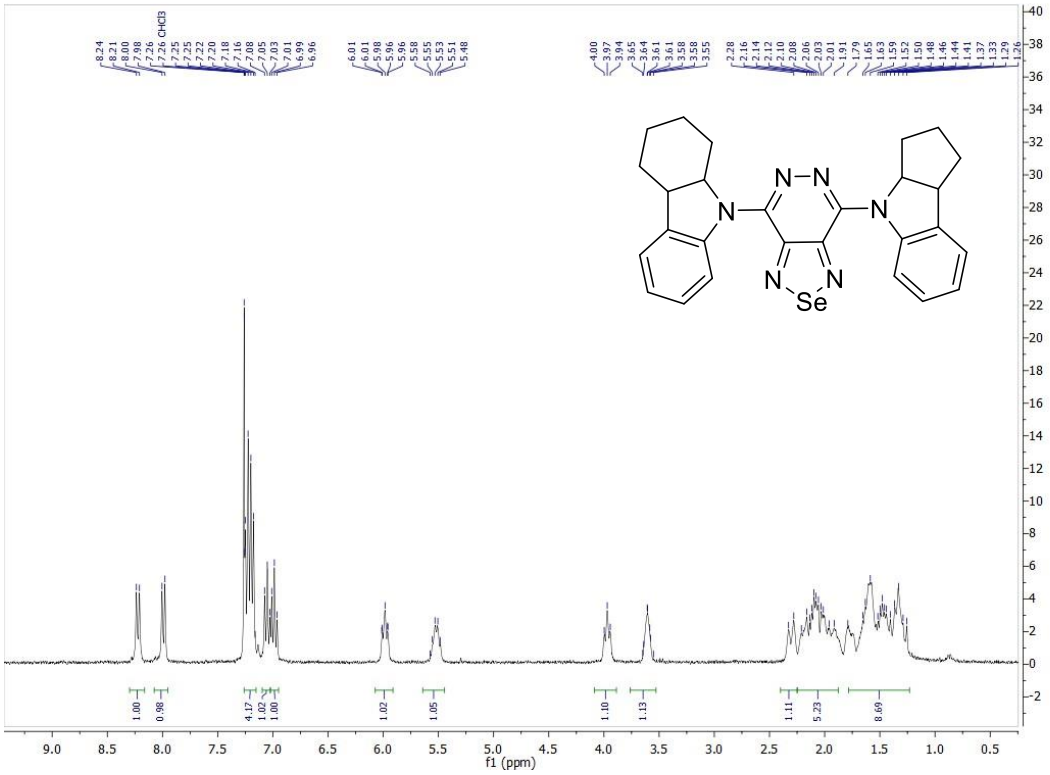


^{13}C NMR(75 MHz)

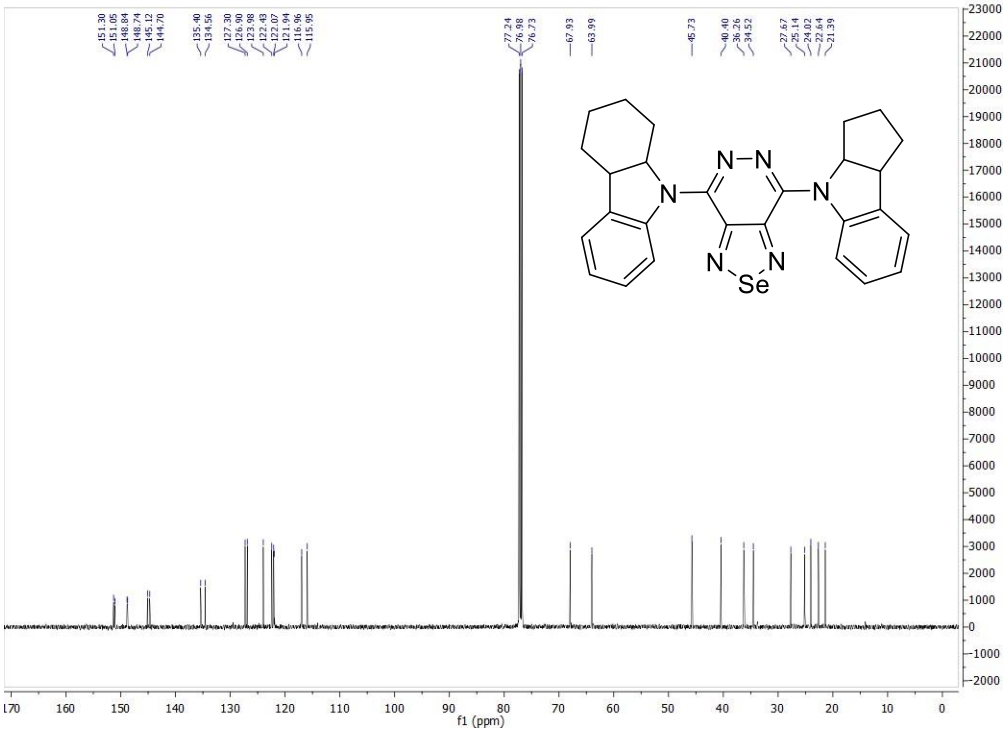


4-(1,2,3,4,4a,9a-Hexahydro-9H-carbazol-9-yl)-7-(2,3,3a,8b-tetrahydrocyclopenta[b]indol-4(1H)-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (7c)

