Supporting Information for

Impact of Molecular Arrangement and Torsional Motion on the Fluorescence of Salophen and its Metal Complexes

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Table of contents

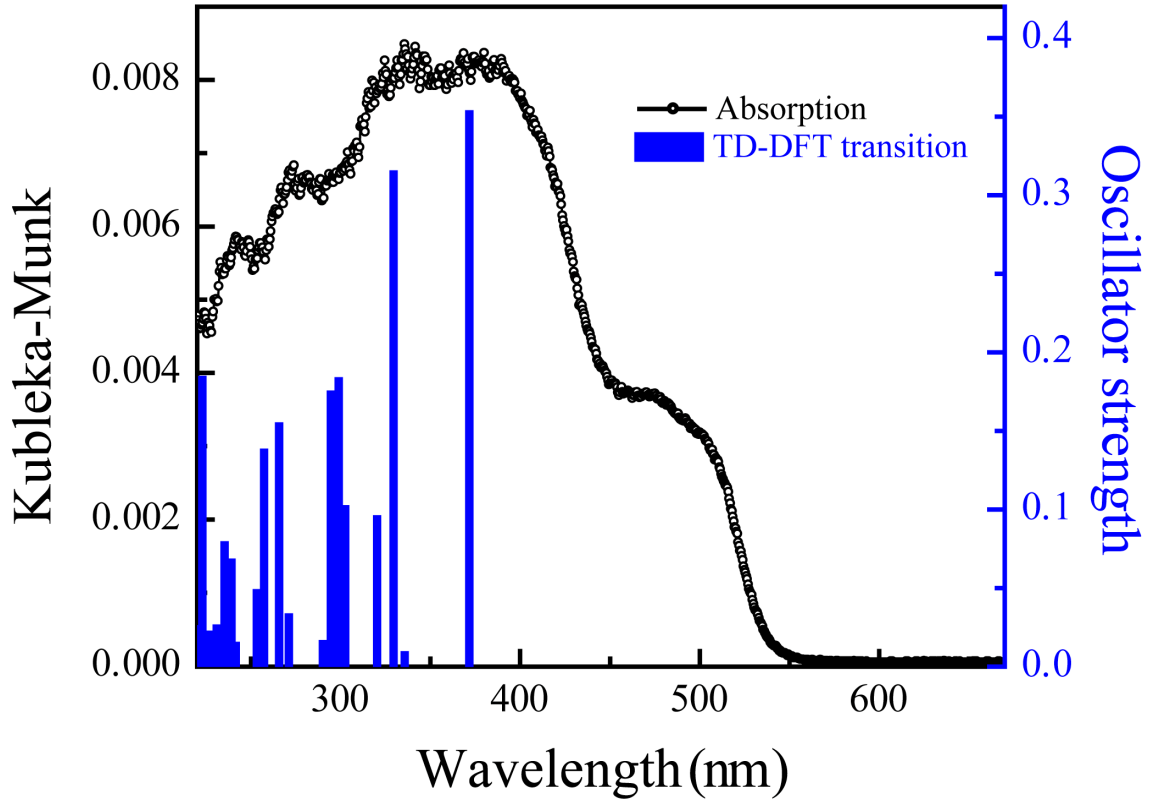

Figure S1. Solid state absorption spectrum of salophen crystal (black) and TD-DFT transitions of salophen (blue) in its crystal geometry (B3LYP/6-311++G(d,p)/Acetonitrile). In order to construct the absorption spectrum, salophen crystals are crushed to a powder and mixed with $BaSO_4$ with a final sample concentration of ~5% (v/v). Diffuse reflectance of this powder is measured on a Shimadzu-3600 spectrometer fitted with MPC-3100 multi-purpose compartment. The absorption spectrum is then generated from measured reflectance via Kubelka-Munk transformation.

