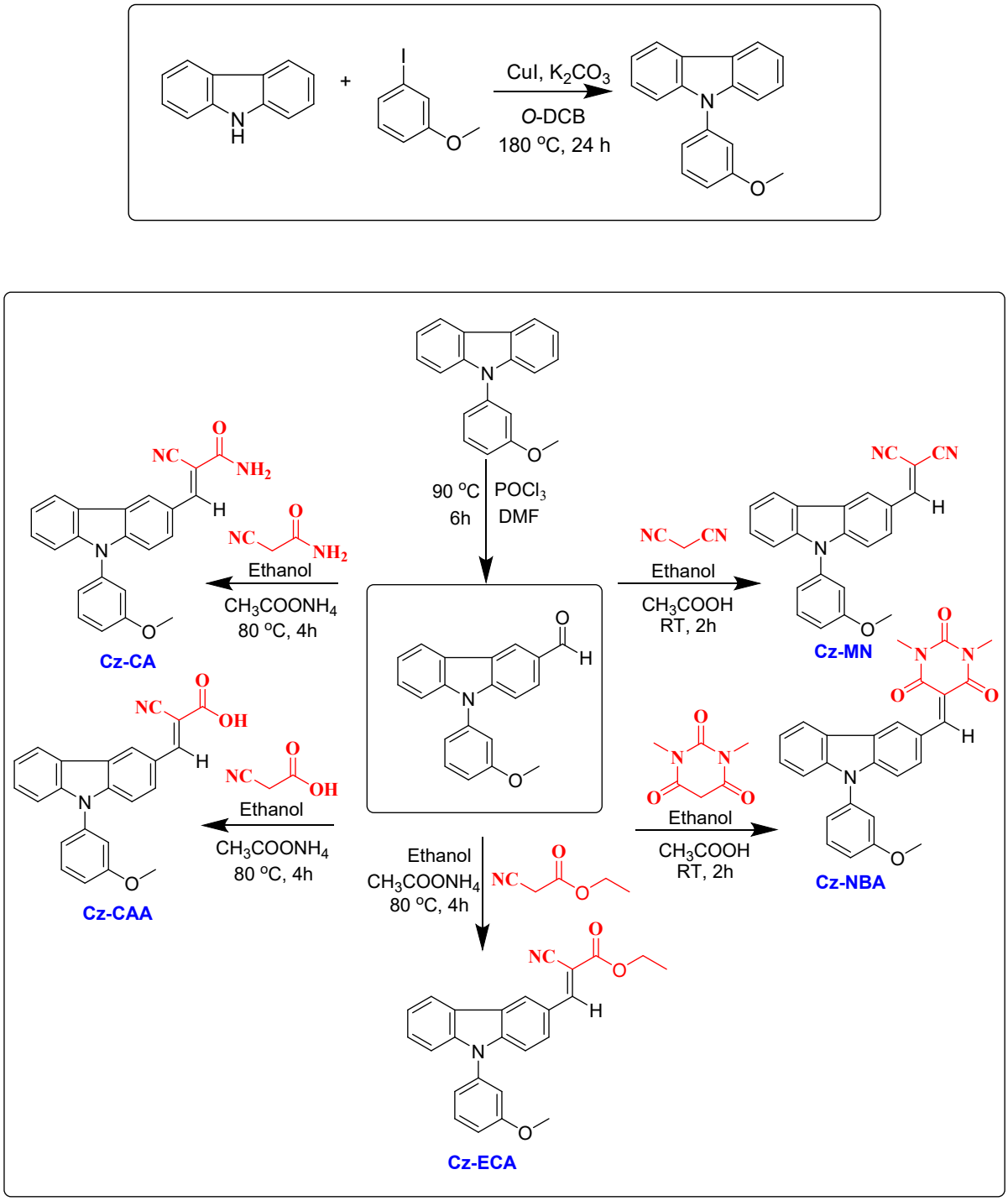
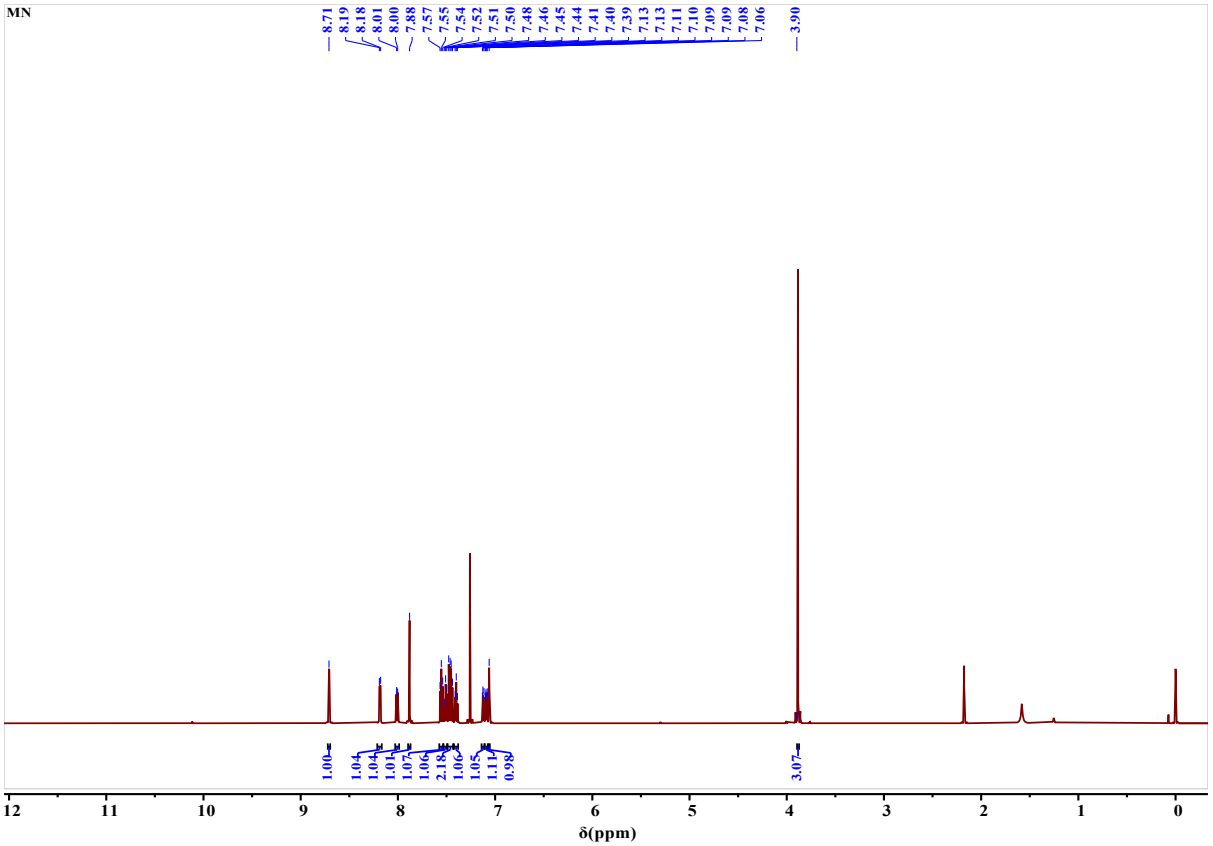
