Supporting Information

Zinc Donor-Acceptor Schiff Base Complexes as Thermally Activated Delayed Fluorescence Emitters

Andreas Russegger, Lisa Eiber, Andreas Steinegger and Sergey M. Borisov*

Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology,

Stremayrgasse 9, 8010, Graz, Austria

* sergey.borisov@tugraz.at

1 Photophysical Properties

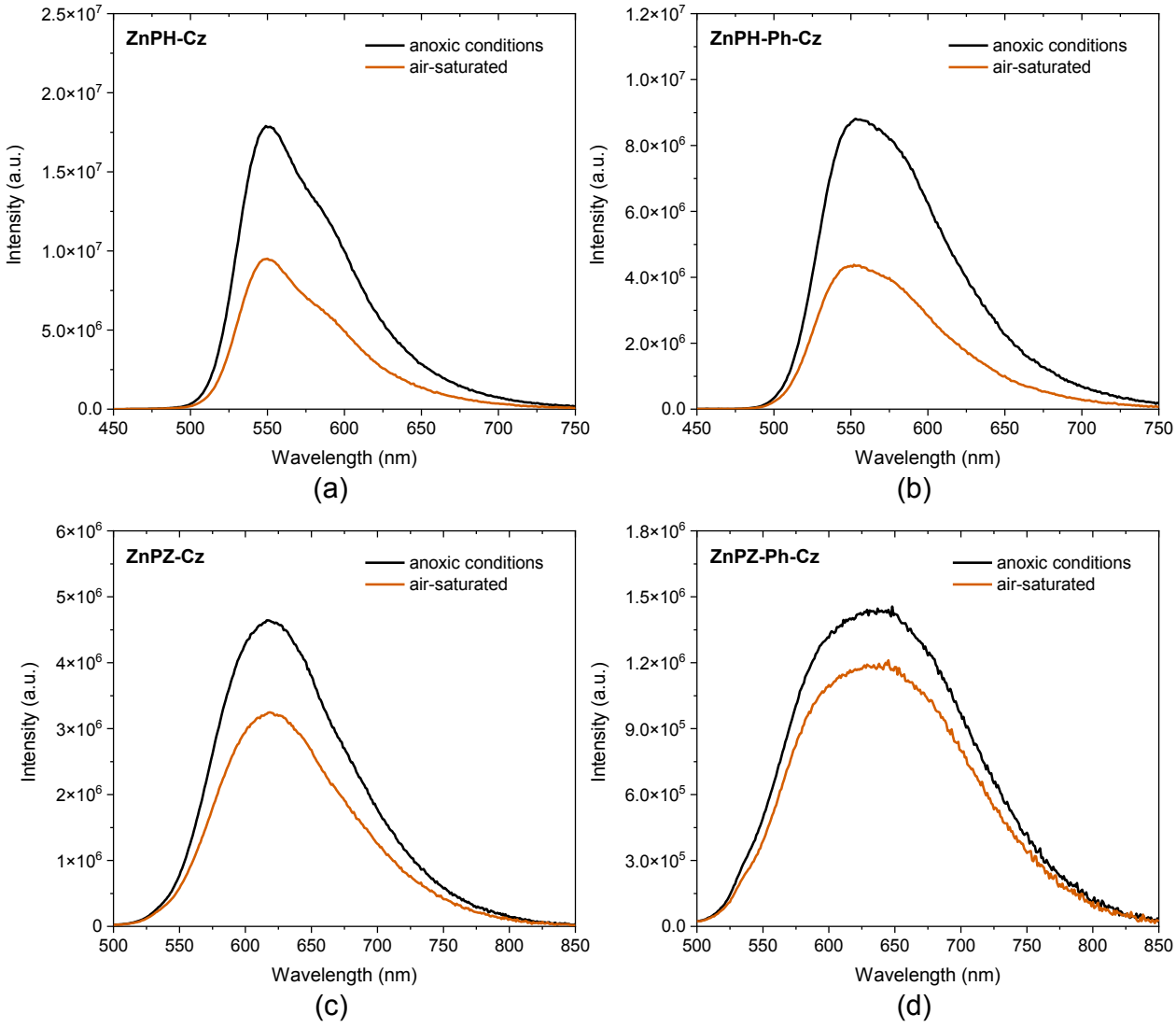

Figure S1. Emission spectra of **ZnPH-Cz** (a), **ZnPH-Ph-Cz** (b), **ZnPZ-Cz** (c) and **ZnPZ-Ph-Cz** (d) in toluene under anoxic (degassed with high purity nitrogen) and air-saturated conditions.

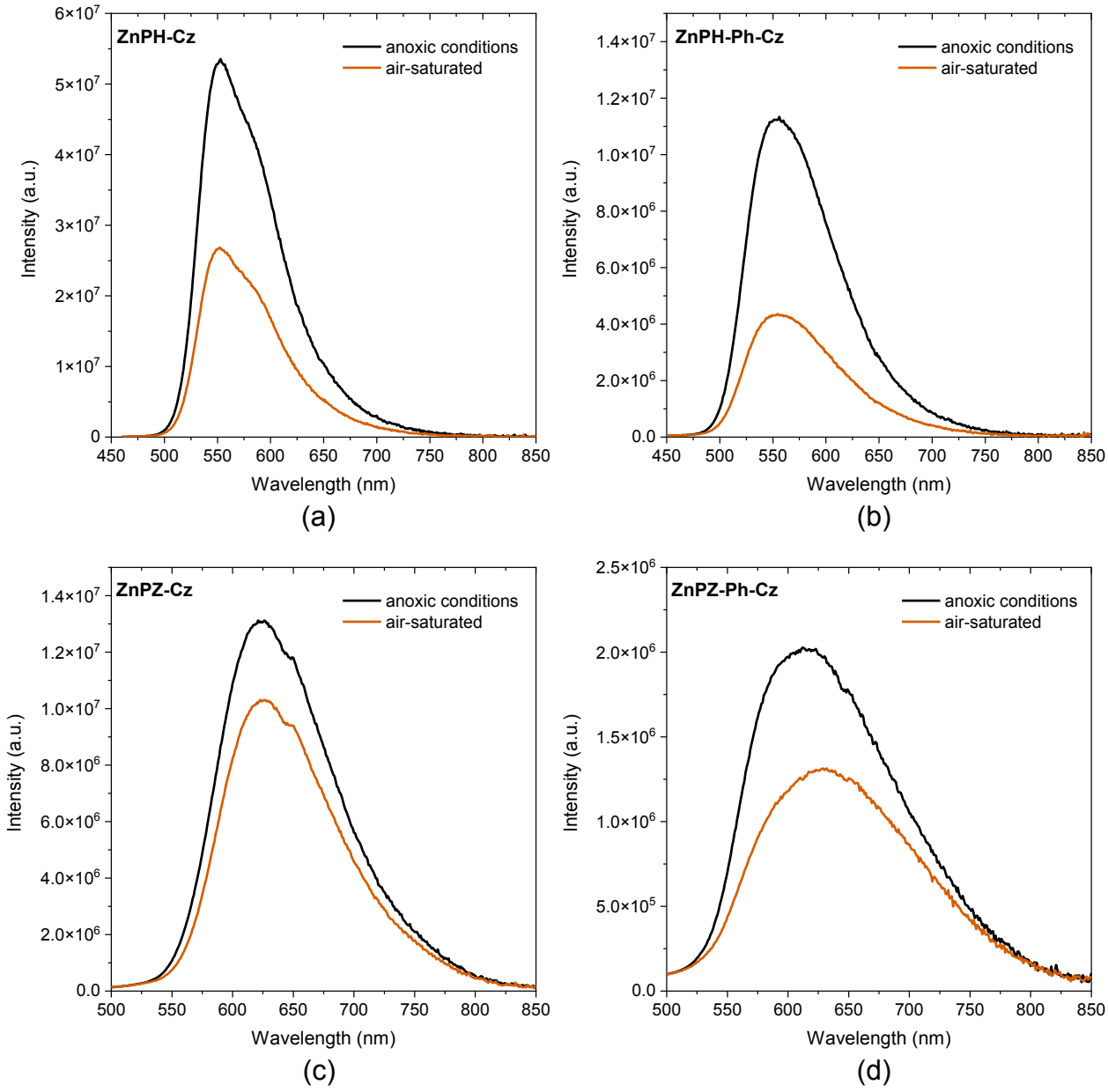

Figure S2. Emission spectra of **ZnPH-Cz** (a), **ZnPH-Ph-Cz** (b), **ZnPZ-Cz** (c) and **ZnPZ-Ph-Cz** (d) measured in polystyrene under anoxic conditions (aqueous solution with 5 w% Na_2SO_3 and traces of $CoCl_2$) and air-saturated conditions.

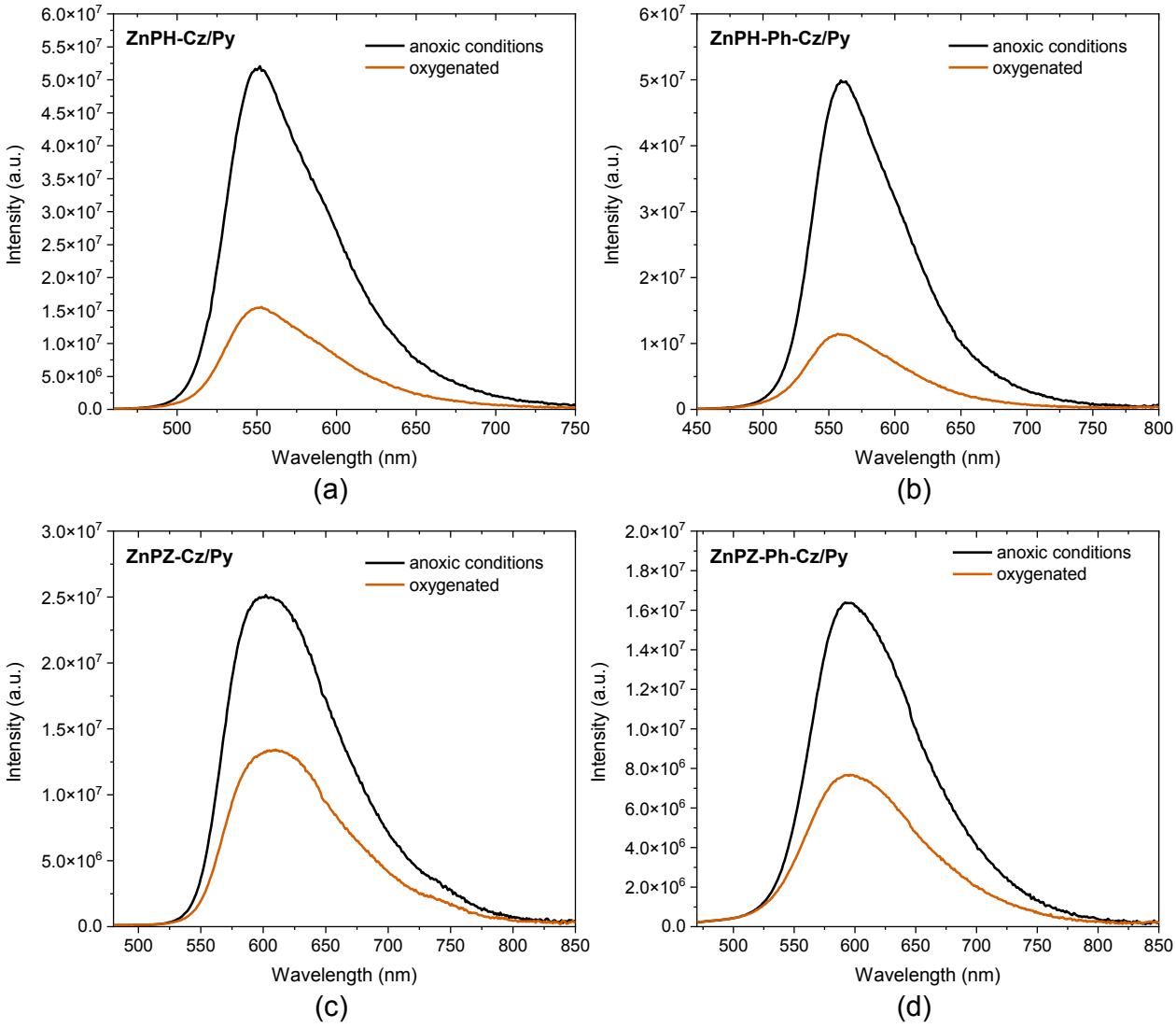

Figure S3. Emission spectra of **ZnPH-Cz** (a), **ZnPH-Ph-Cz** (b), **ZnPZ-Cz** (c) and **ZnPZ-Ph-Cz** (d) with pyridine as axial ligands measured in polystyrene under anoxic conditions (aqueous solution with 5 w% Na_2SO_3 and traces of $CoCl_2$) and air-saturated conditions.