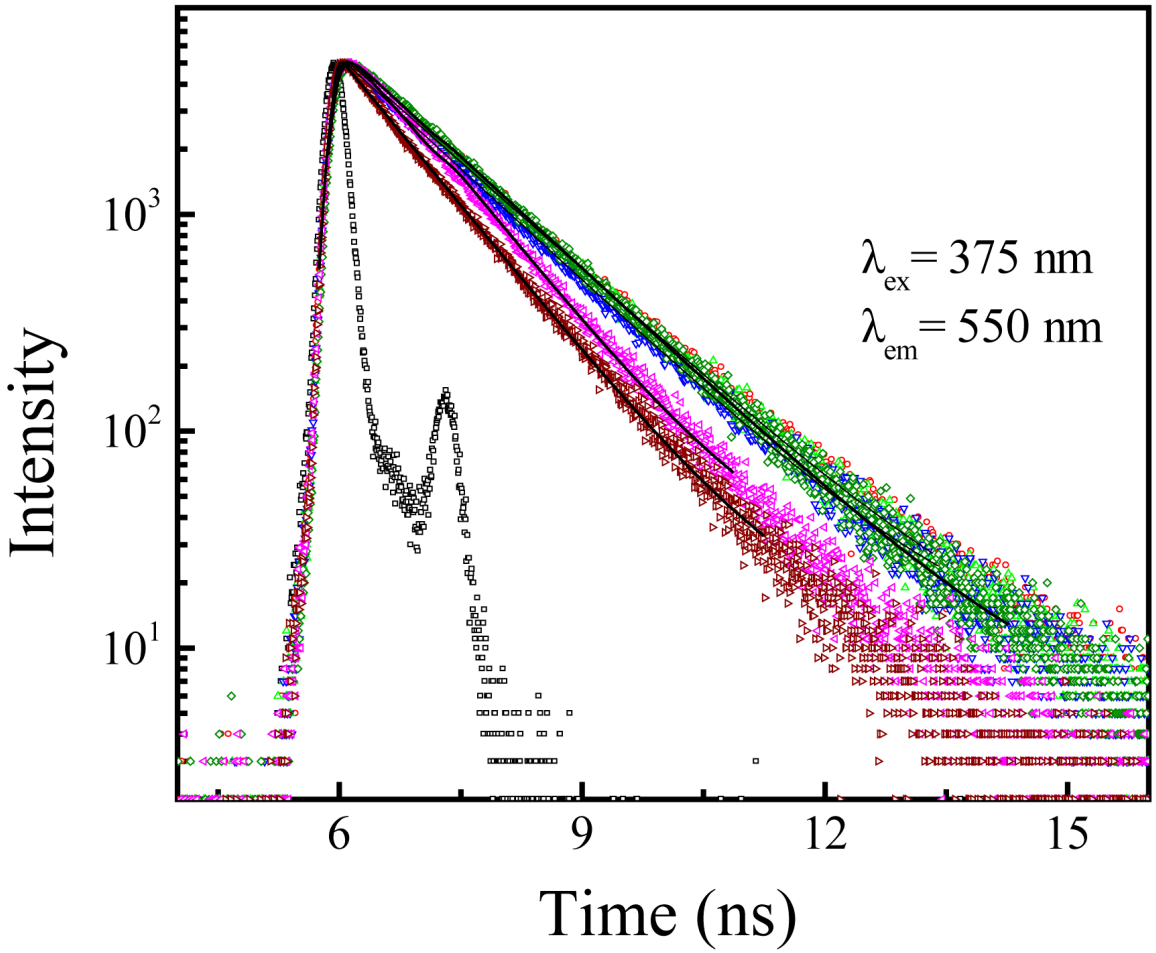

Figure S2. Decay profiles of dropcasted salophen at different spots. The smallest lifetime is 0.95 ns whereas the median lifetime is 1.2 ns.

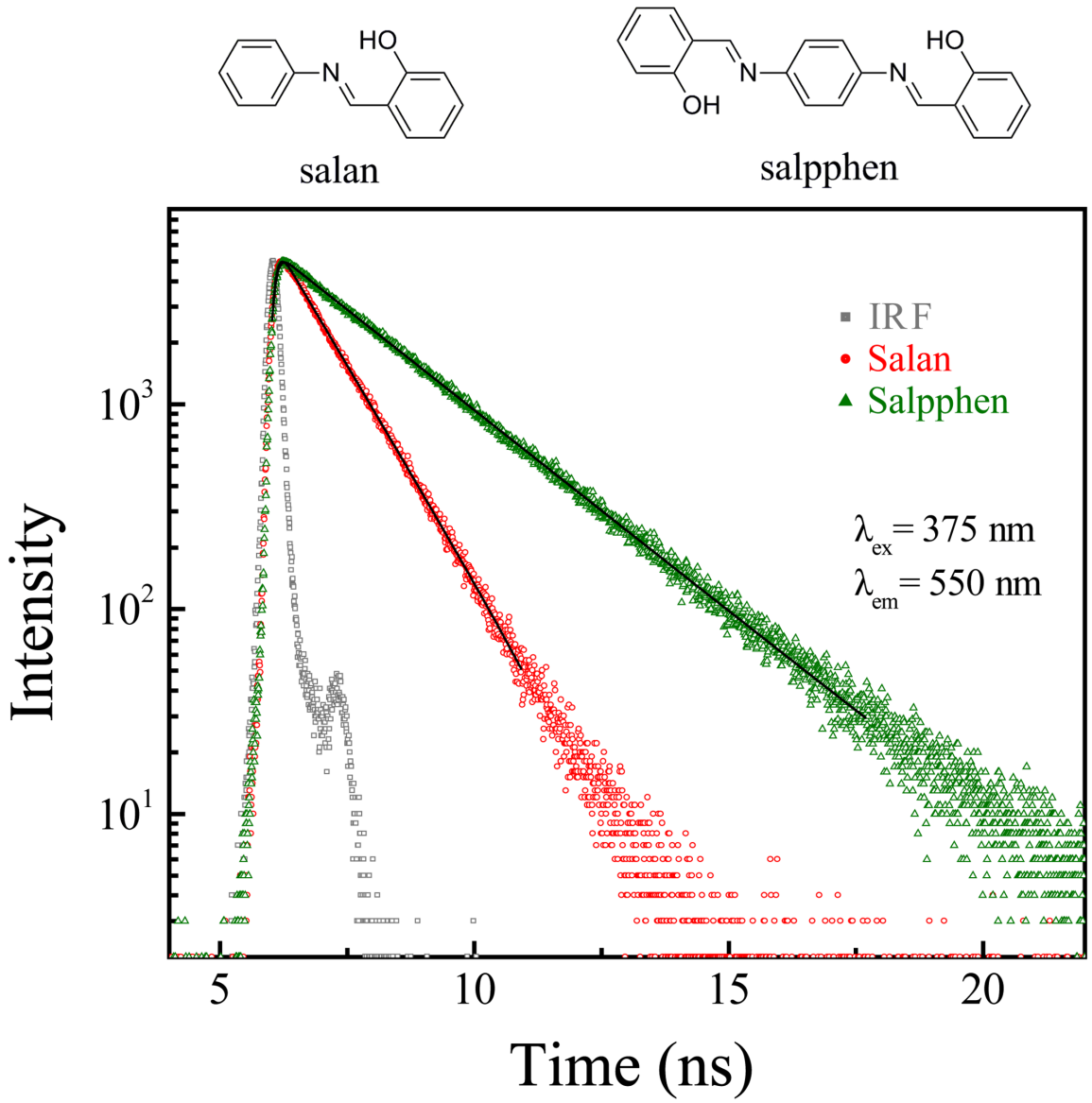

Figure S3. Nanosecond fluorescence decay of salan and salpphen in crystal form.