^{1}H NMR(300 MHz)

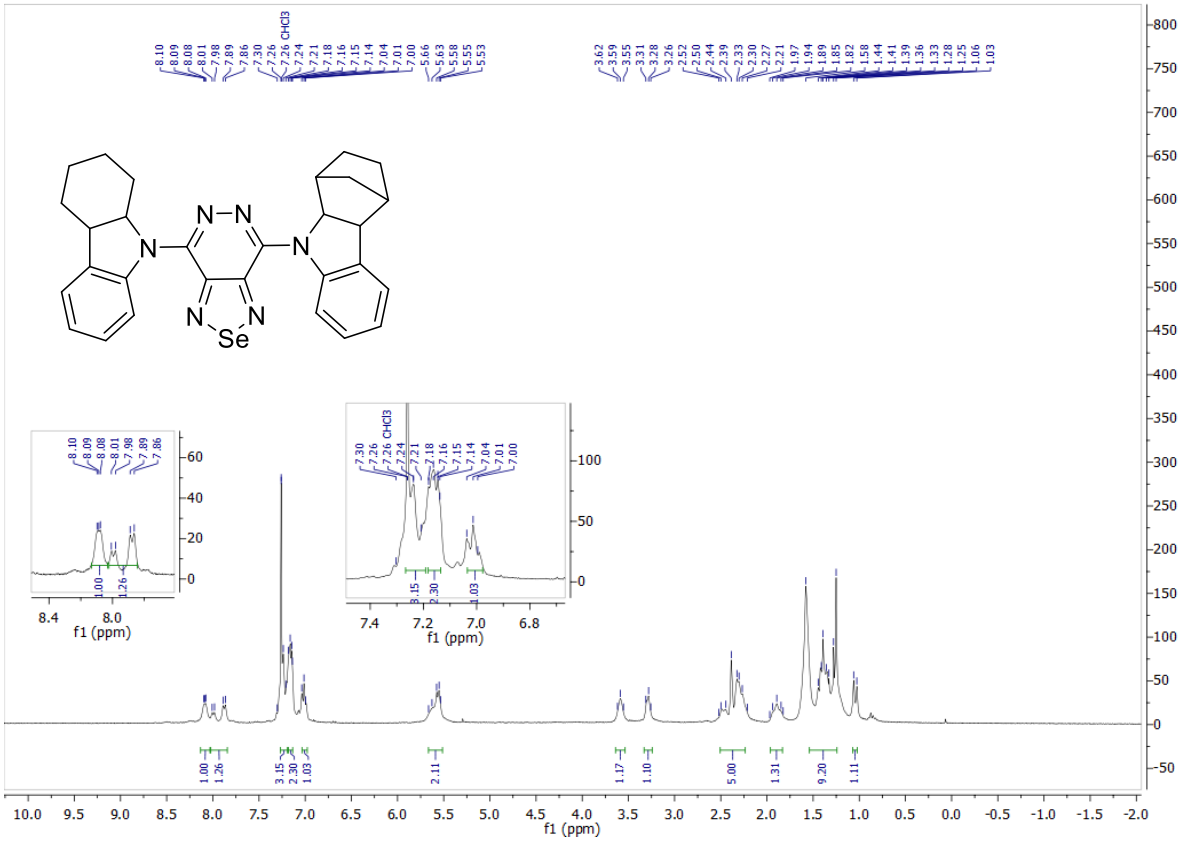


^{13}C NMR(75 MHz)