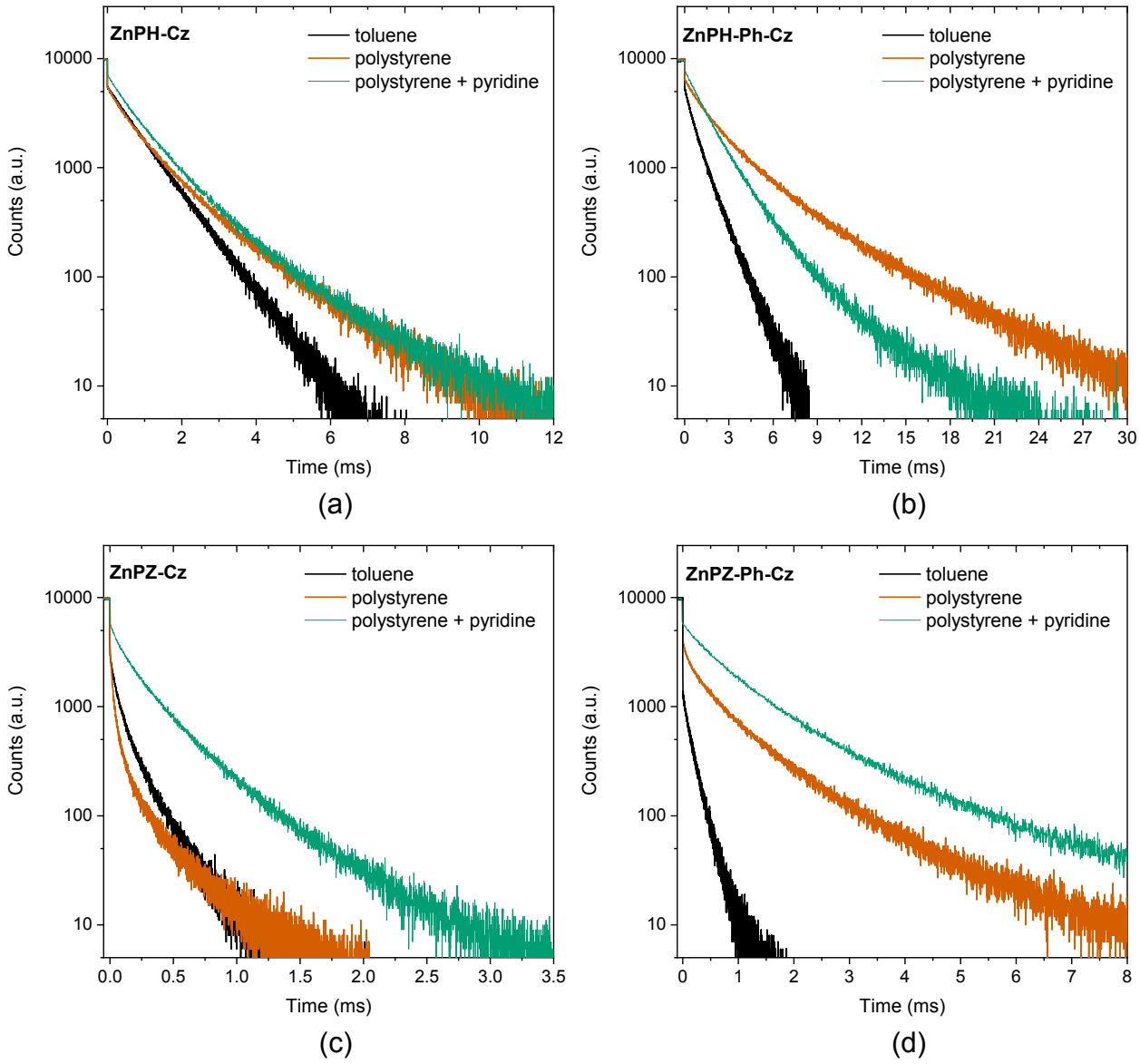

Figure S4. TADF decay of **ZnPH-Cz** (a), **ZnPH-Ph-Cz** (b), **ZnPZ-Cz** (c) and **ZnPZ-Ph-Cz** (d) in toluene and polystyrene (with and without pyridine) under anoxic conditions at 25 °C.

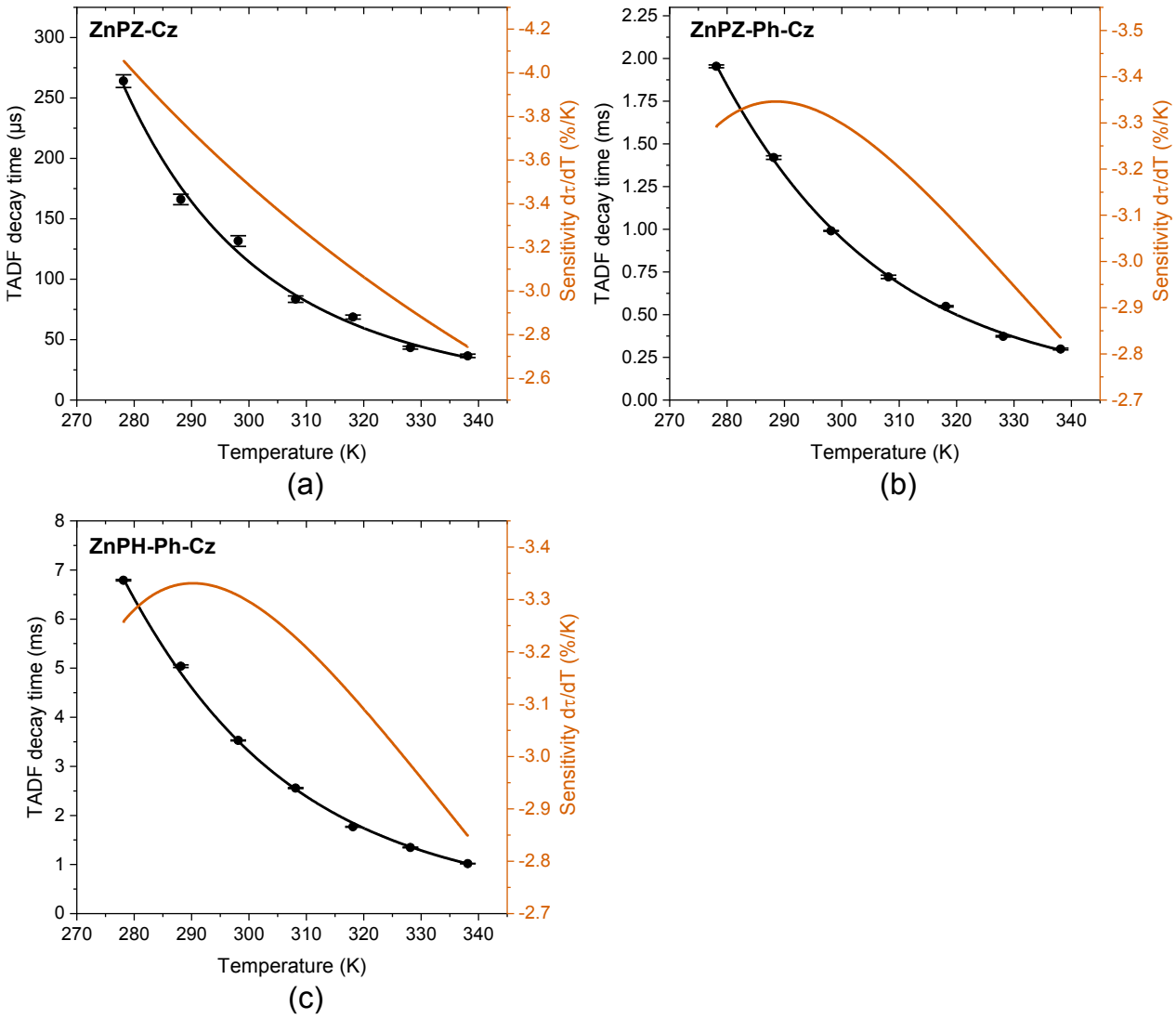

Figure S5. Temperature dependency of TADF lifetimes between 5 and 65 °C for **ZnPZ-Cz** (a), **ZnPZ-Ph-Cz** (b) and **ZnPH-Ph-Cz** (c) in PS matrix under anoxic conditions (aqueous solution with 5 w% Na_2SO_3 and traces of $CoCl_2$). In each temperature calibration cycle, three decay time measurements were made at each temperature. The calibration cycle was repeated three times.

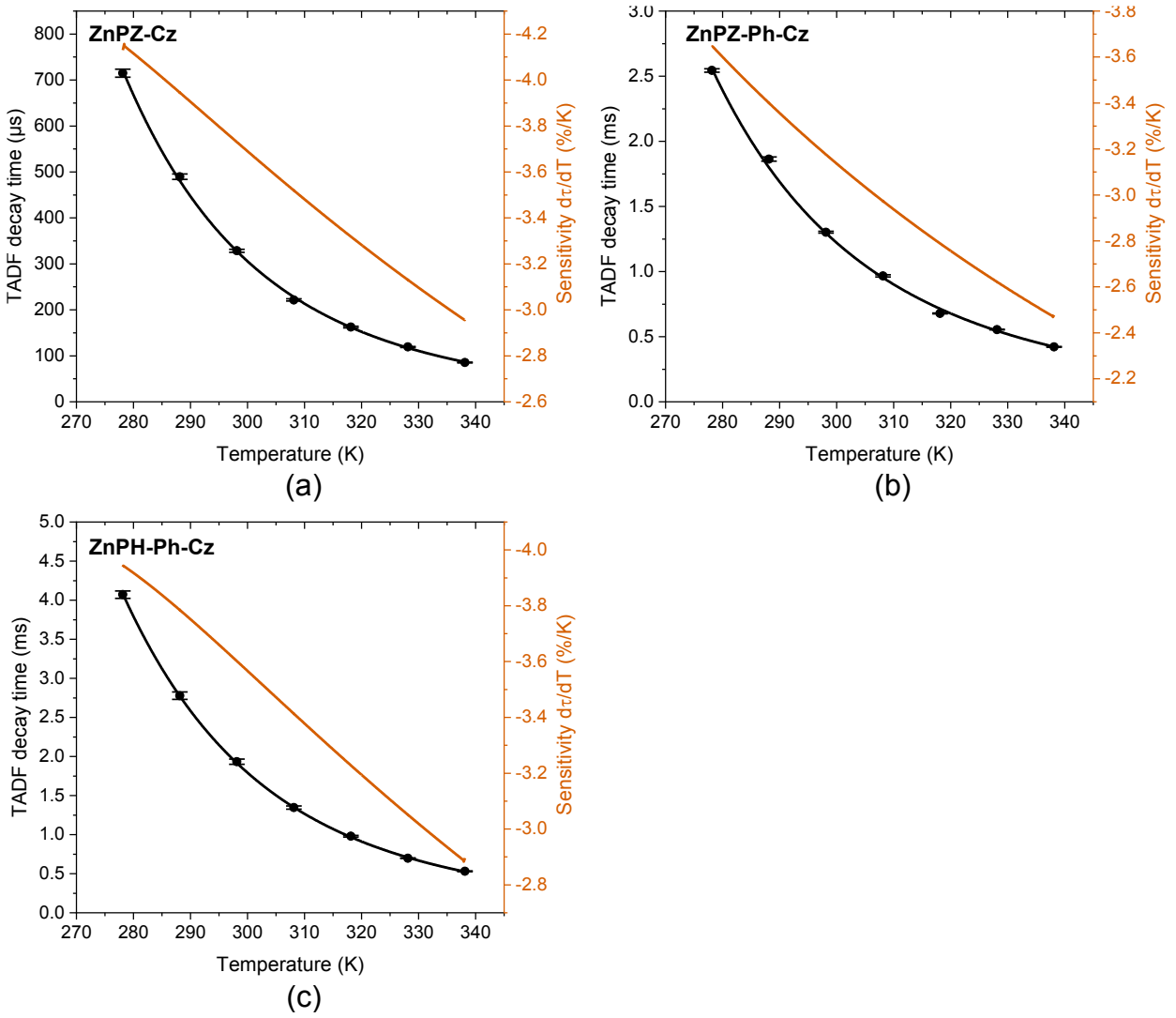

Figure S6. Temperature dependency of TADF lifetimes between 5 and 65 °C for **ZnPZ-Cz** (a), **ZnPZ-Ph-Cz** (b) and **ZnPH-Ph-Cz** (c) with pyridine in PS matrix under anoxic conditions (aqueous solution with 5 w% Na_2SO_3 and traces of $CoCl_2$). In each temperature calibration cycle, three decay time measurements were made at each temperature. The calibration cycle was repeated three times.

2 NMR Spectra

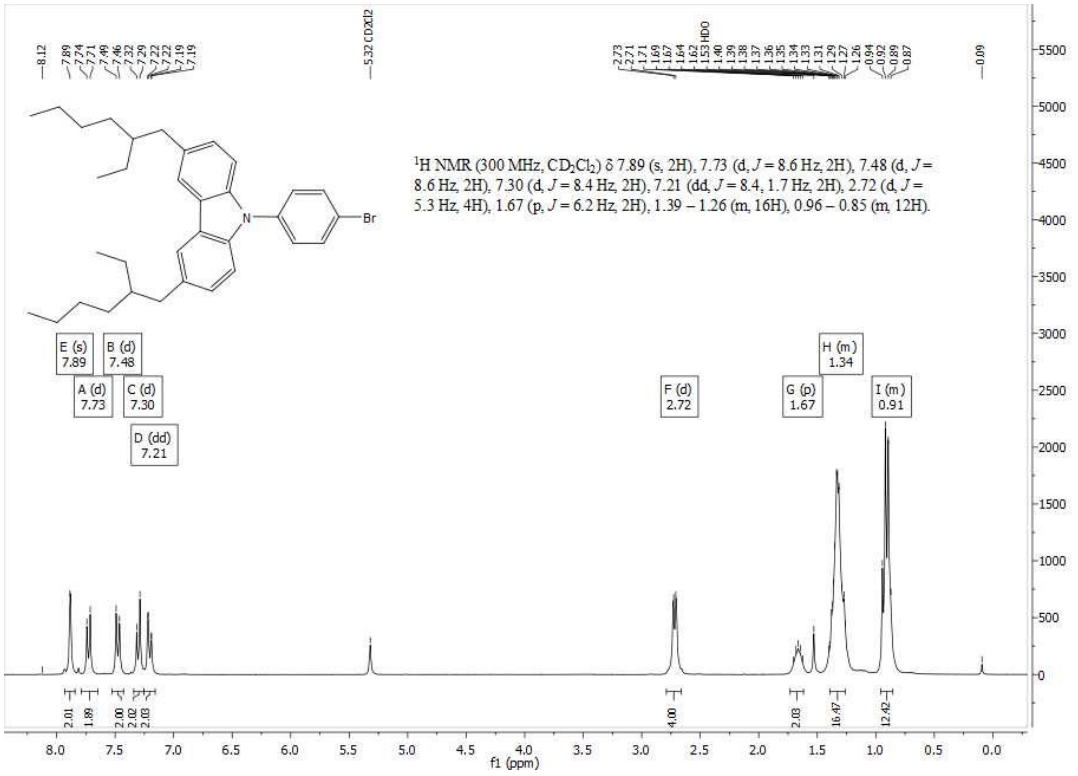

Figure S7. ^{1}H NMR (300 MHz, CD_2Cl_2) of **2**.