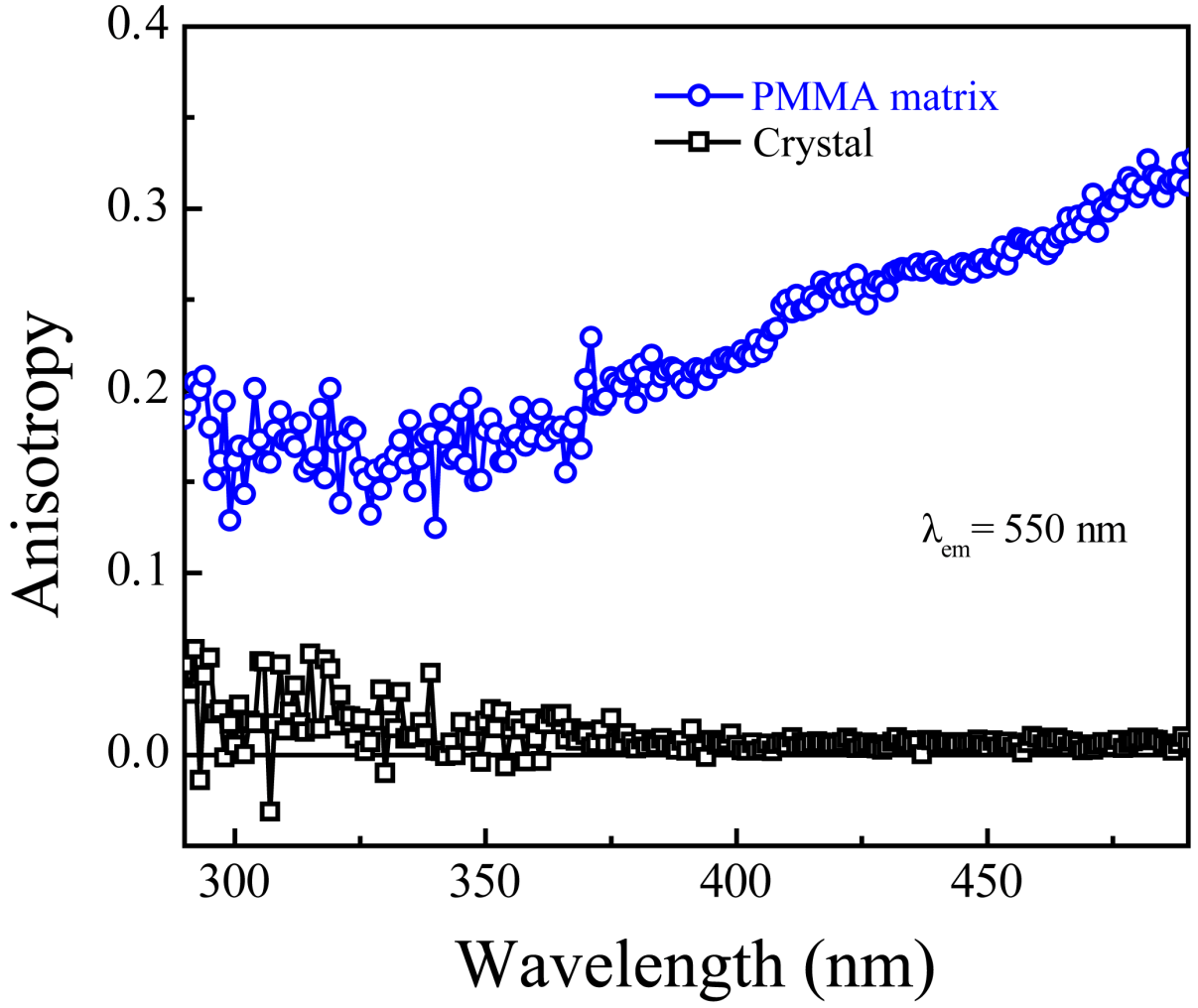

Figure S4. Steady state excitation anisotropy of salophen in crystalline form and PMMA matrix monitored at 550 nm.