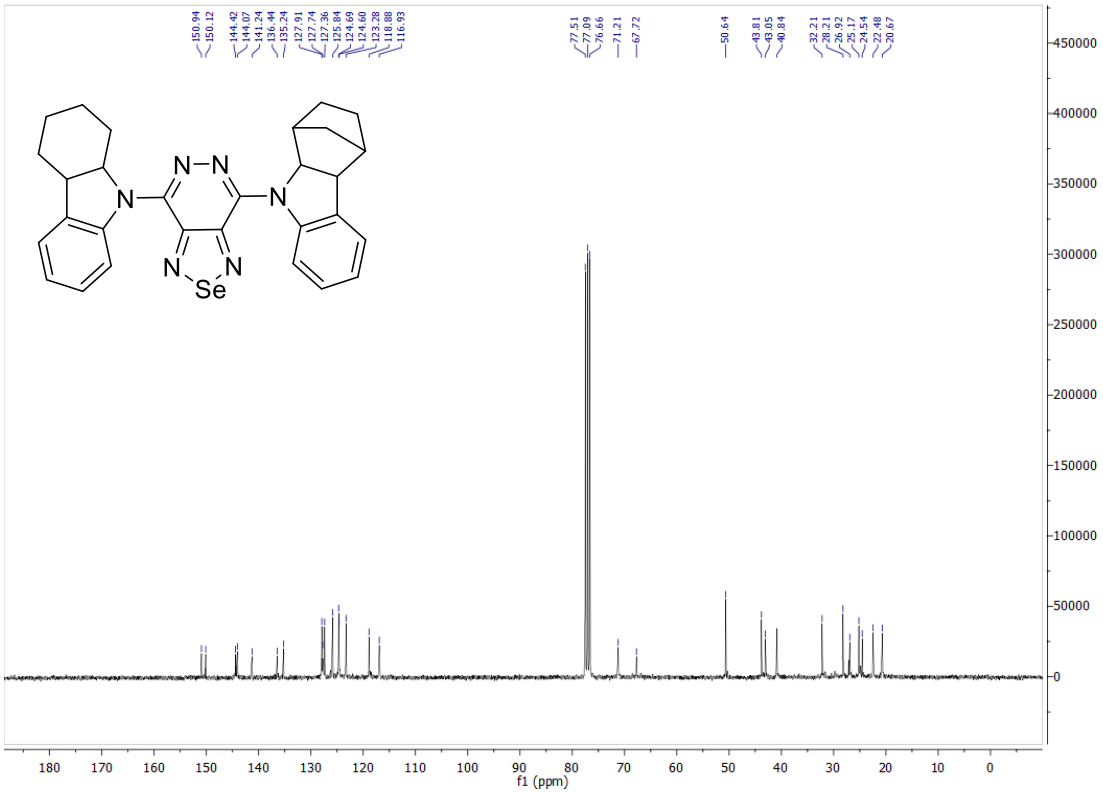


4-(1,2,3,4,4a,9a-Hexahydro-9H-1,4-methanocarbazol-9-yl)-7-(1,2,3,4,4a,9a-hexahydro-9H-carbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (7d)

^{1}H NMR(300 MHz)

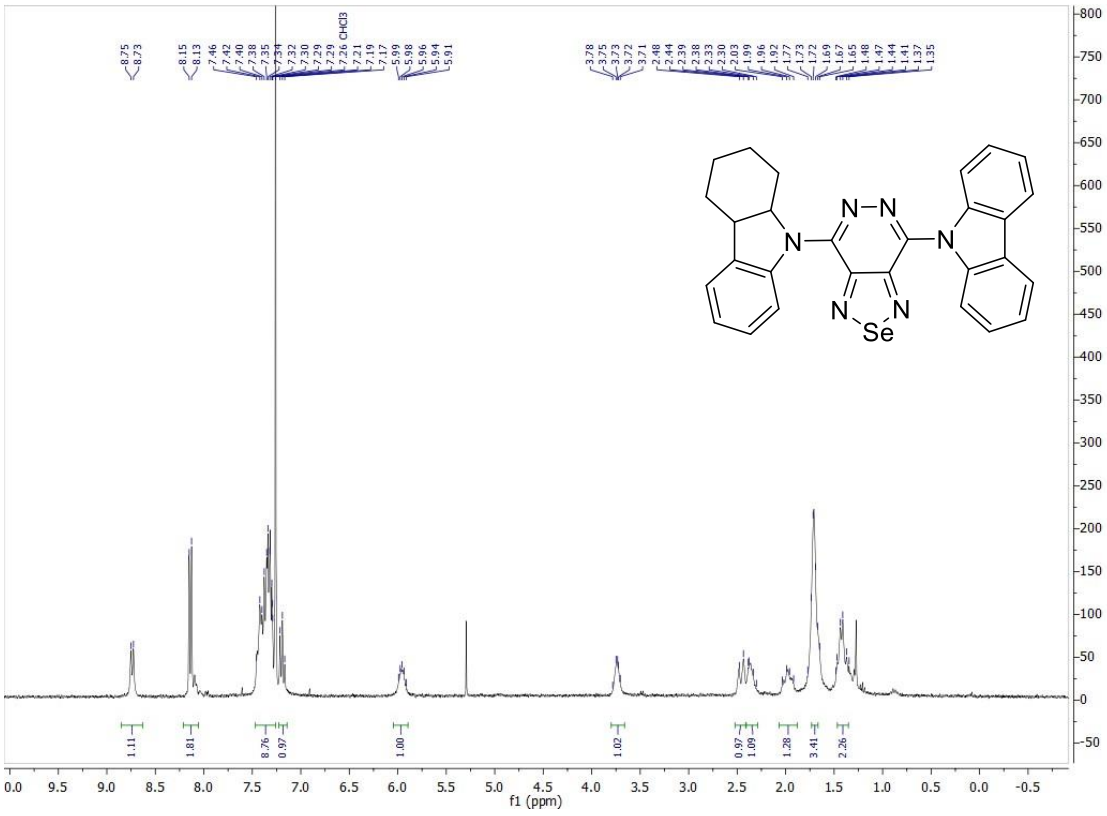


^{13}C NMR(75 MHz)