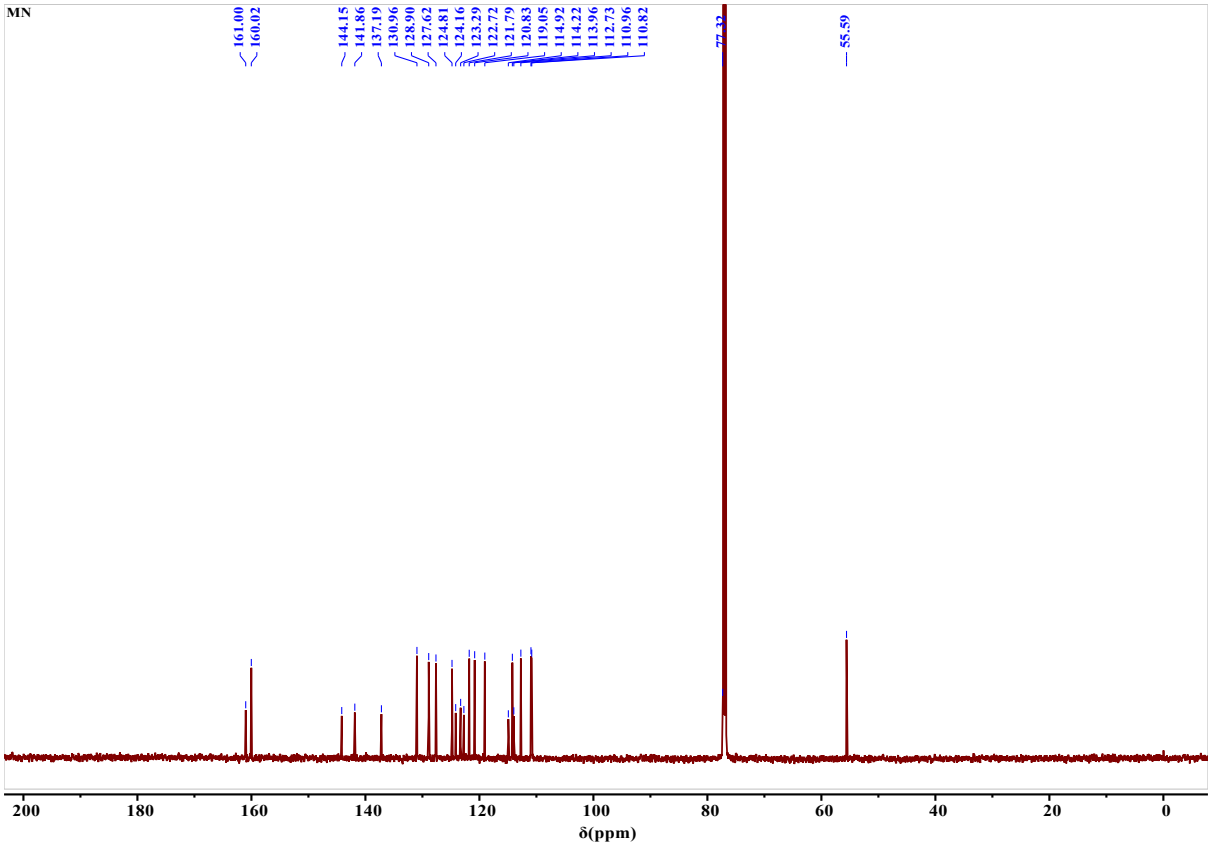
Electronic Supplementary Information (ESI)

Self-reversible mechanofluorochromic