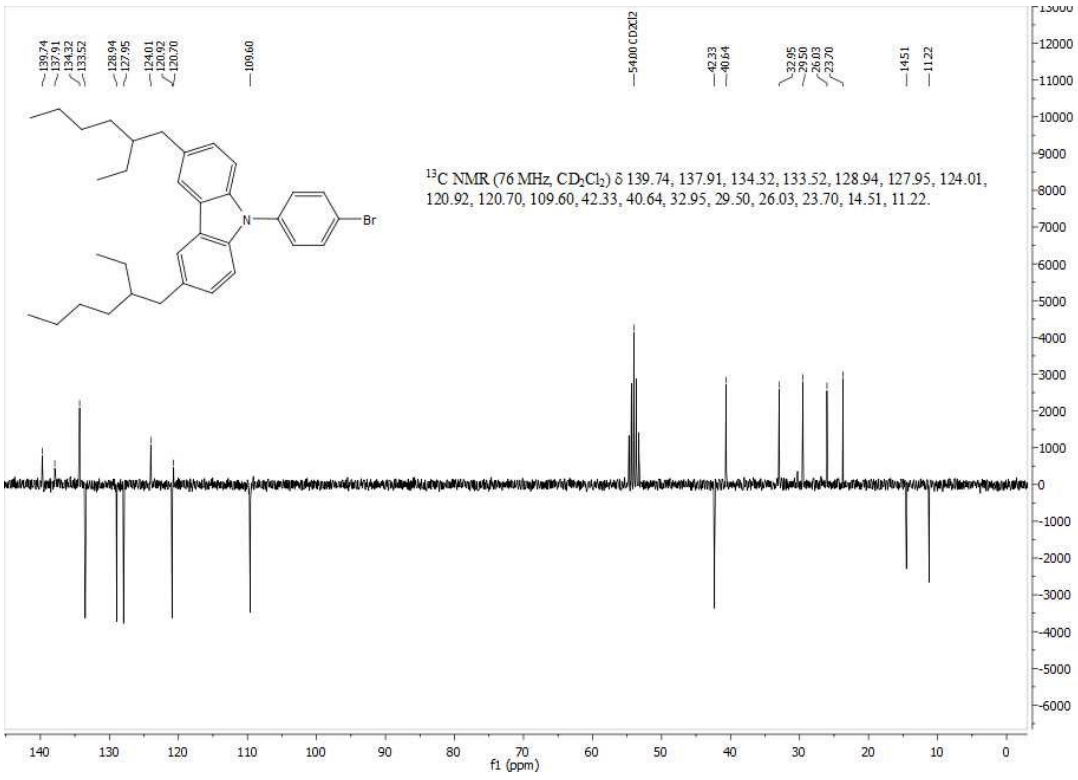

Figure S8. ^{13}C-APT NMR (76 MHz, CD_2Cl_2) of **2**.

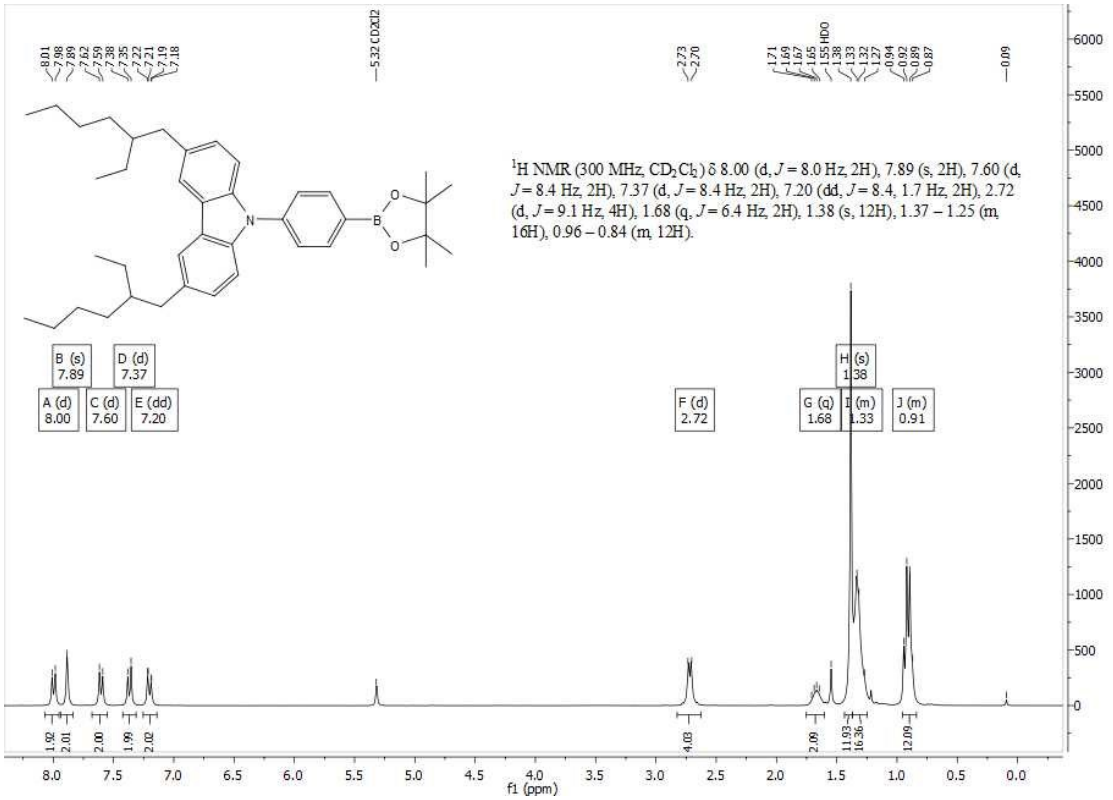

Figure S9. ^{1}H NMR (300 MHz, CD_2Cl_2) of **3**.

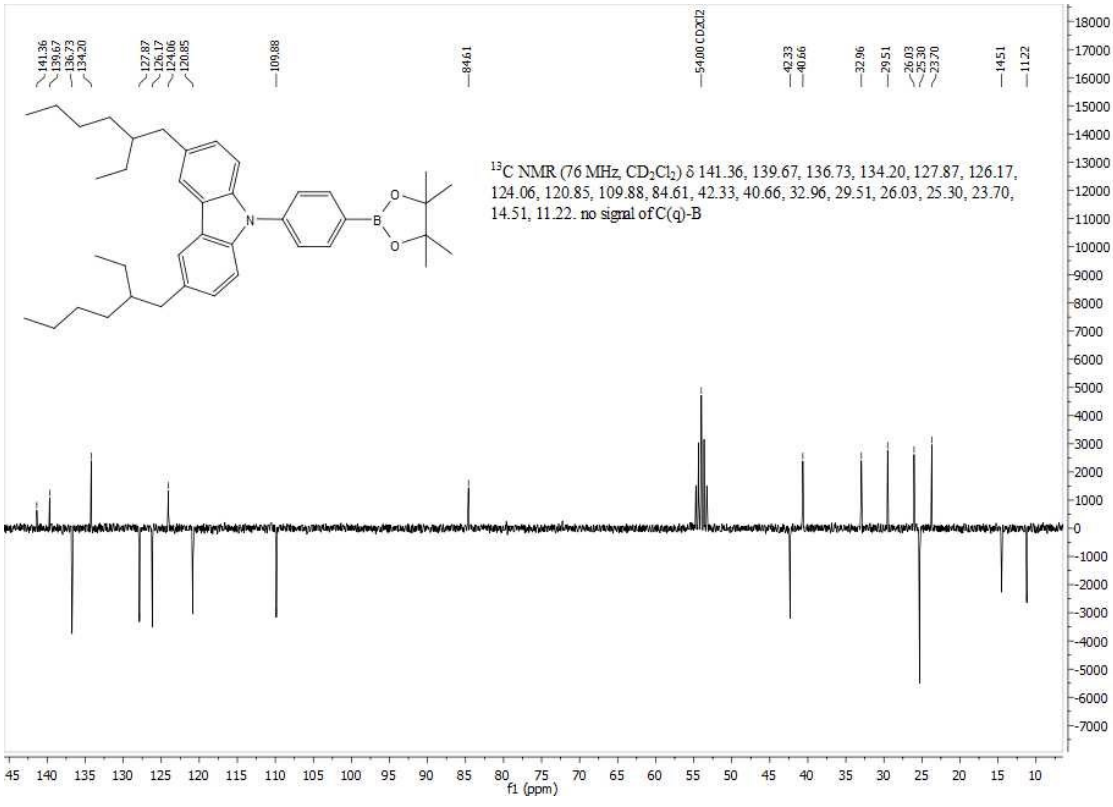

Figure S10. ^{13}C-APT NMR (76 MHz, CD_2Cl_2) of **3**.

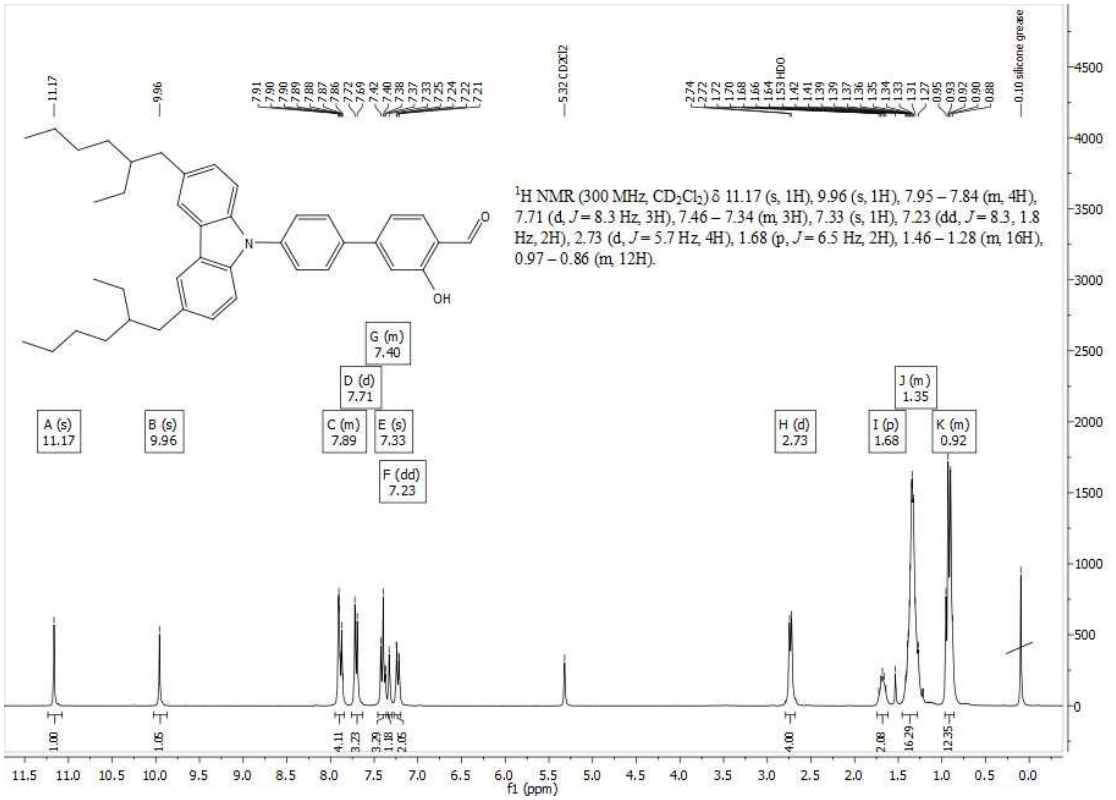

Figure S11. ^{1}H NMR (300 MHz, CD_2Cl_2) of **4**.