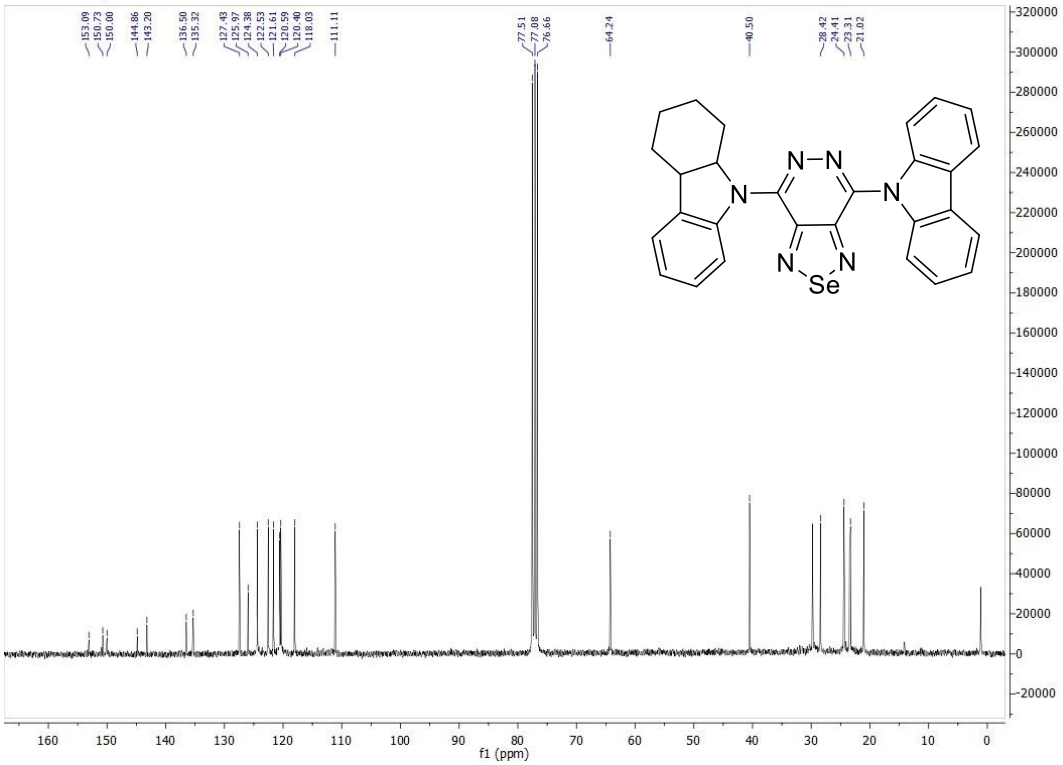


4-(9H-carbazol-9-yl)-7-(1,2,3,4,4a,9a-hexahydro-9H-carbazol-9-yl)-[1,2,5]selenadiazolo[3,4-d]pyridazine (7e)

^{1}H NMR(300 MHz)



^{13}C NMR(75 MHz)



SI-2 Crystal data

Table 1. Crystal data and structure refinement for compound (**5a**)

Empirical formula	$C_9H_{10}BrN_5$ Se
Formula weight	347.09
Temperature	100.00(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 32.5188(3) Å α= 90°.
b = 6.73250(10) Å	β= 95.2020(10)°.
c = 20.1942(2) Å	γ = 90°.
Volume	4402.96(9) $Å^3$
Z	16
Density (calculated)	2.094 Mg/m^3
Absorption coefficient	8.714 mm^{-1}
F(000)	2688
Crystal size	0.459 x 0.096 x 0.067 mm^3
Theta range for data collection	2.729 to 80.389°.
Index ranges	-41<=h<=41, -8<=k<=8, -25<=l<=25
Reflections collected	9133
Independent reflections	9133
Completeness to theta = 67.684°	99.9 %
Absorption correction	Gaussian
Max. and min. transmission	-0.010 and 10000000.000
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9133 / 30 / 309
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1292
R indices (all data)	R1 = 0.0427, wR2 = 0.1308
Largest diff. peak and hole	1.014 and -1.142 $e.Å^{-3}$