AIEgens with tunable solid-state fluorescence: effectof acceptor and intermolecular interactions

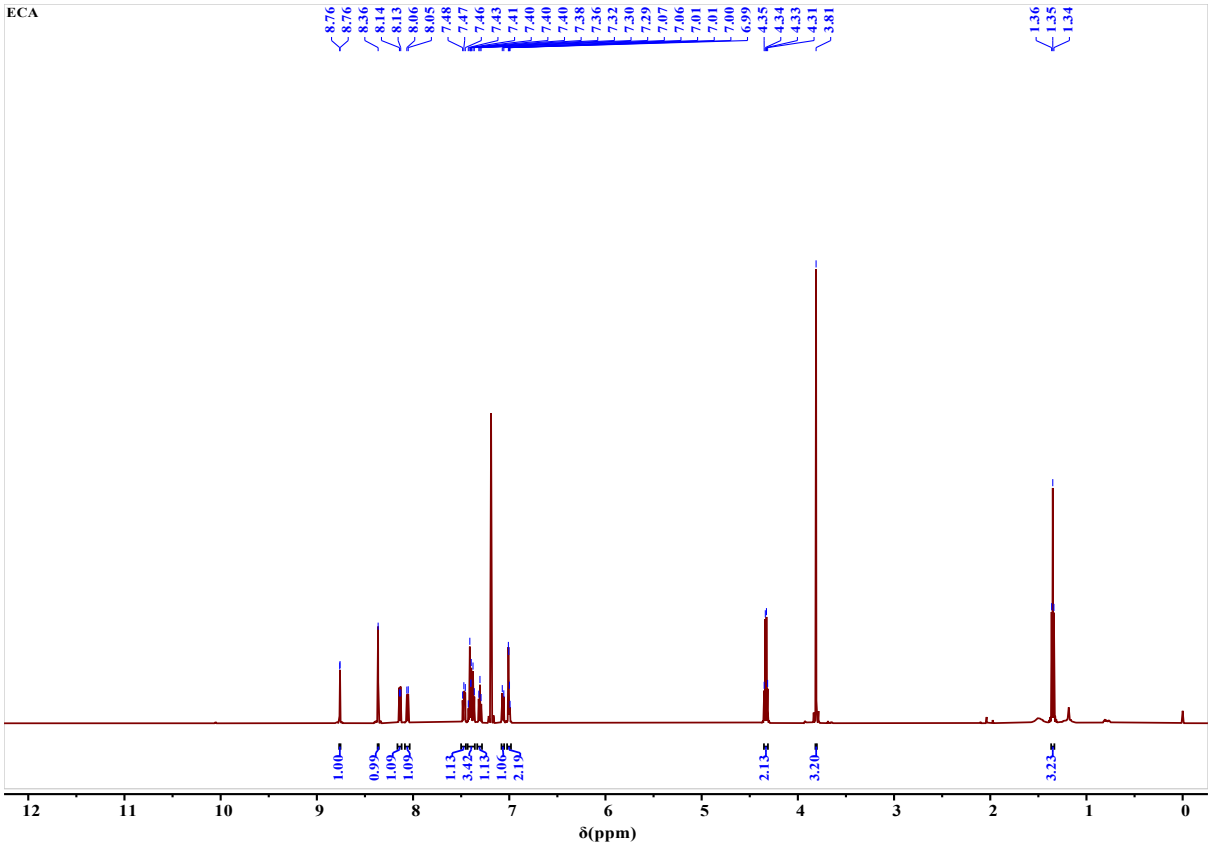


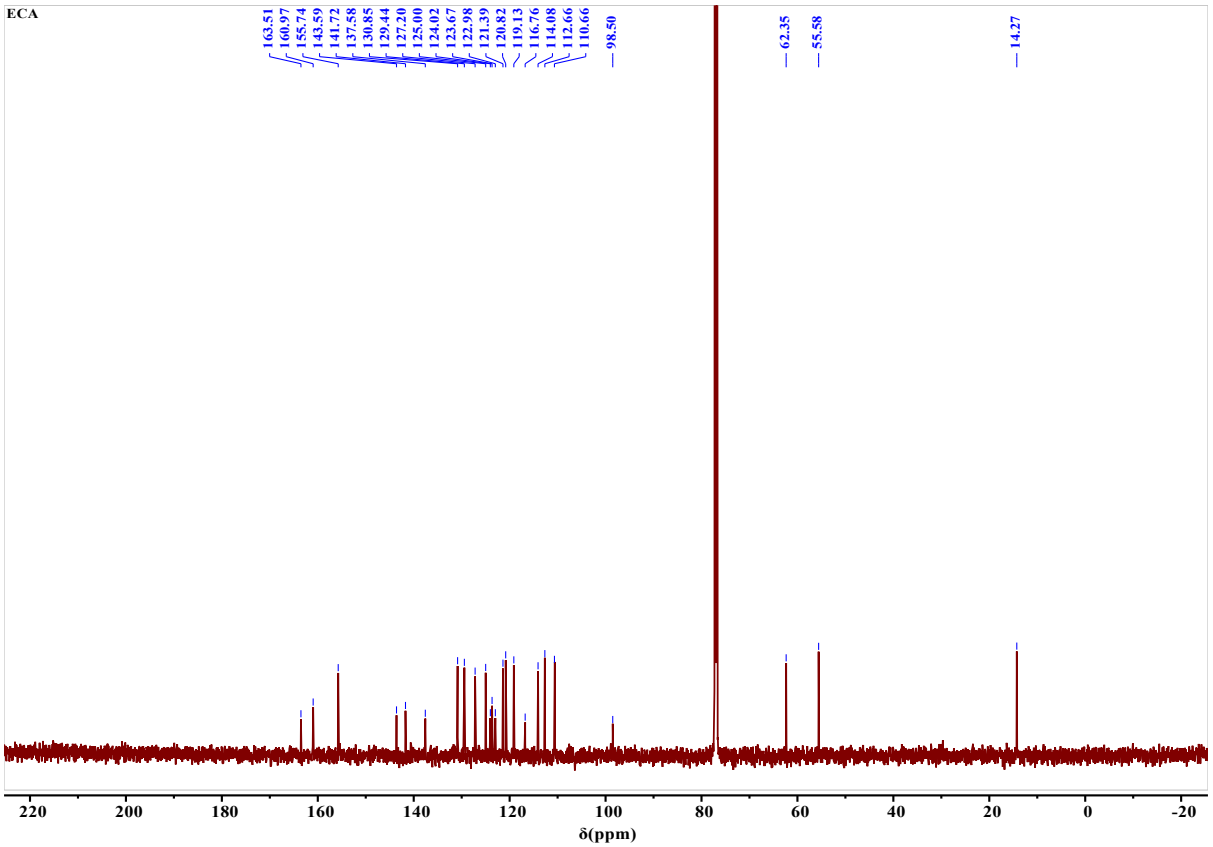