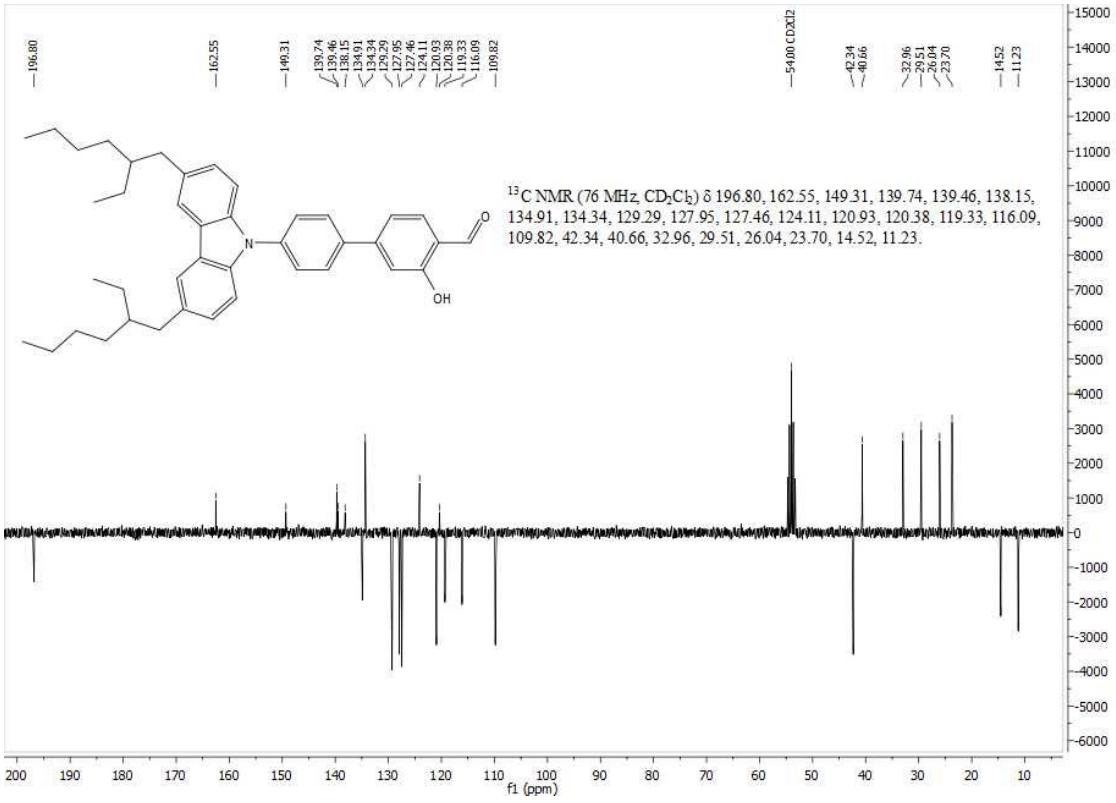

Figure S12. ^{13}C-APT NMR (76 MHz, CD_2Cl_2) of **4**.

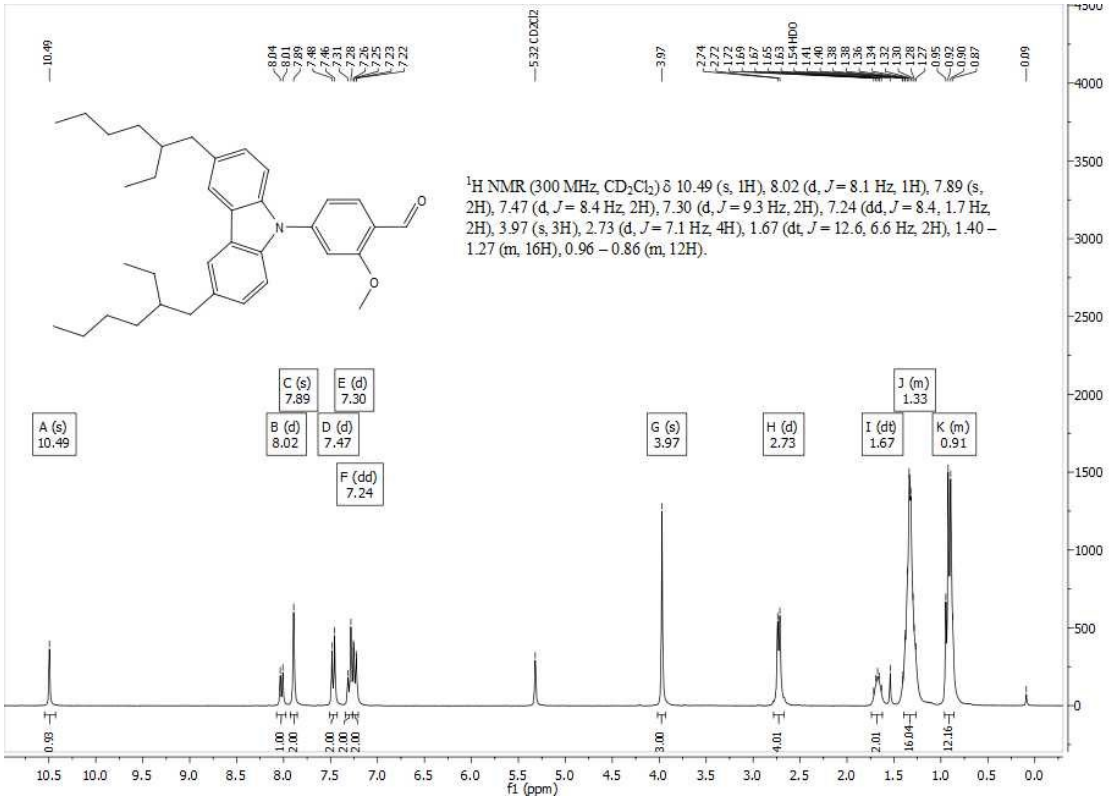

Figure S13. ^{1}H NMR (300 MHz, CD_2Cl_2) of **5**.

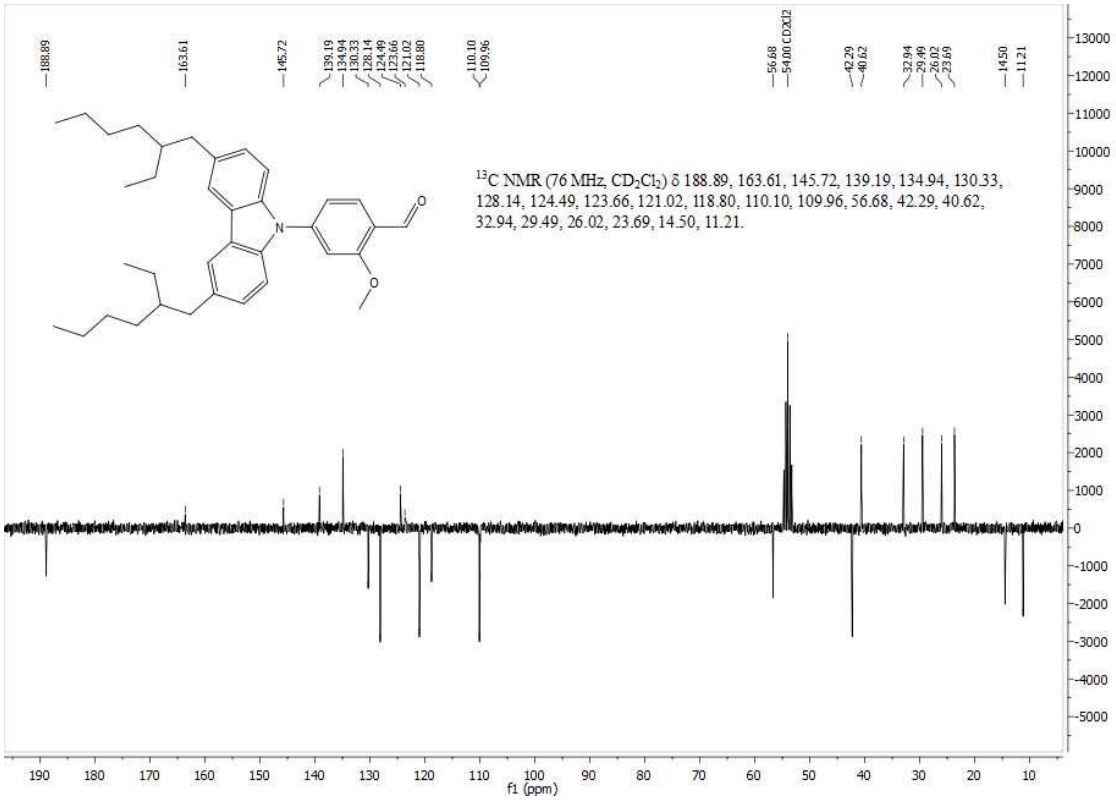

Figure S14. ^{13}C-APT NMR (76 MHz, CD_2Cl_2) of **5**.

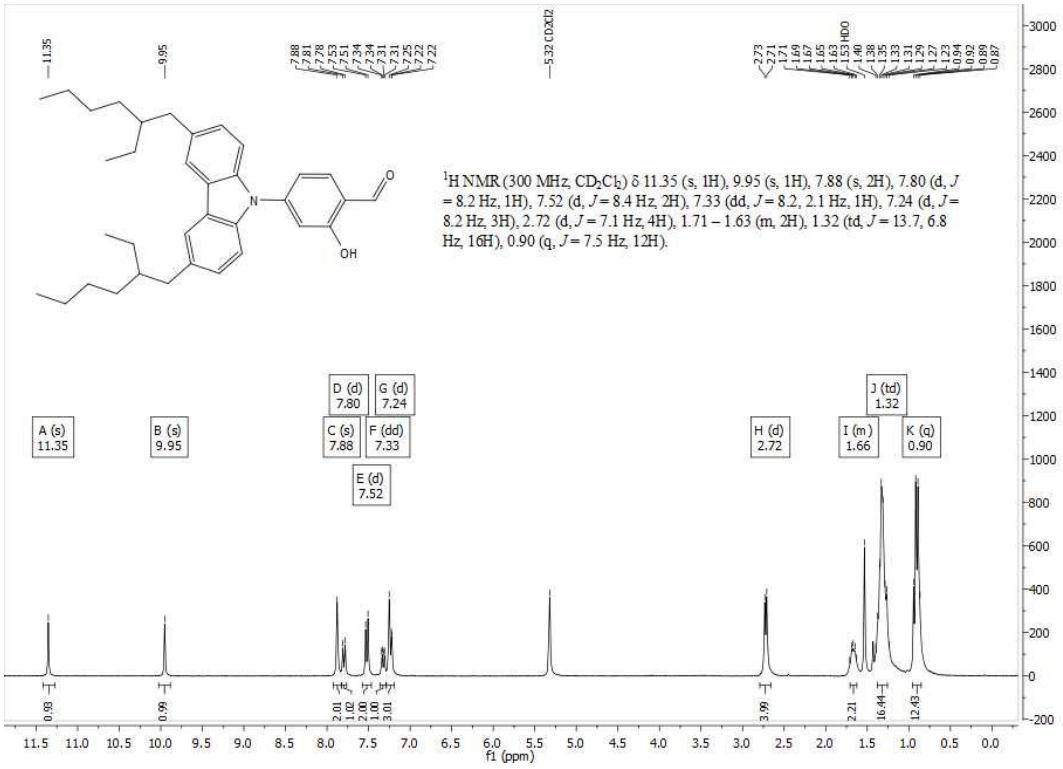

Figure S15. ^{1}H NMR (300 MHz, CD_2Cl_2) of **6**.

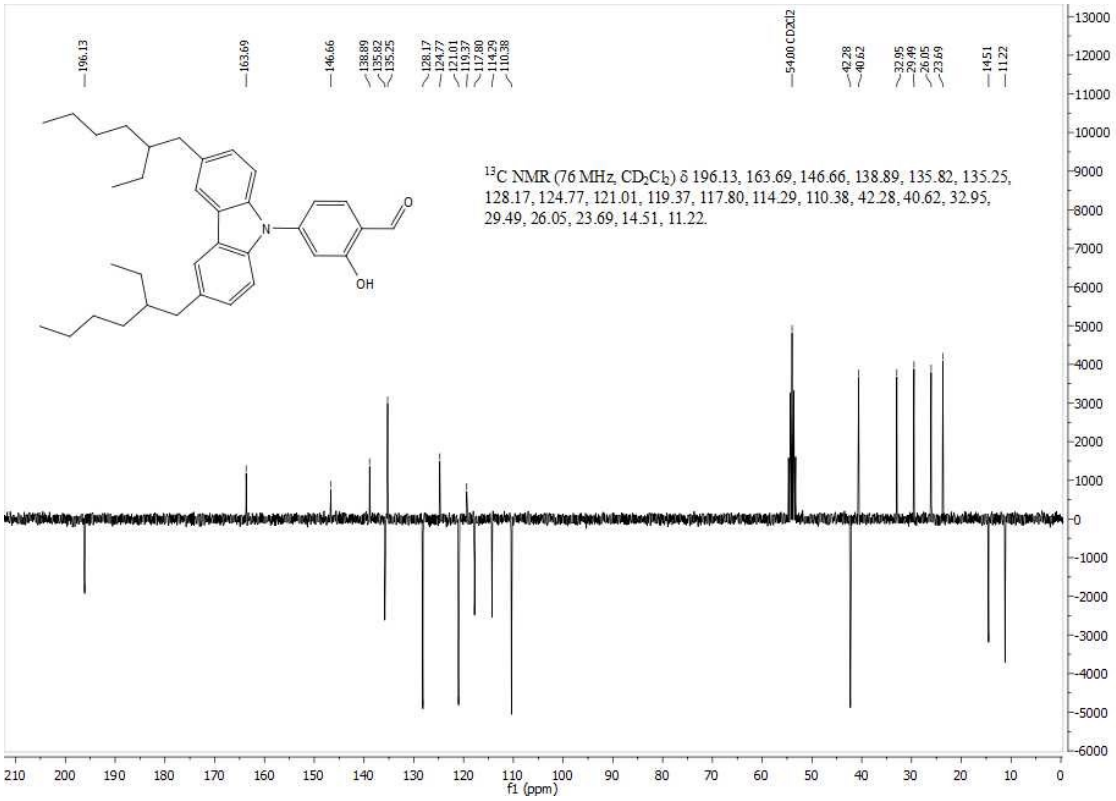

Figure S16. ^{13}C-APT NMR (76 MHz, CD_2Cl_2) of **6**.