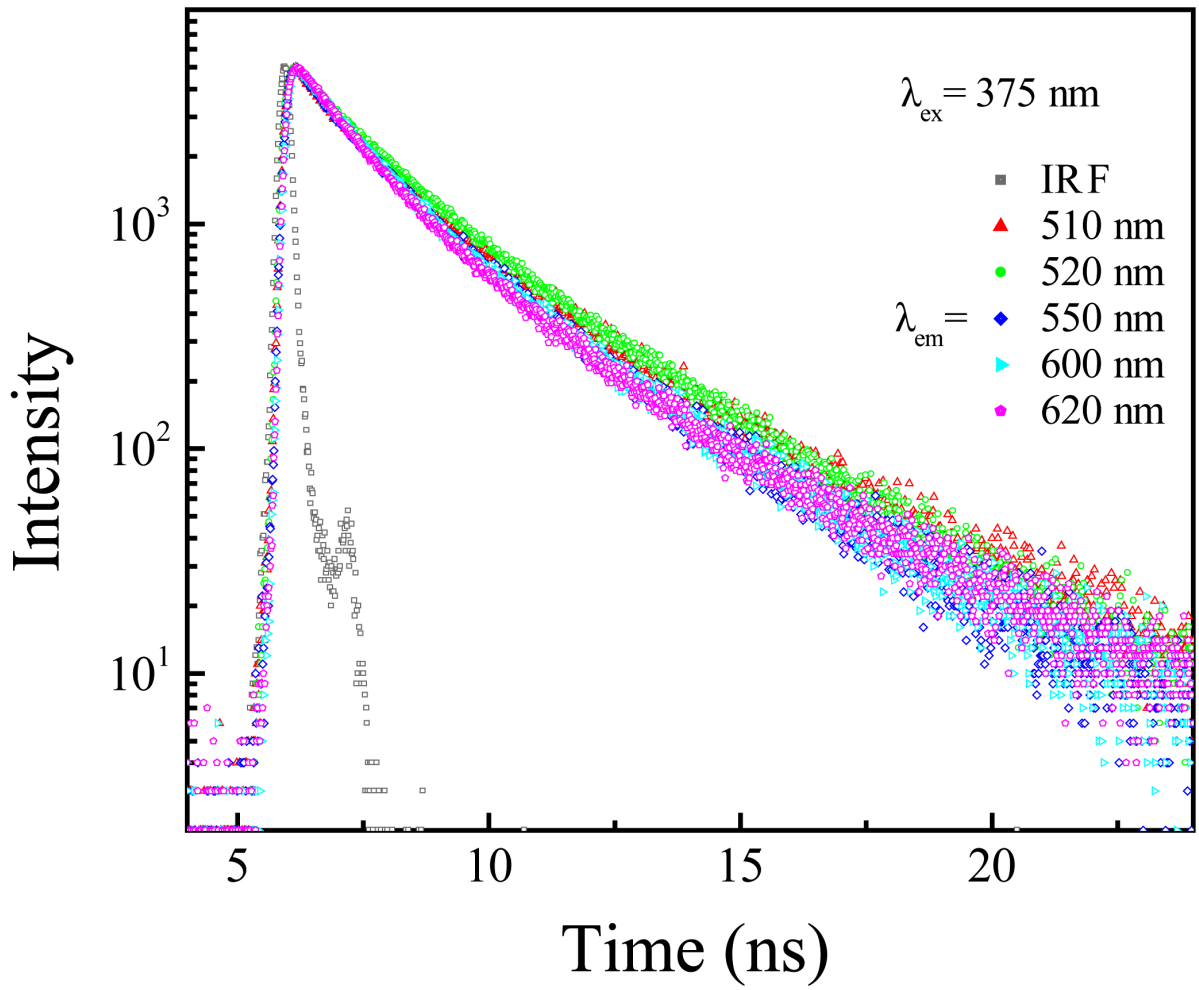

Figure S5. Fluorescence decays of salophen for different emission wavelengths at 77K.

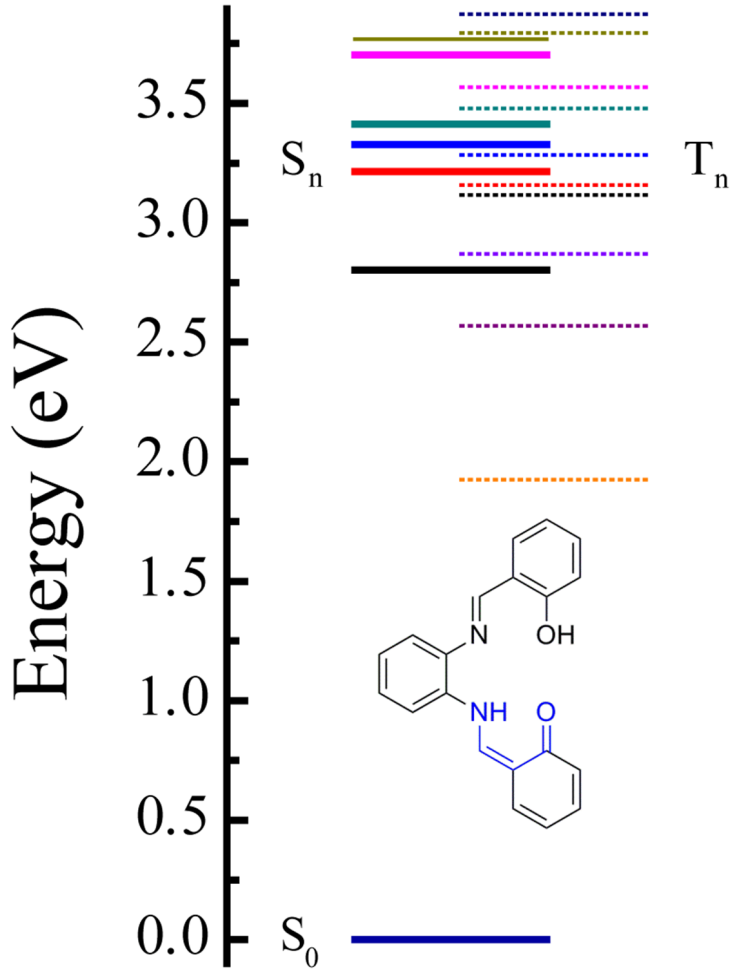

Figure S6. Energy level diagram of cis-mono keto form of salophen showing both its singlet (solid line) and triplet states (dotted line).