Scheme S1. Synthesis of carbazole derivatives with different acceptor units.



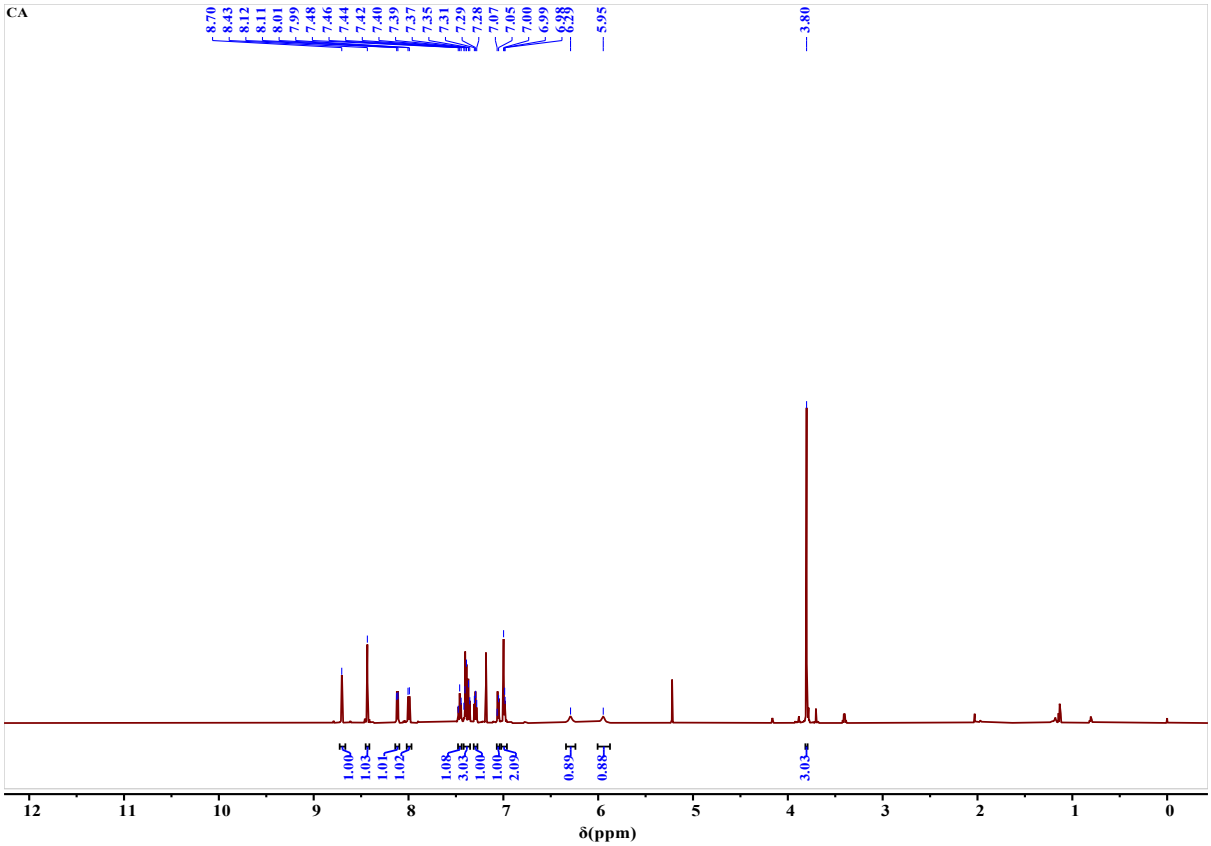