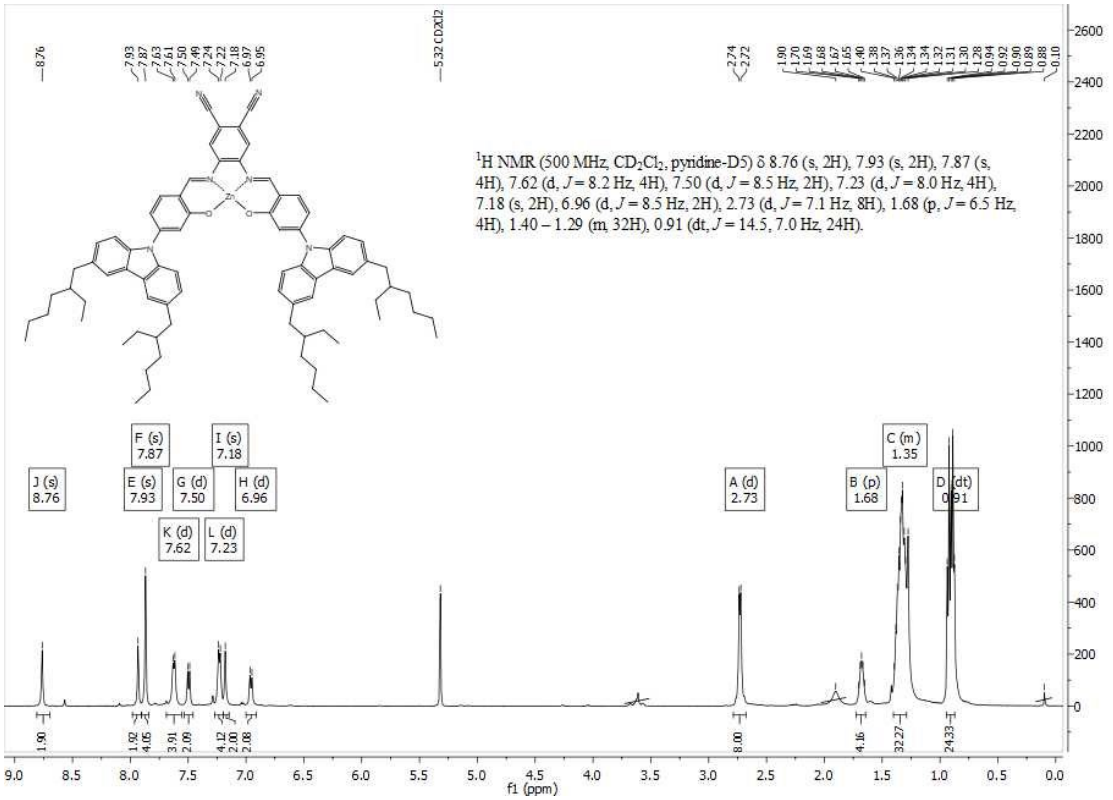

Figure S17. ^{1}H NMR (500 MHz, CD_2Cl_2, pyridine-D5) of **ZnPH-Cz**.

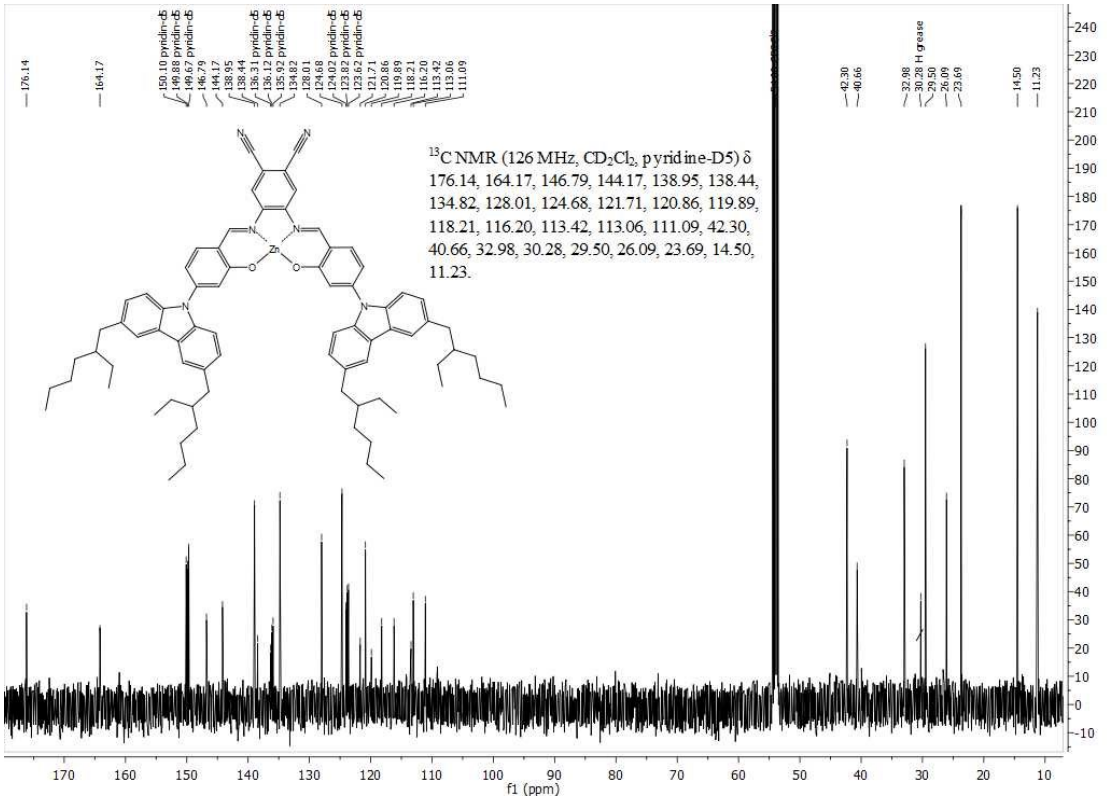

Figure S18. ^{13}C-NMR (126 MHz, CD_2Cl_2, pyridine-D5) of **ZnPH-Cz**.

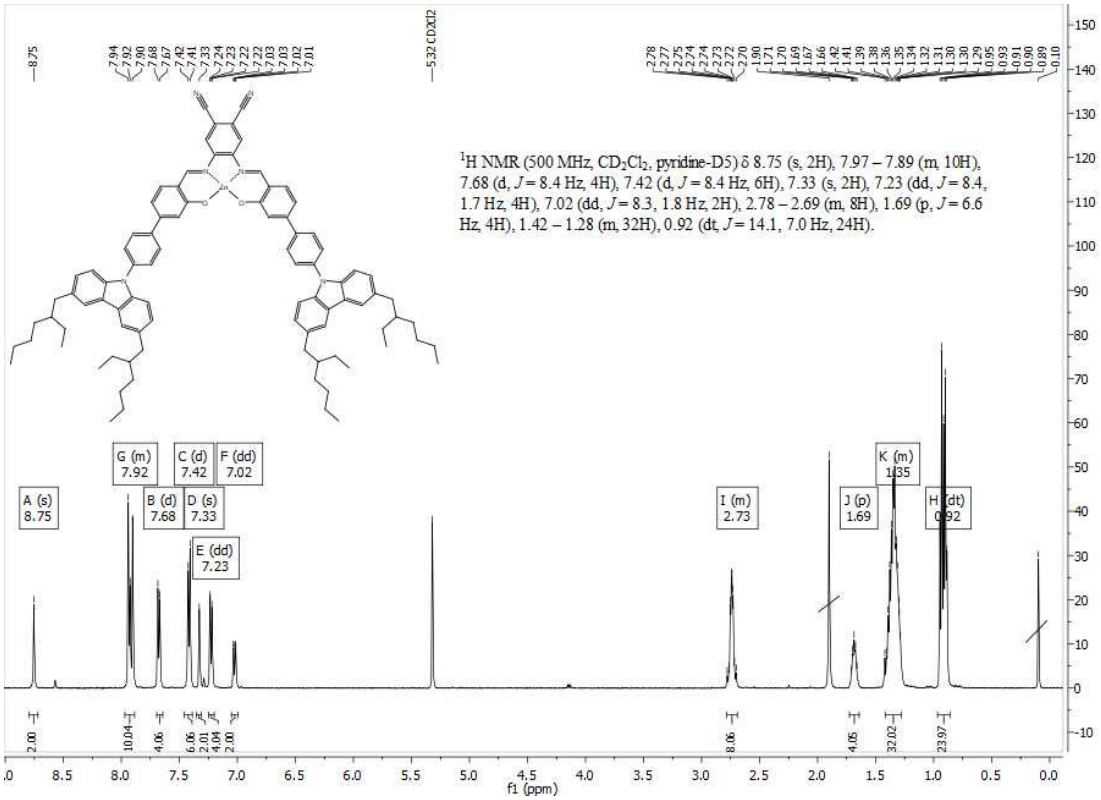

Figure S19. ^{1}H NMR (500 MHz, CD_2Cl_2, pyridine-D5) of **ZnPH-Ph-Cz**.

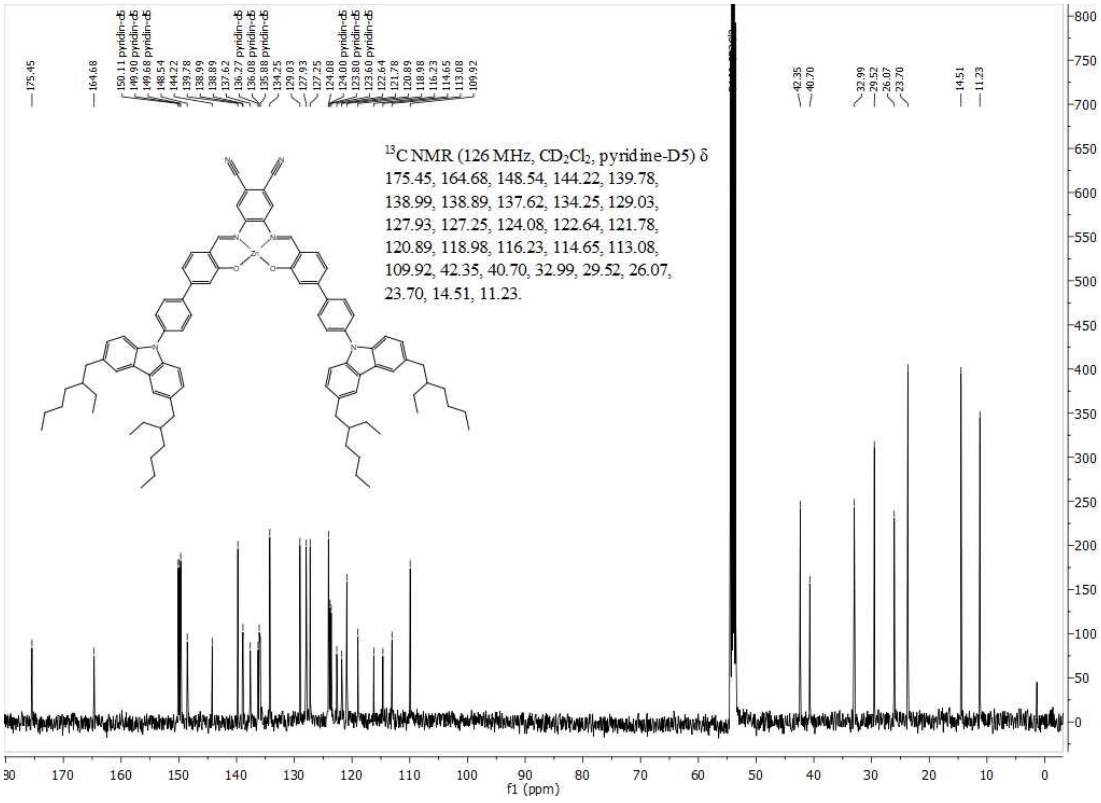

Figure S20. ^{13}C- NMR (126 MHz, CD_2Cl_2, pyridine-D5) of **ZnPH-Ph-Cz**.