SI-3 Spectroscopy

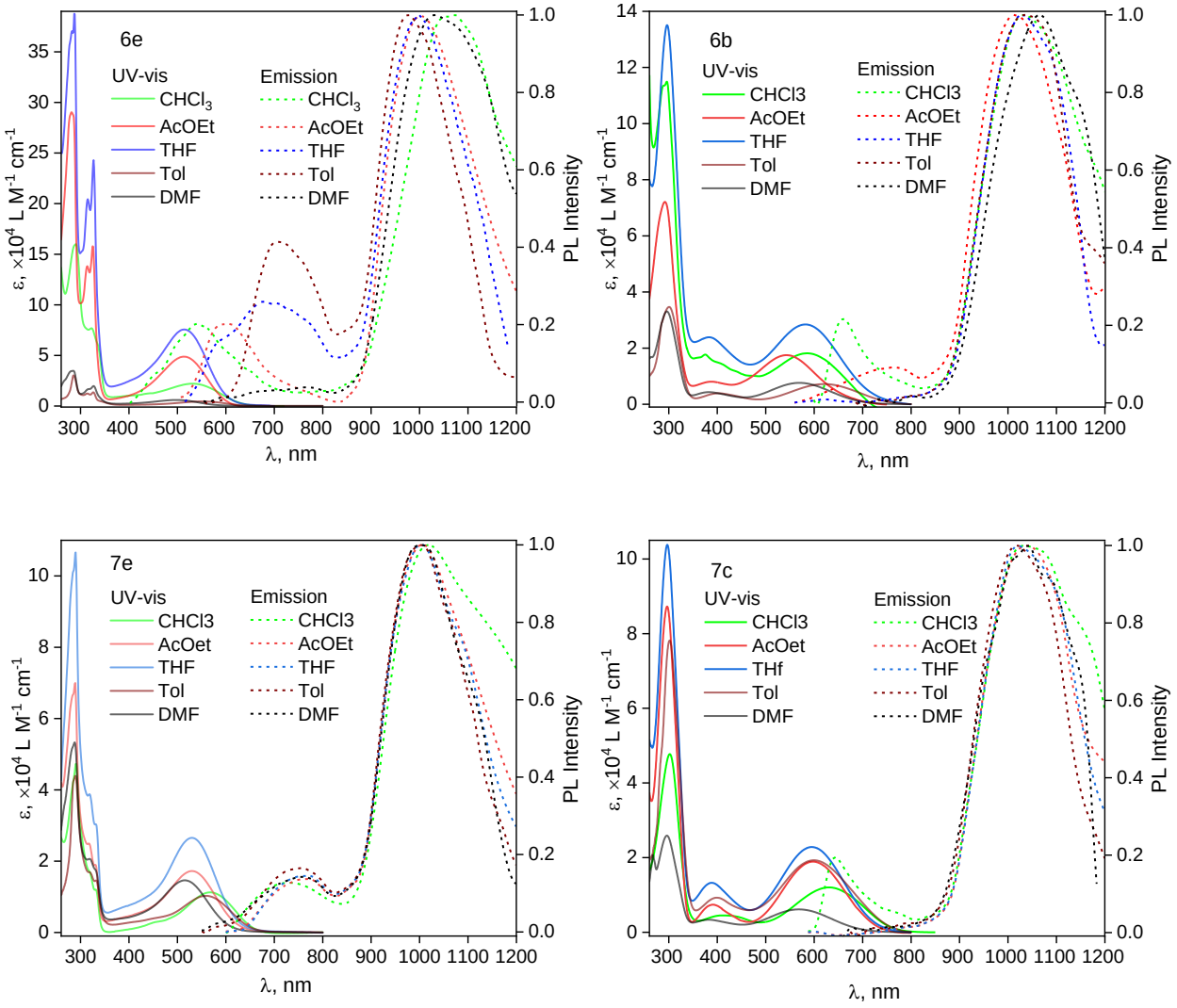
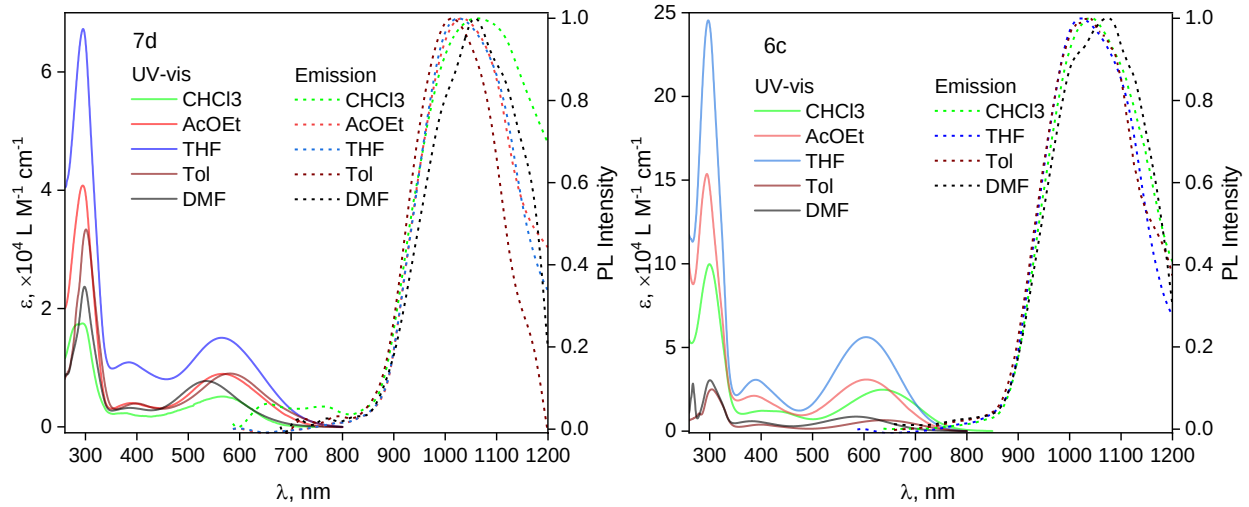


Рисунок 1 7d-худшая интенсивность



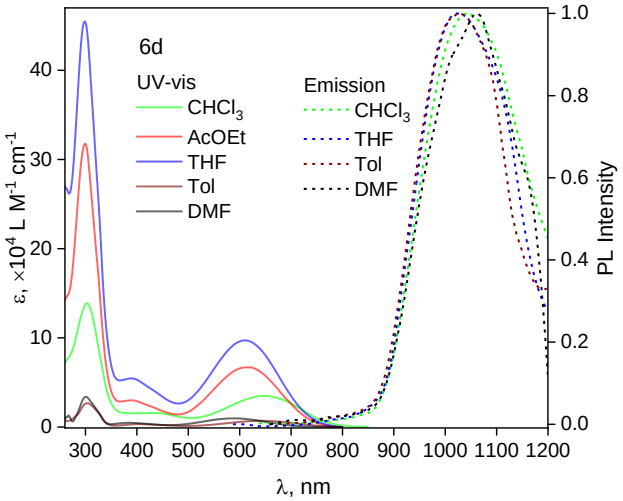


Figure S1. Absorption and luminescence spectra recorded upon excitation at the wavelength of absorption maximum (λ_{abs} ICT) for the 6e, **6b, 7e, 7c, 7d, 6c** and **6d** compounds dissolved in different solvents.