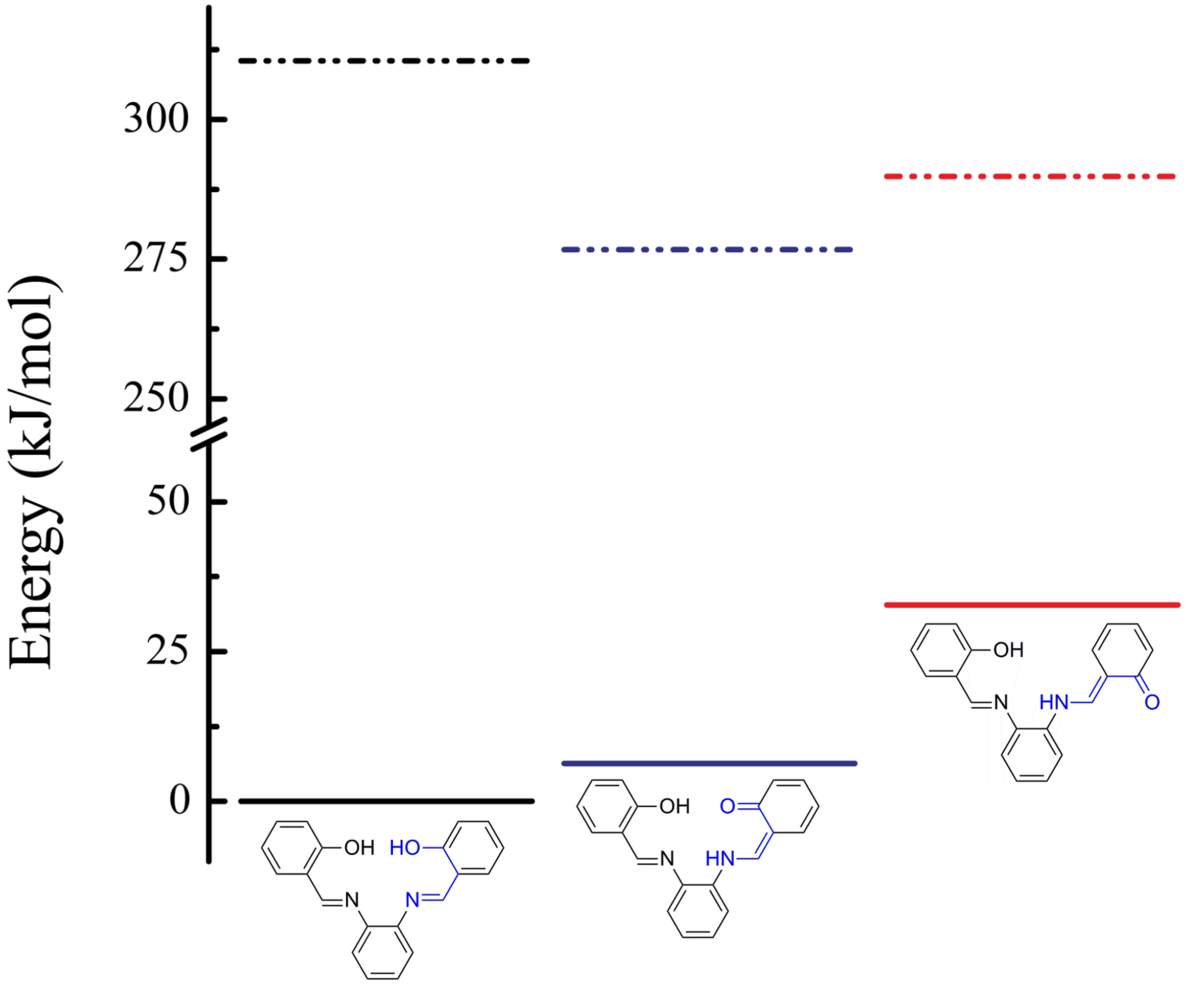

Figure S7. Ground state (solid line) and their corresponding excited state (dotted line) energy level of enol, cis-mono keto form and trans mono-keto form of salophen.