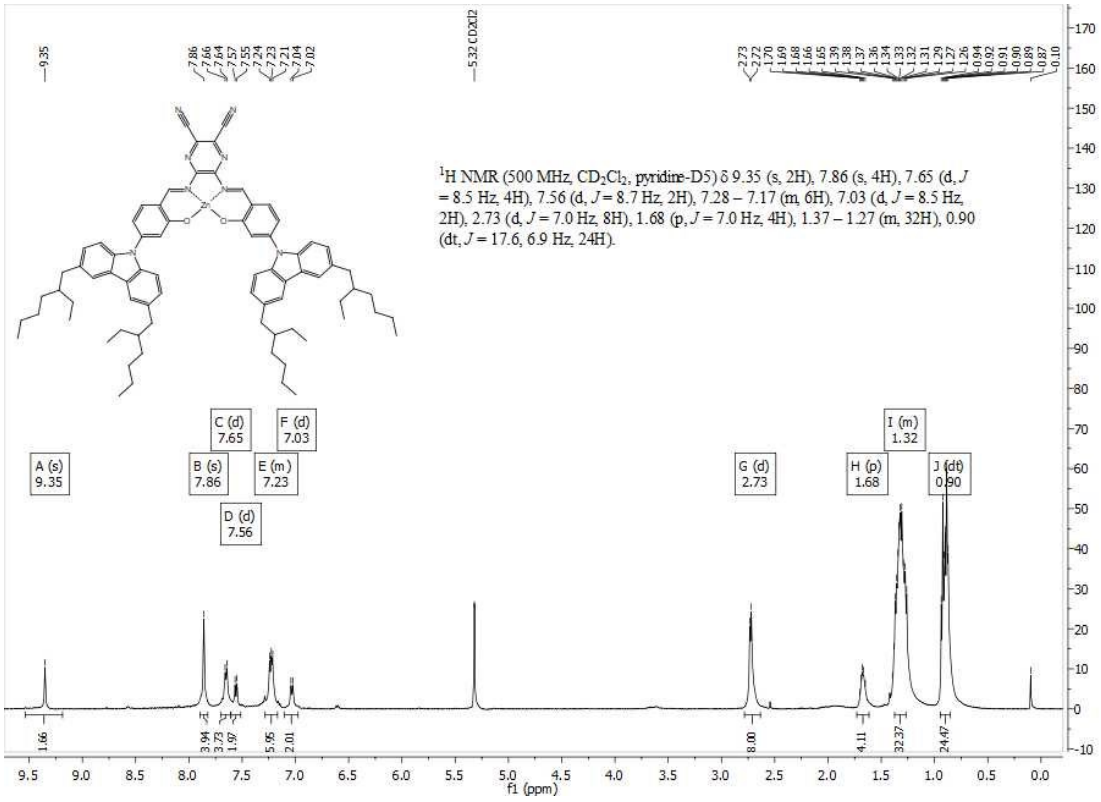

Figure S21. ^{1}H NMR (500 MHz, CD_2Cl_2, pyridine-D5) of **ZnPZ-Cz**.

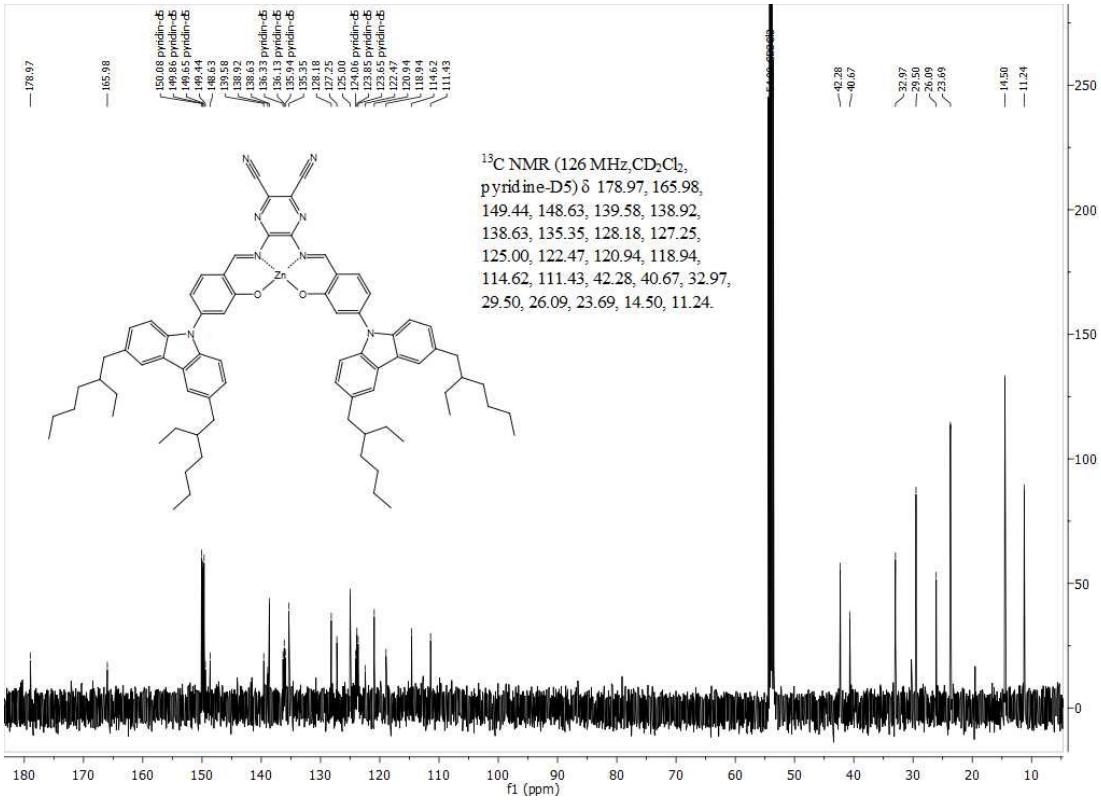

Figure S22. ^{13}C- NMR (126 MHz, CD_2Cl_2, pyridine-D5) of **ZnPZ-Cz**.

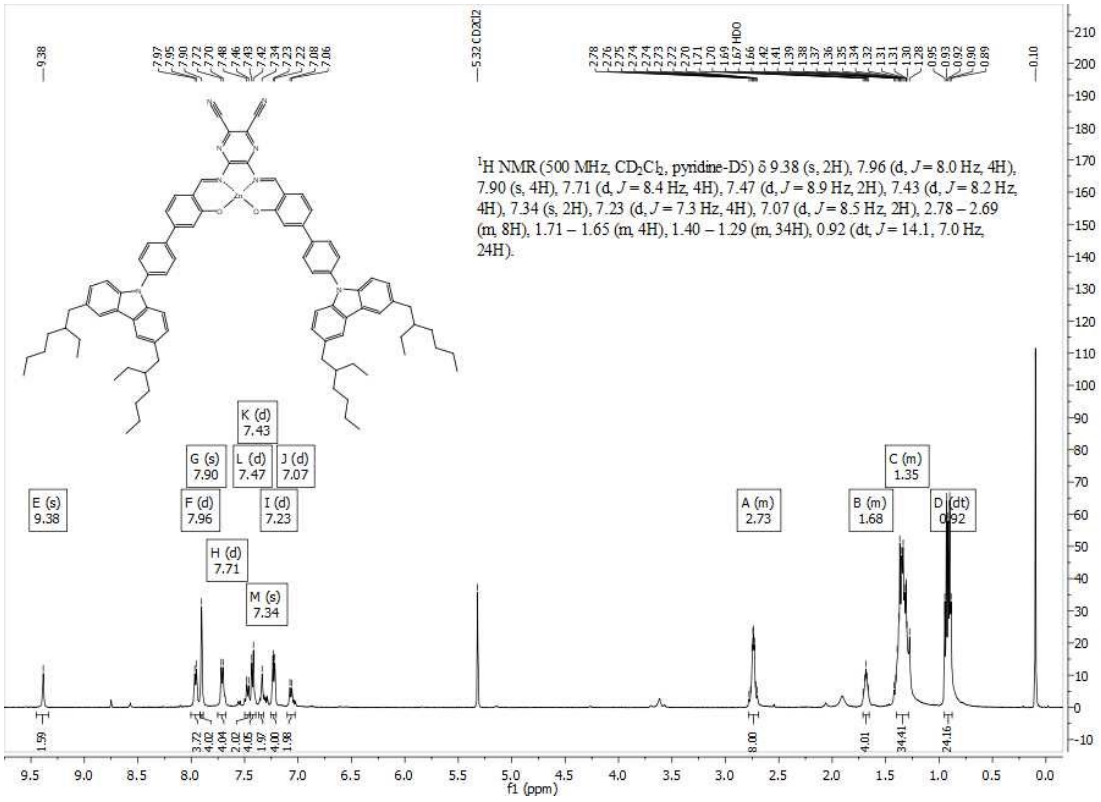

Figure S23. ^{1}H NMR (500 MHz, CD_2Cl_2, pyridine-D5) of **ZnPZ-Ph-Cz**.

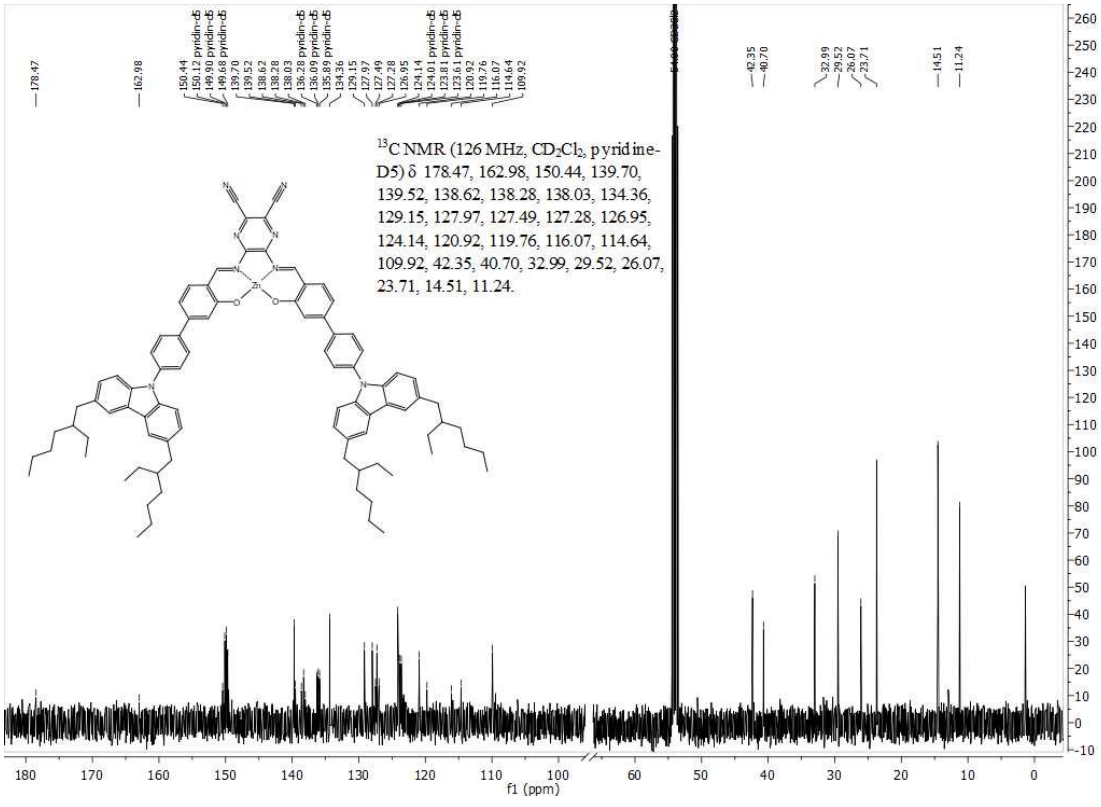

Figure S24. ^{13}C- NMR (126 MHz, CD_2Cl_2, pyridine-D5) of **ZnPZ-Ph-Cz**.

3 MS Spectra

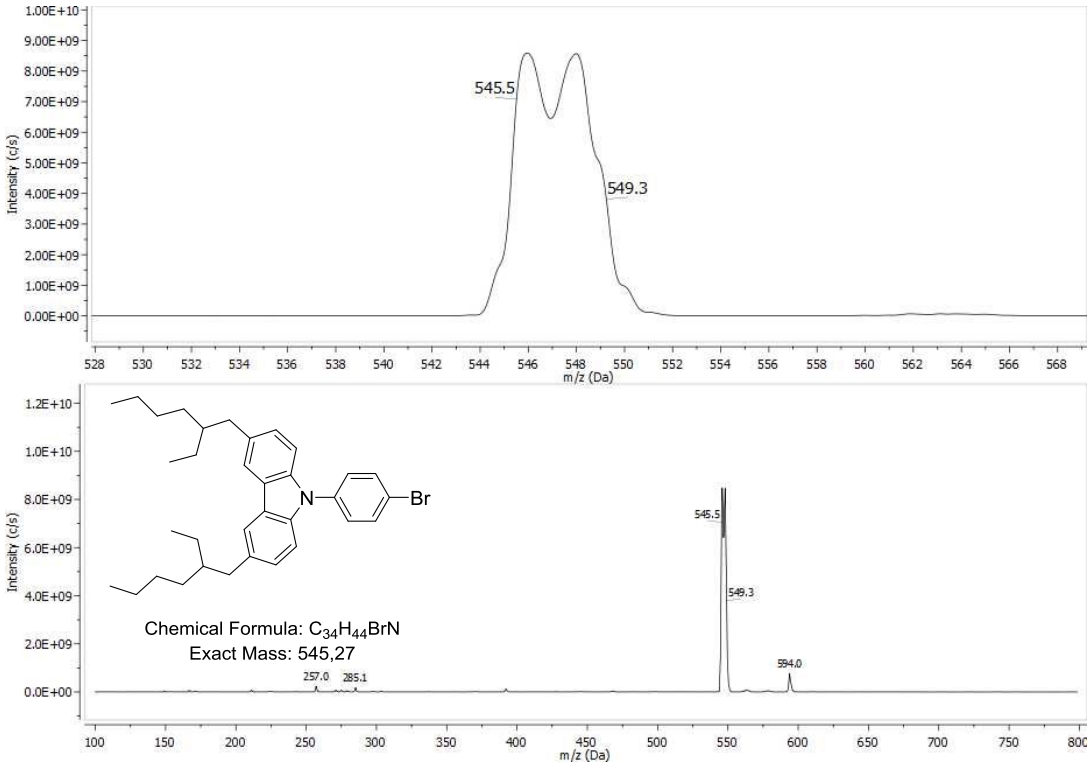

Figure S25. Mass spectrum (APCI-MS) of **2**.