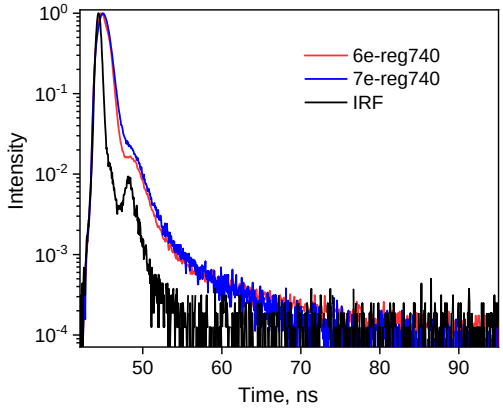
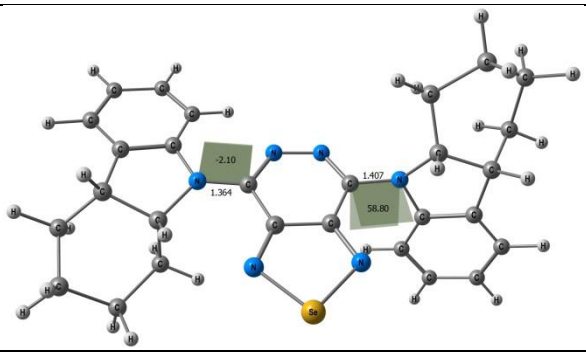
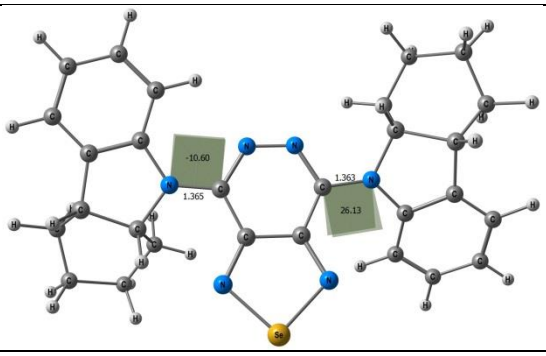


Figure S2. PL decays measured under excitation at 450 nm for **6e** and **7e** recorded at 740 nm at T=300 K.

For **6e** compound the phosphorescence lifetime (τ) is 10.1 ± 0.8 ns, for **7e** τ = 7.0 ± 0.4 ns.