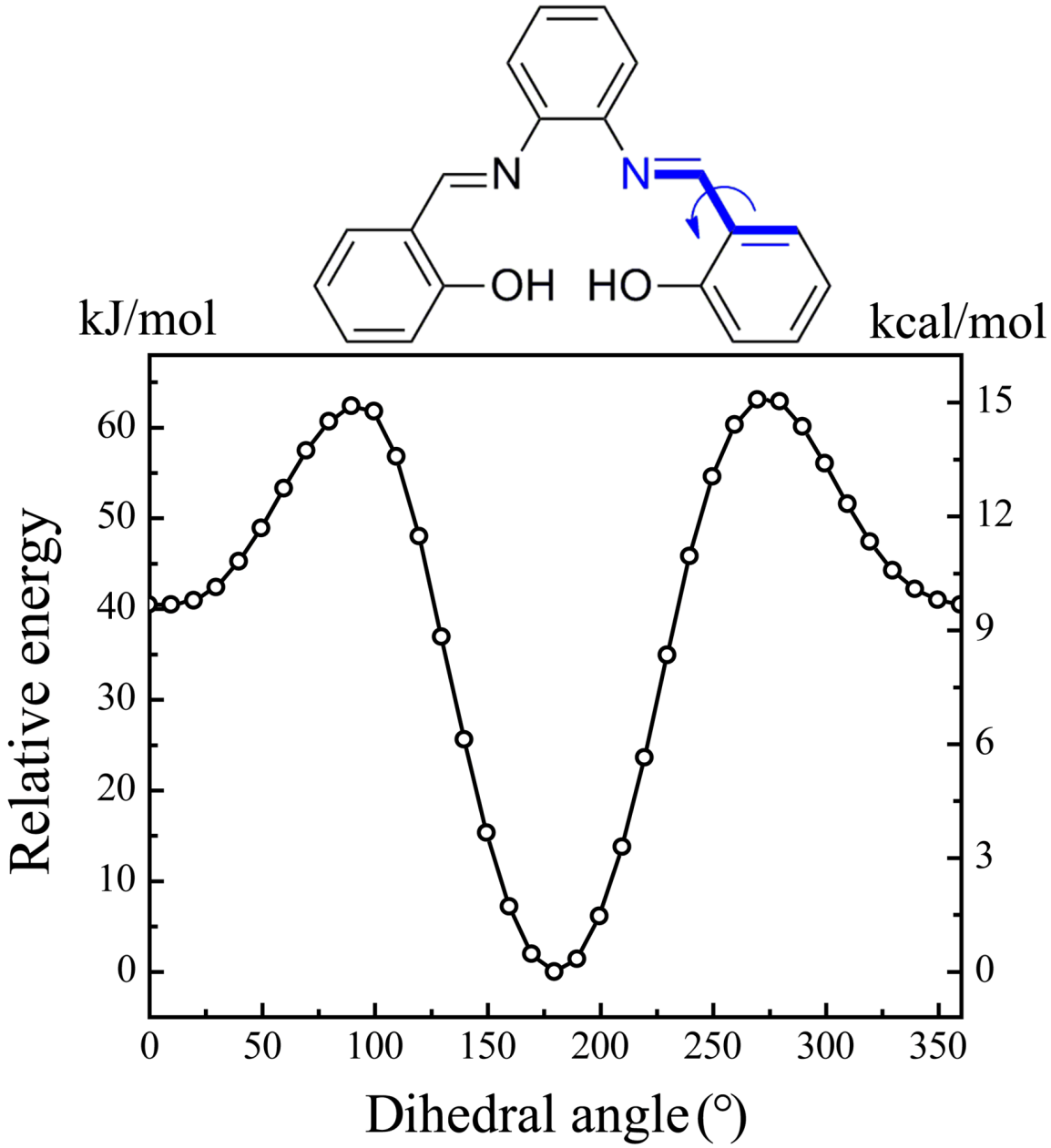

Figure S8. Energy profile for rotation indicated in blue.

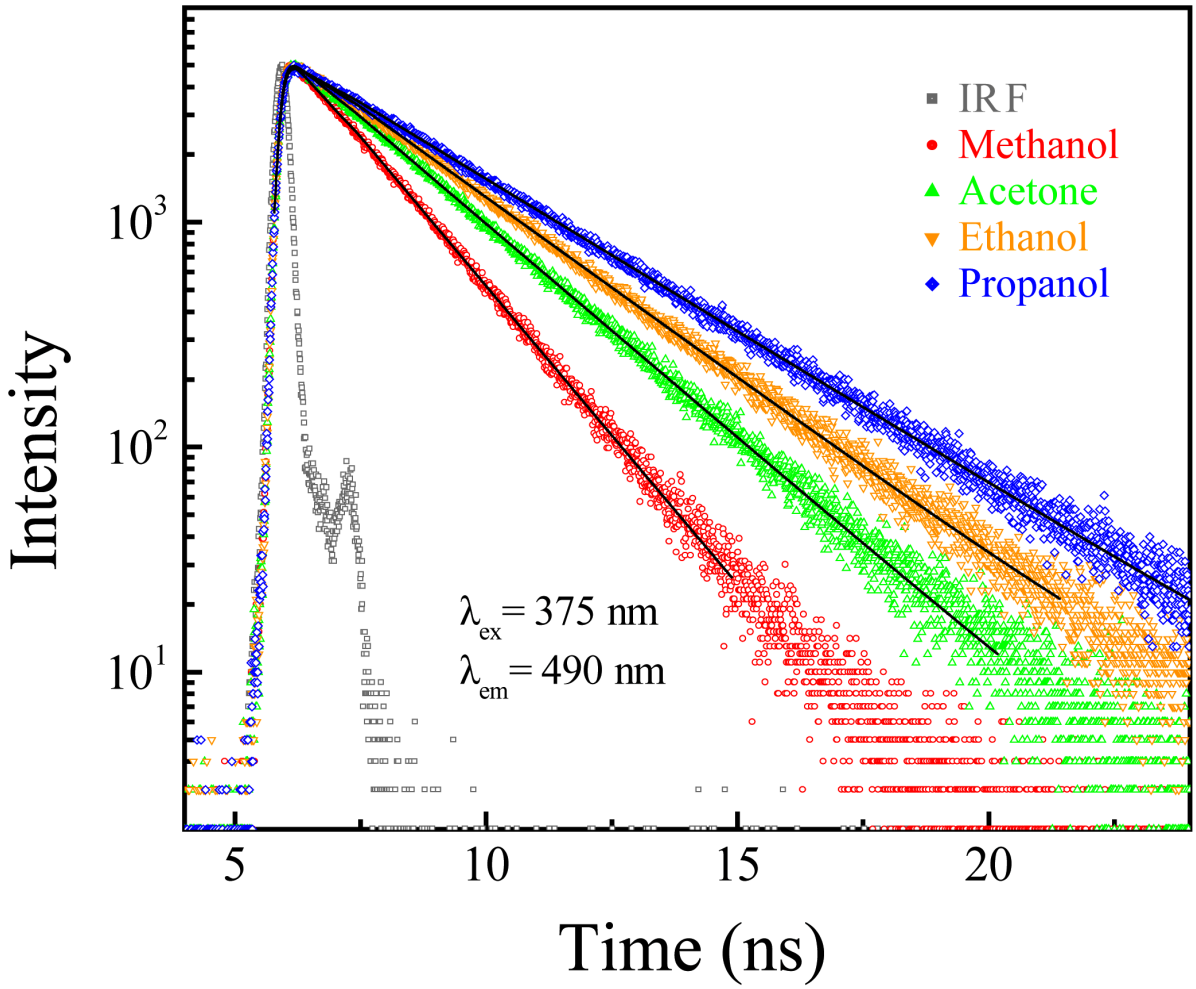

Figure S9. Fluorescence decays of $SalAl^+$ in methanol (red), acetone (green), ethanol (orange) and propanol (blue).