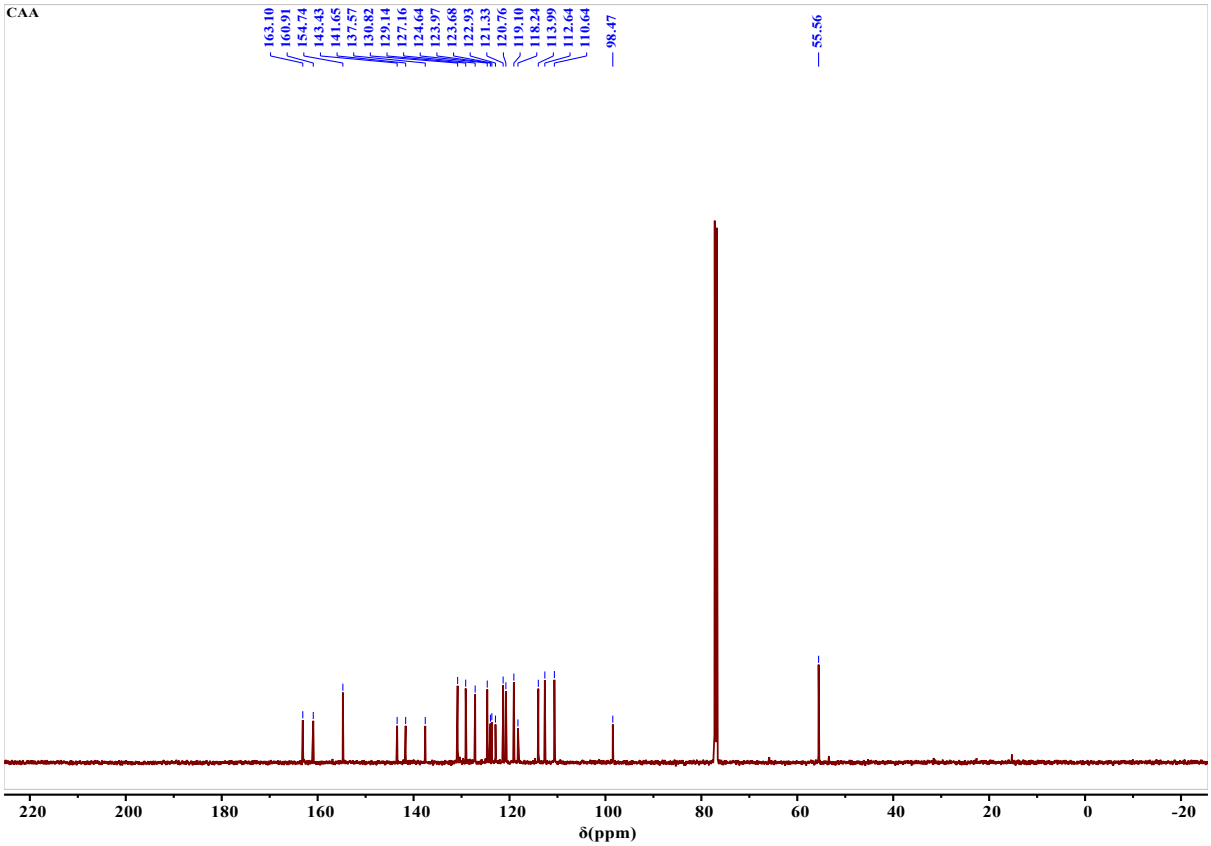
^{1}H and ^{13}C NMR of **Cz-MN** in $CDCl_3$.