SI-4 Theoretical calculations

	S_0	S_1
6b		

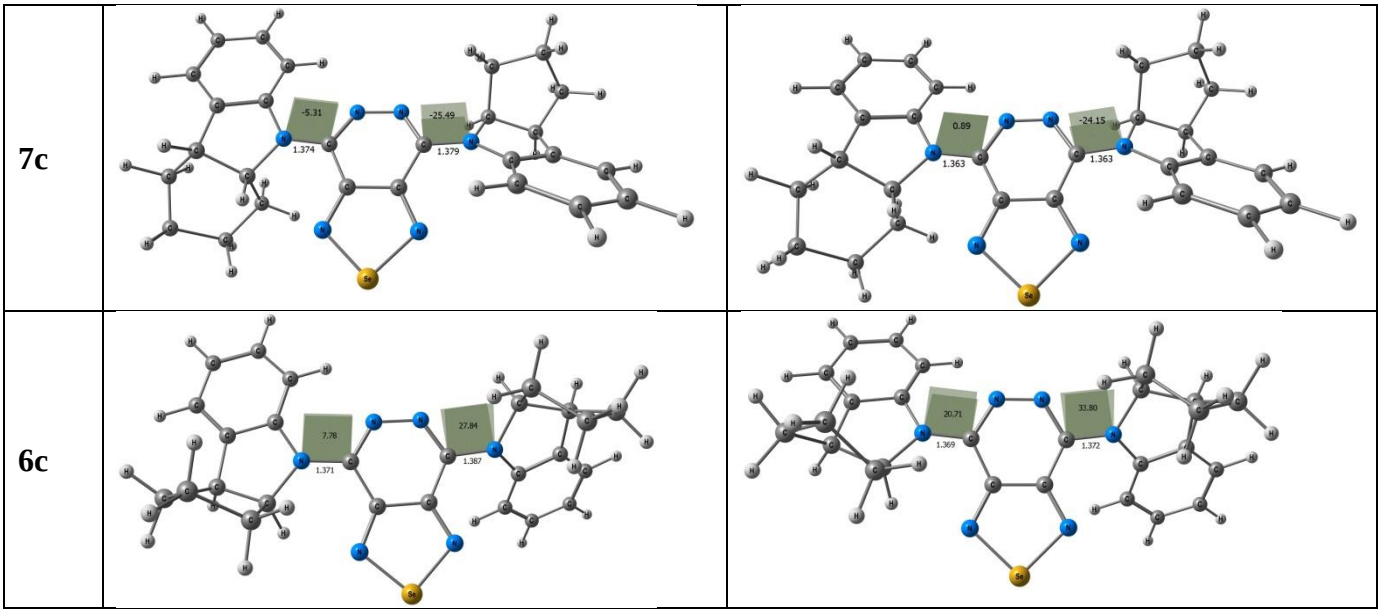
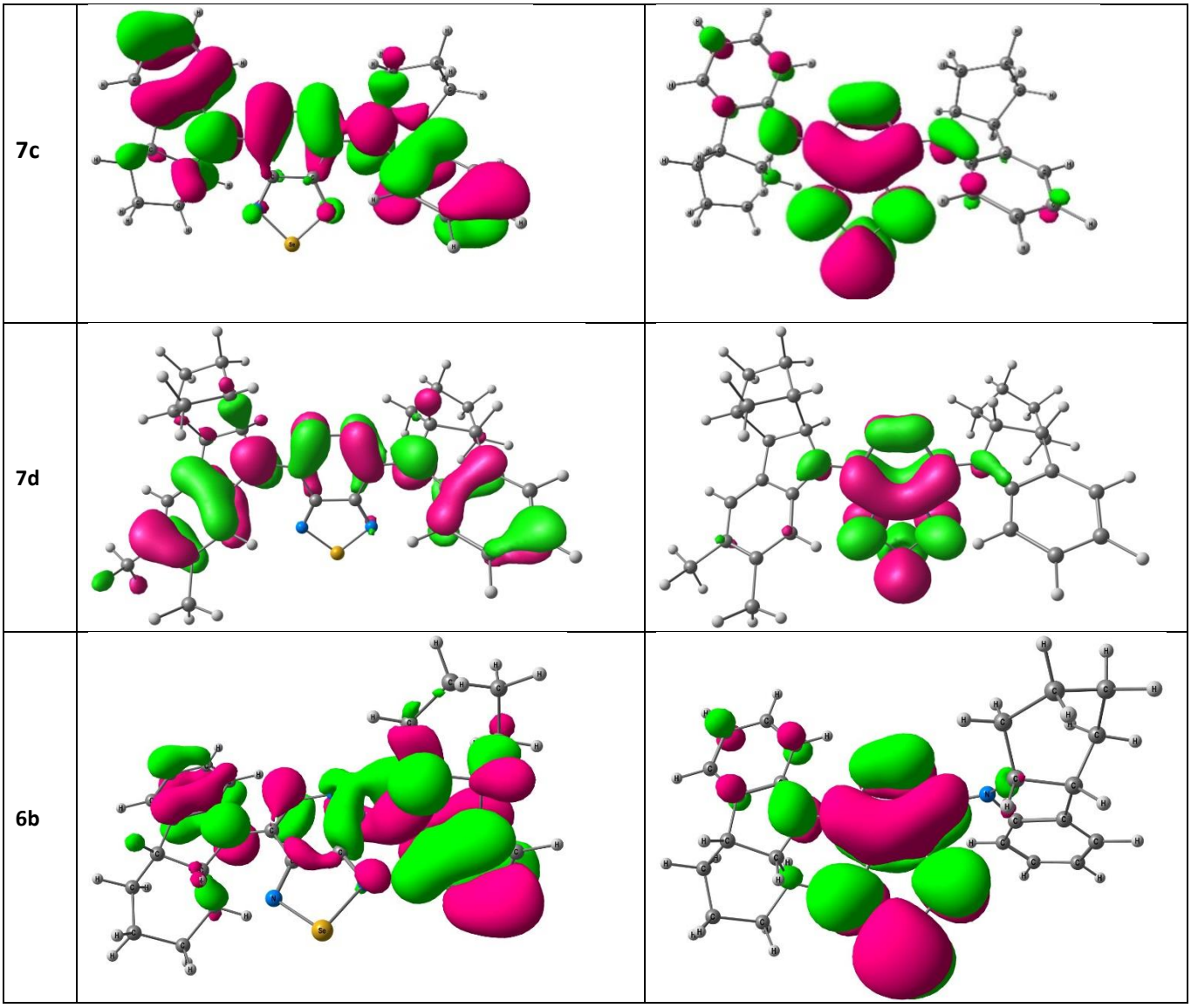


Figure S2. Optimized ground state (S_0) and first excited singlet state (S_1) geometries for **6b**, **7c**, **6c** and **6d**.



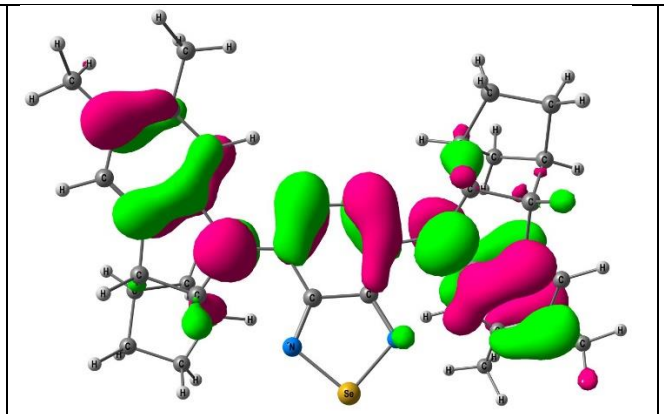
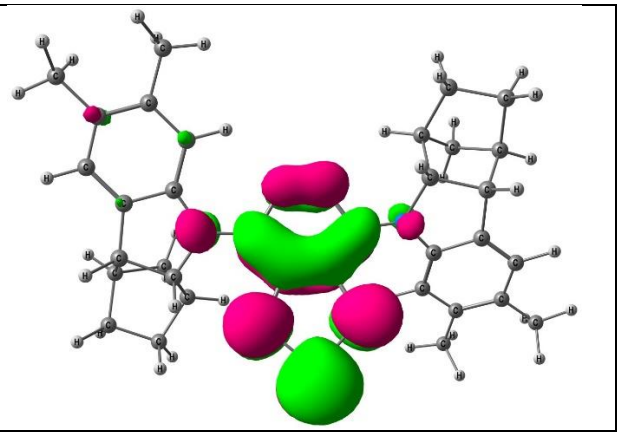
6d		