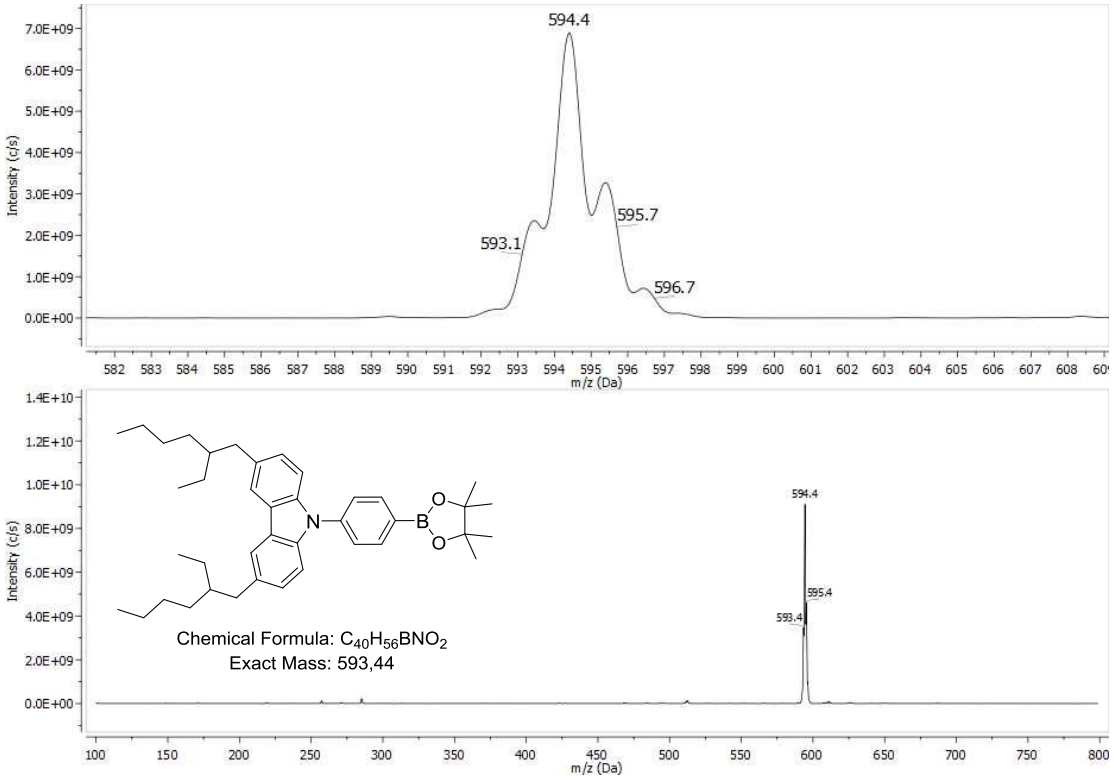

Figure S26. Mass spectrum (APCI-MS) of **3**.

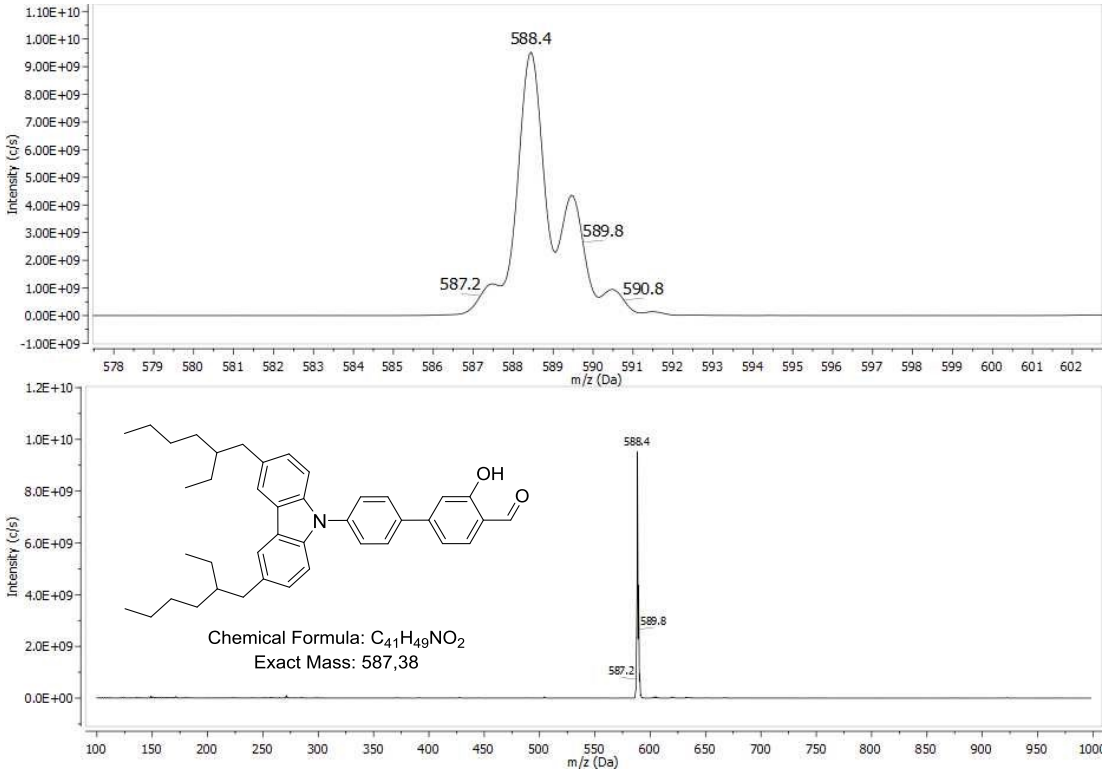

Figure S27. Mass spectrum (APCI-MS) of **4**.

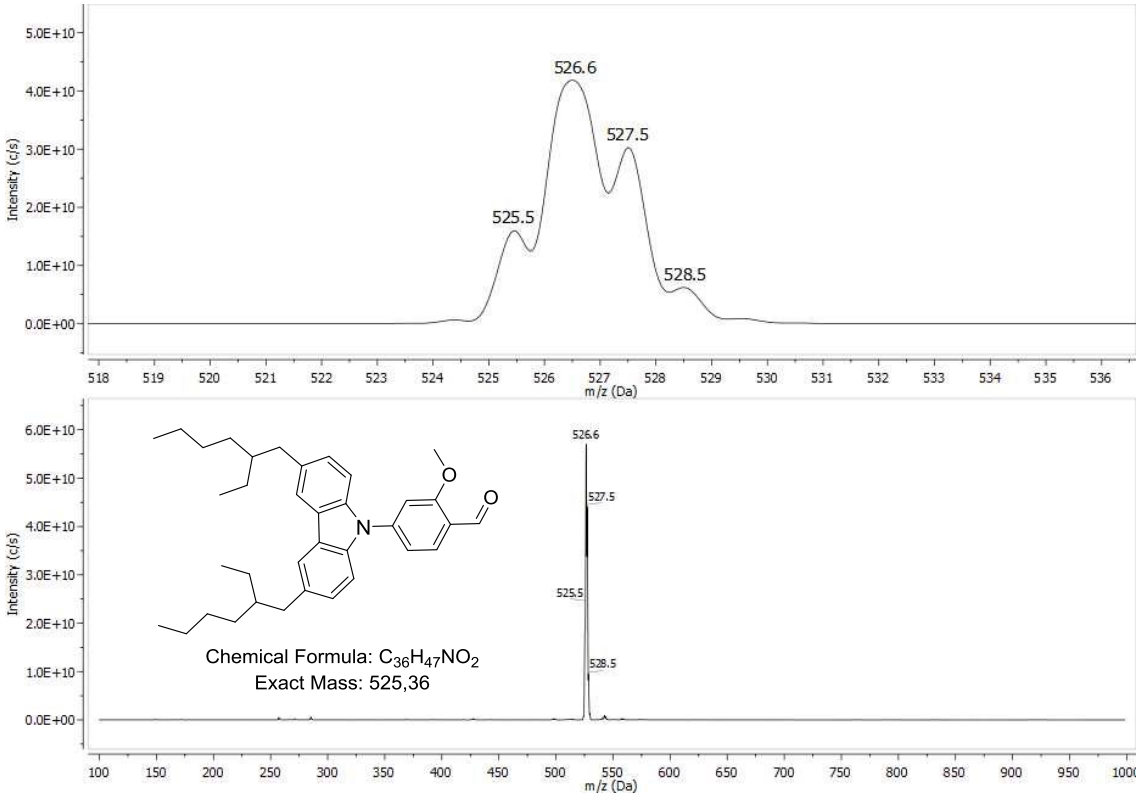

Figure S28. Mass spectrum (APCI-MS) of **5**.

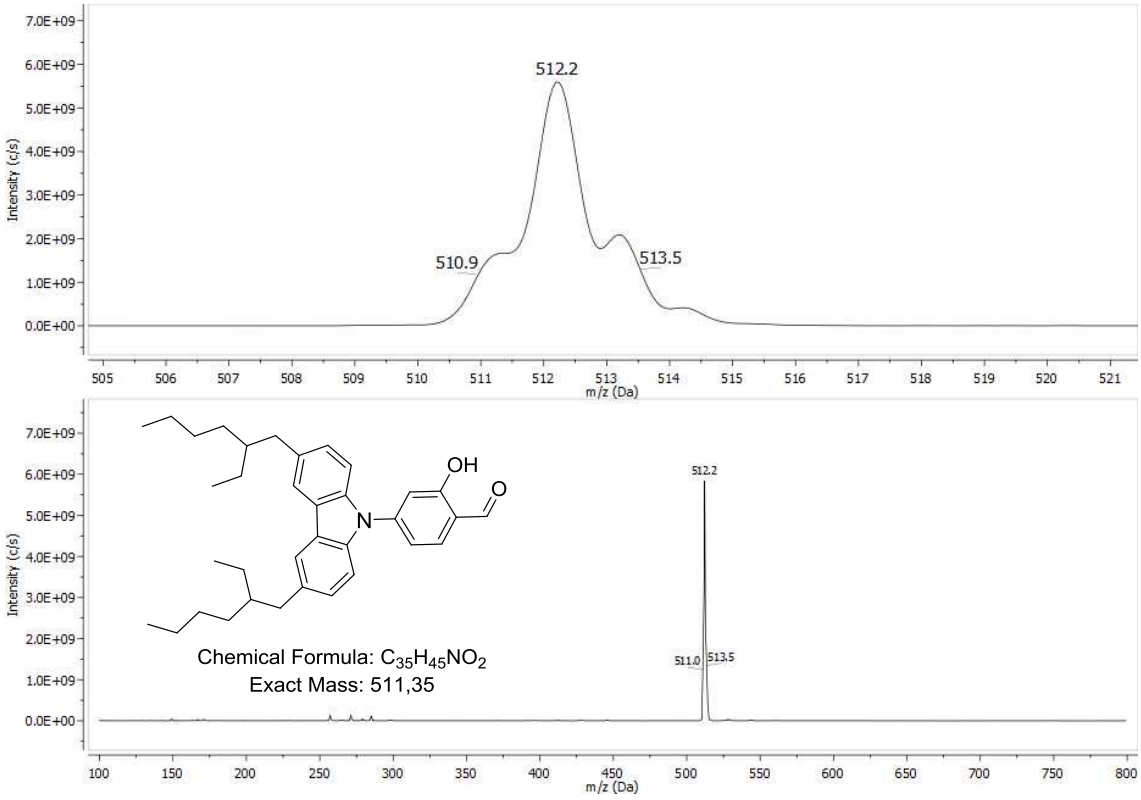

Figure S29. Mass spectrum (APCI-MS) of **6**.

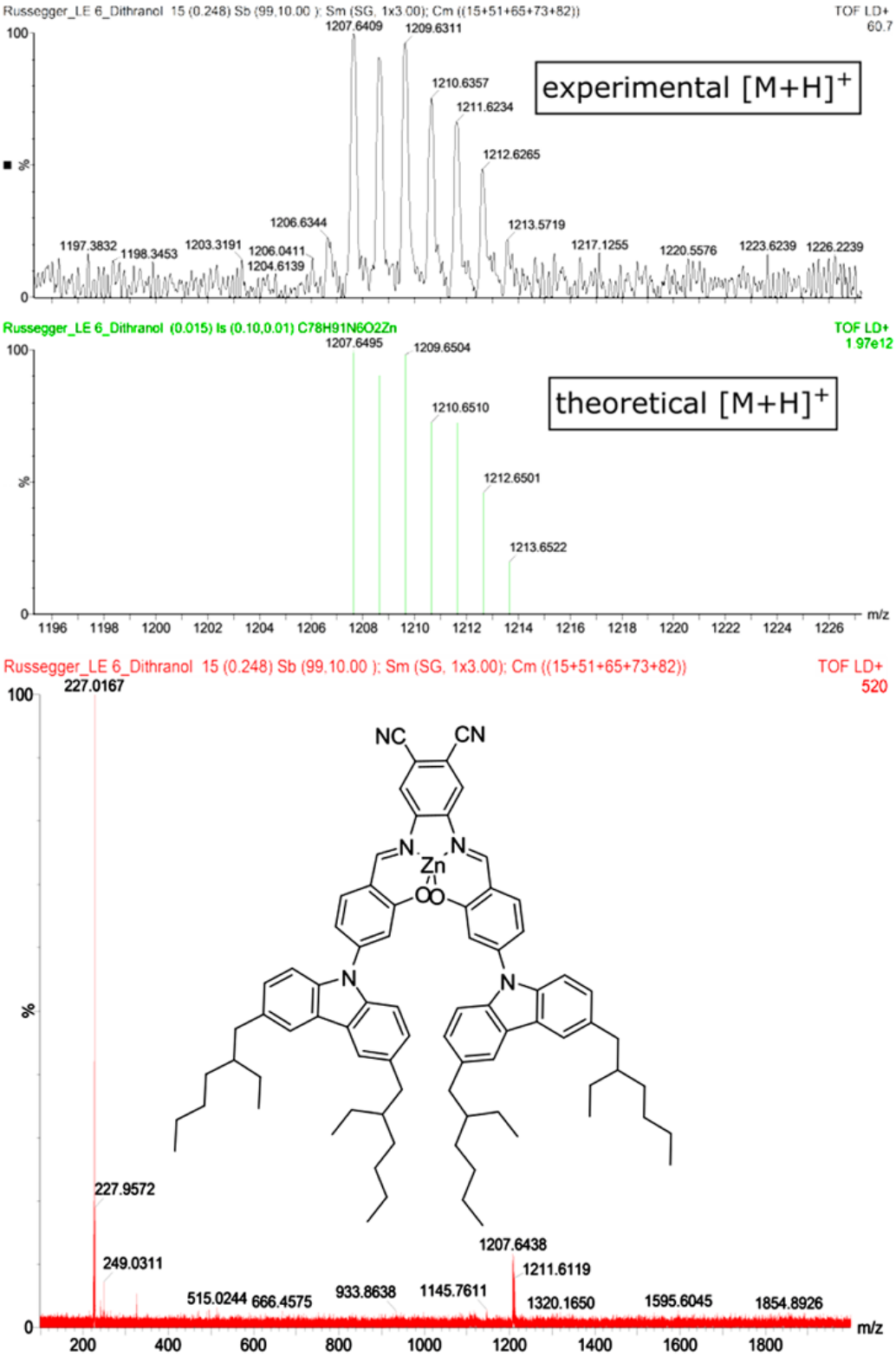

Figure S30. Mass spectra (MALDI-TOF) of **ZnPH-Cz** in dithranol matrix.