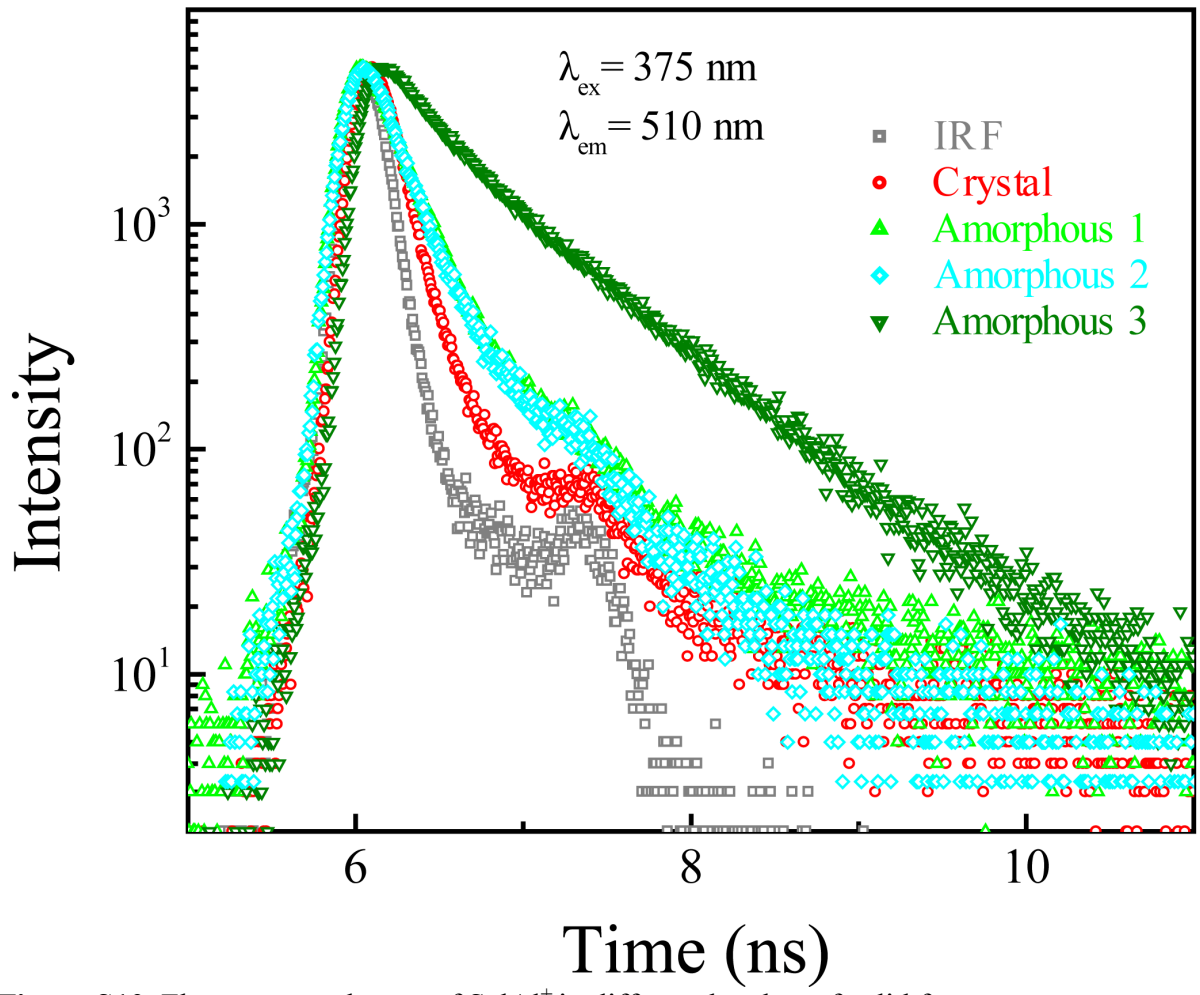

Figure S10. Fluorescence decays of $SalAl^+$ in different batches of solid form.