Figure S3: Frontier molecular orbitals calculated for equilibrium S_0 geometries of the **7c, 7d, 6b** and **6d** compounds.

SI-5 Cytotoxicity

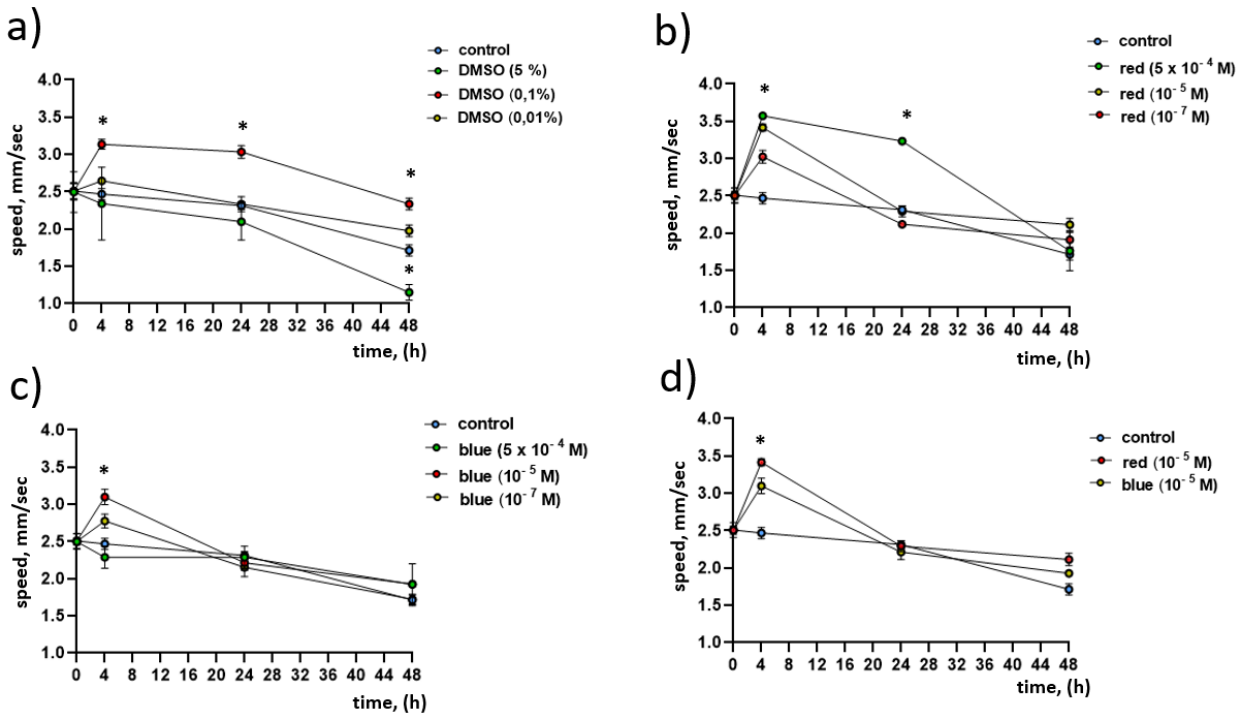


Figure S4: Changes in the swimming speed of Paramecium caudatum in response to the exposure to Red and Blue molecules at different concentrations. (a) Changes in cell movement speed under the influence of DMSO during the 48-hour observation period. Cell concentration - 600±50 cells/ml, * - significant difference from the movement speed of cells in the intact group, $p < 0.05$, two-way ANOVA. (b) Changes in cell movement speed under the influence of Red molecules at concentrations of 5×10^{-4}, 10^{-5}, 10^{-7} M during the 48-hour observation period. Cell concentration - 600±50 cells/ml, * - significant difference from the movement speed of cells in the intact group, $p < 0.05$, two-way ANOVA. (c) Changes in the movement speed of motile cells under the influence of Blue molecules at concentrations of 5×10^{-4}, 10^{-5}, 10^{-7} M during the 48-hour observation period. Cell concentration - 600±50 cells/ml, * - significant difference from the movement speed of cells in the intact group, $p < 0.05$, two-way ANOVA. (d) Comparison of cell movement speed under the influence of **6e** and **6c** molecules at a concentration of 10^{-5} M during the 48-hour observation period. Cell concentration - 600±50 cells/ml, * - significant difference in cell movement speed between the groups with Red and Blue particles, $p < 0.05$, two-way ANOVA.