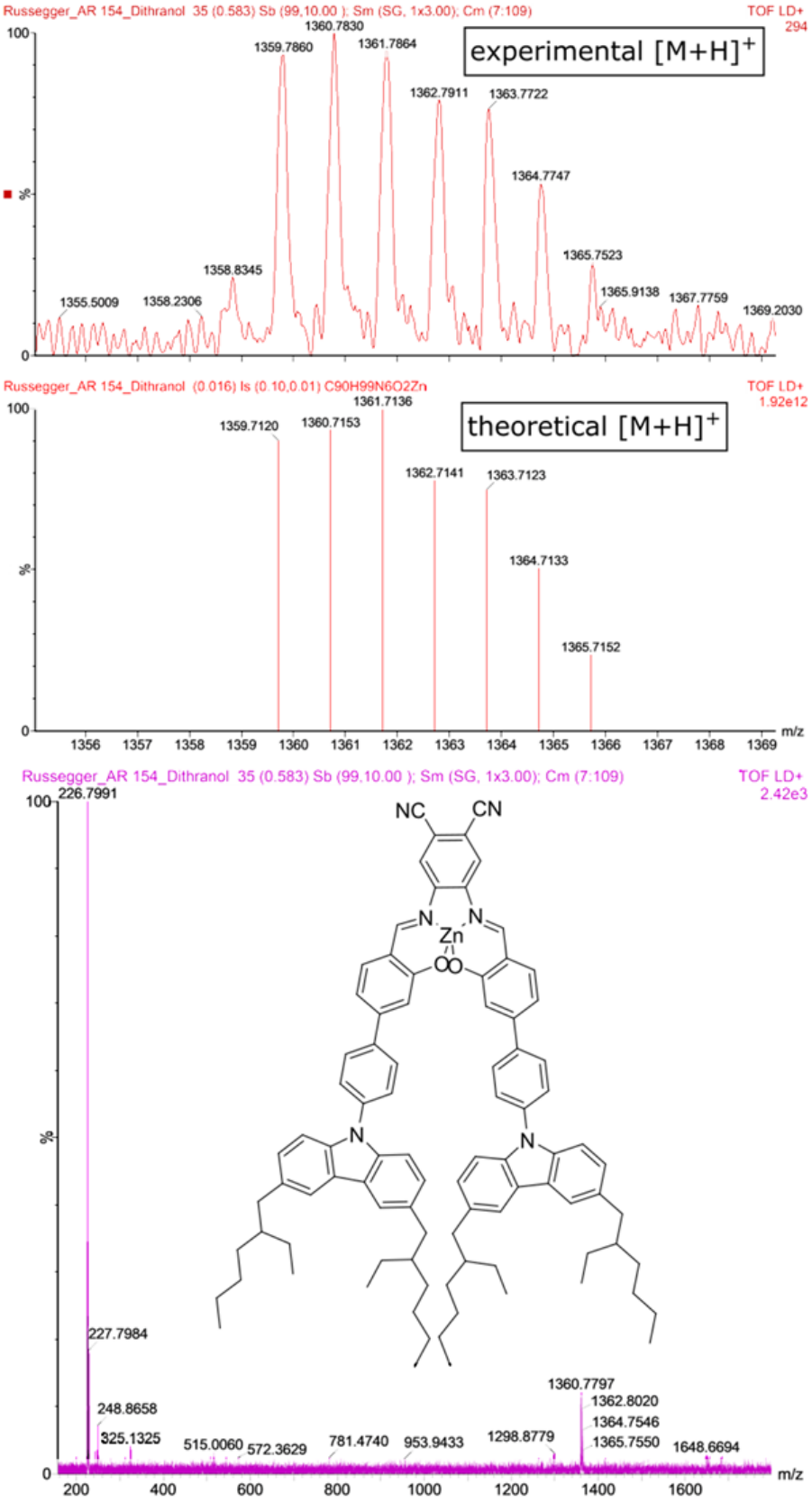

Figure S31. Mass spectra (MALDI-TOF) of **ZnPH-Ph-Cz** in dithranol matrix.

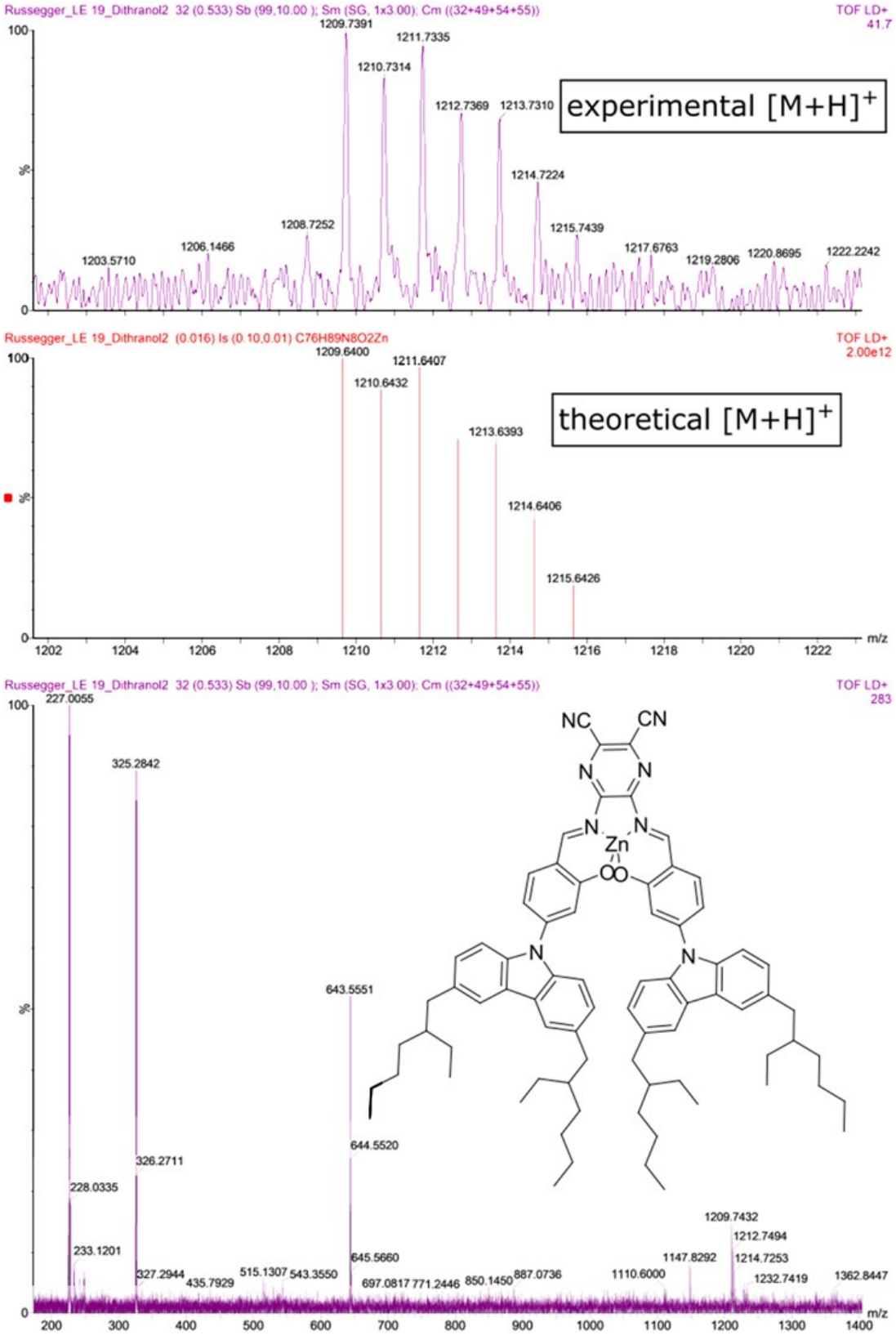

Figure S32. Mass spectra (MALDI-TOF) of **ZnPZ-Cz** in dithranol matrix.

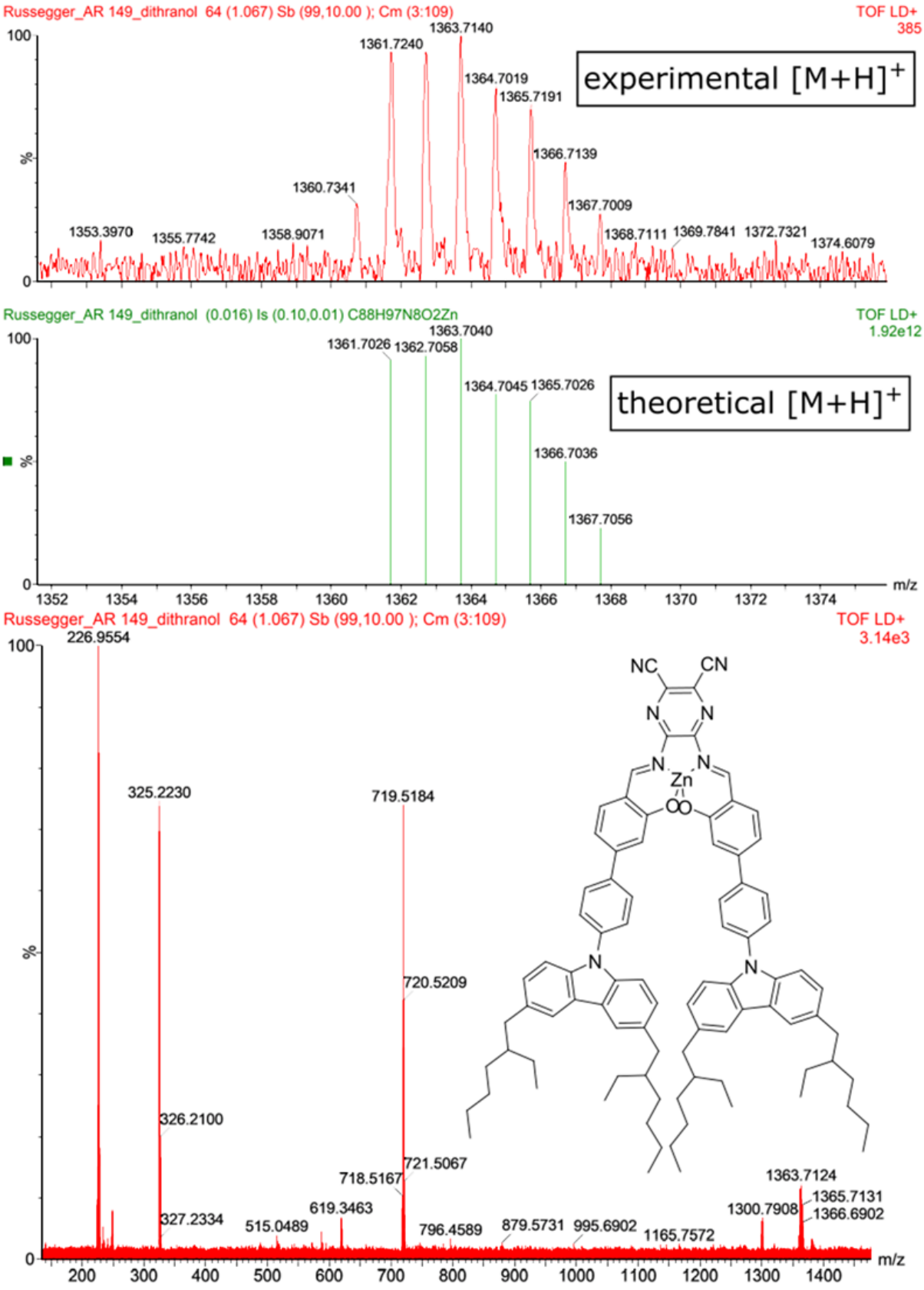

Figure S33. Mass spectra (MALDI-TOF) of **ZnPZ-Ph-Cz** in dithranol matrix.