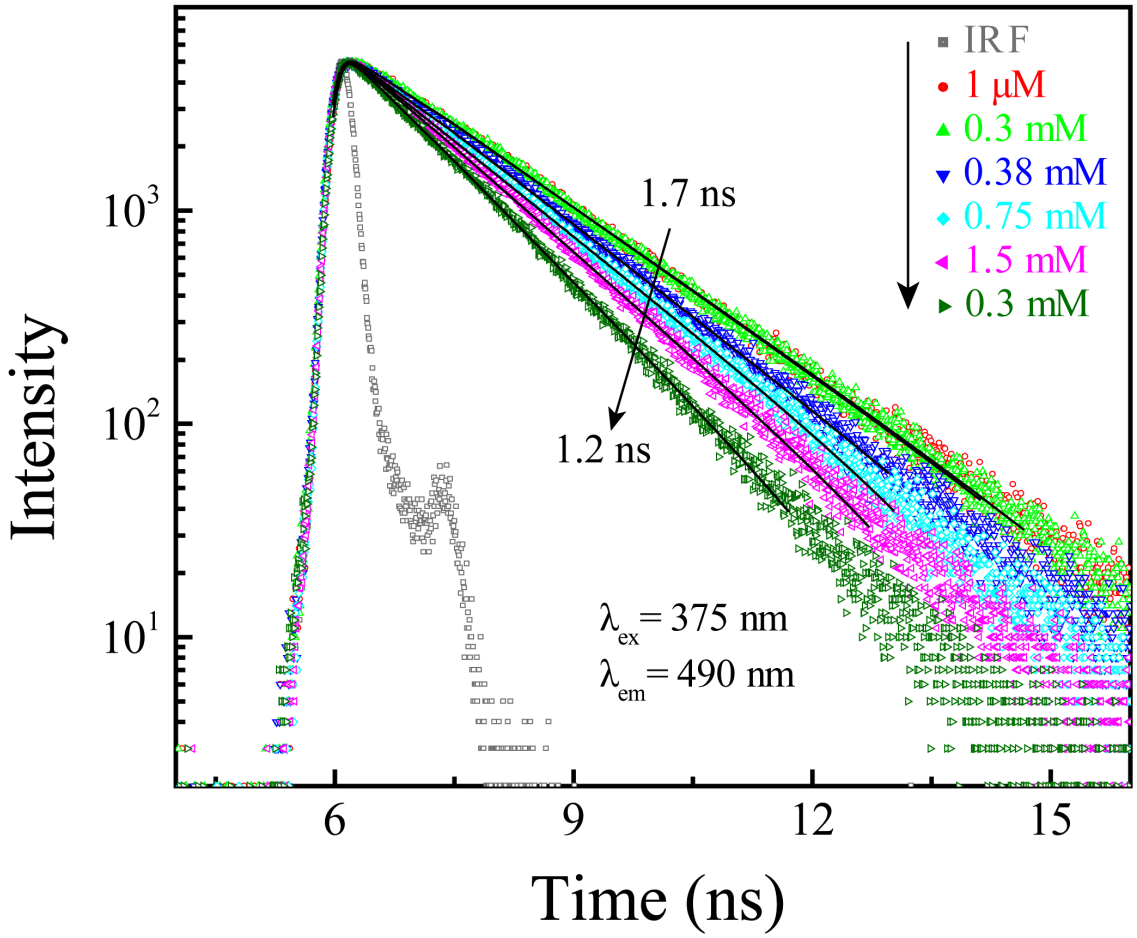

Figure S11. Fluorescence decays of $SalAl^+$ in methanolic solutions, at different concentration. The arrow indicates the direction of increase in concentration. The mentioned concentrations are approximate.

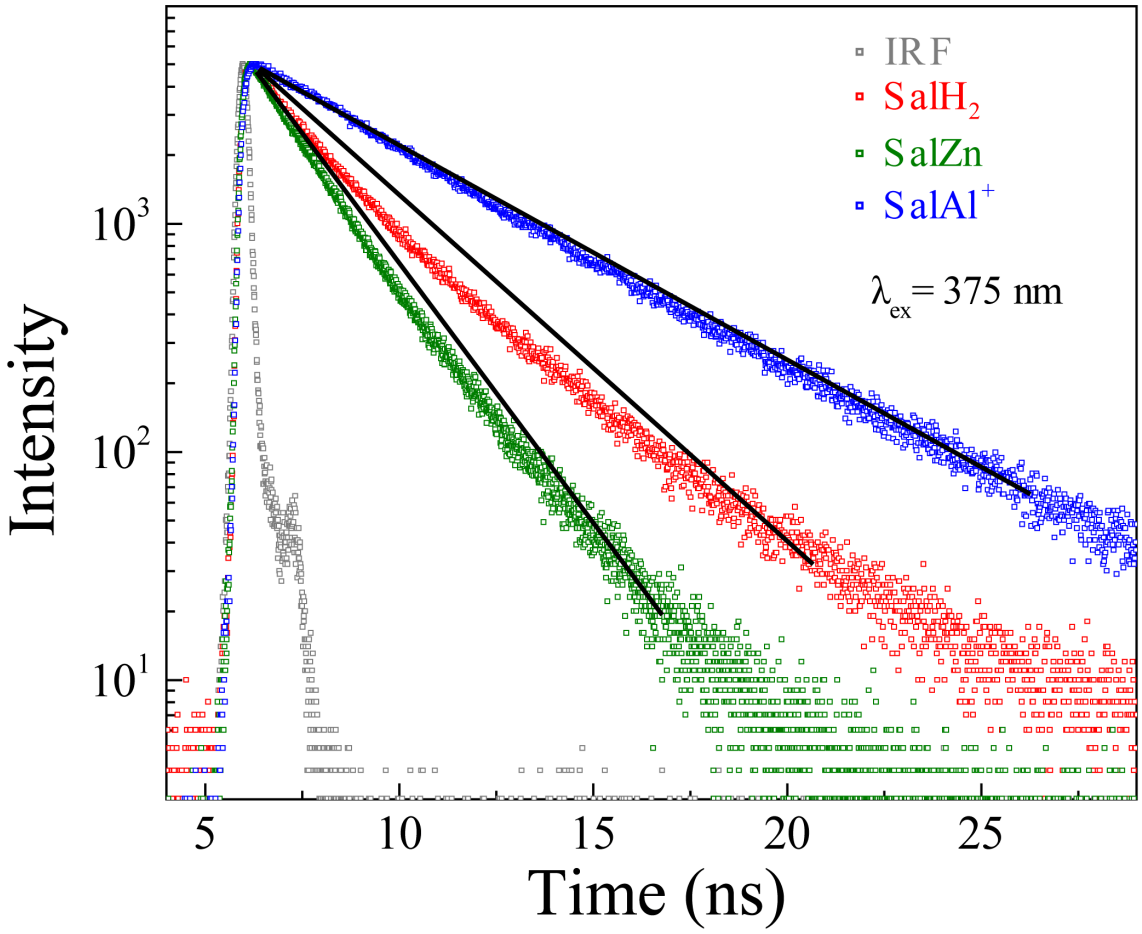

Figure S12. Fluorescence decays of salophen and its complexes at 77K. Straight solid line (black) is used as a reference to indicate the deviation of the decay curve from single exponential behavior.