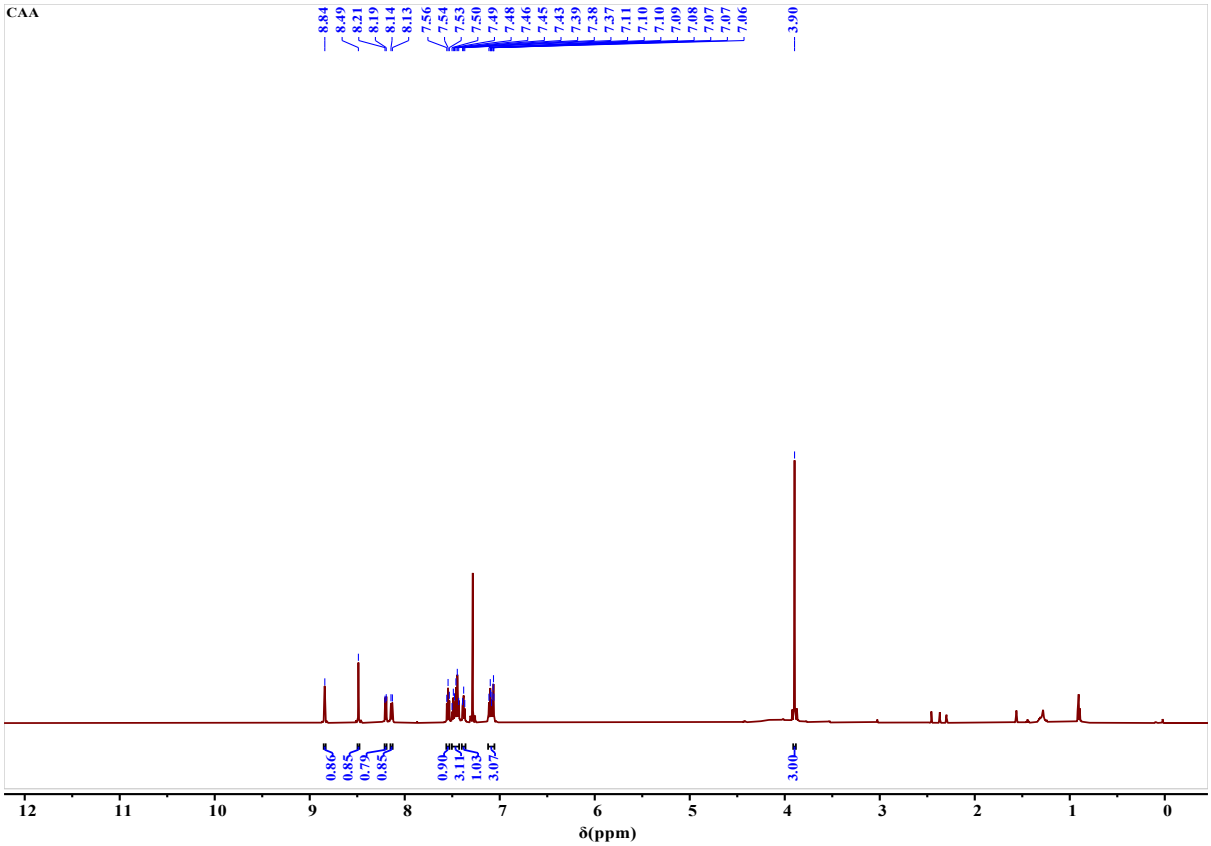


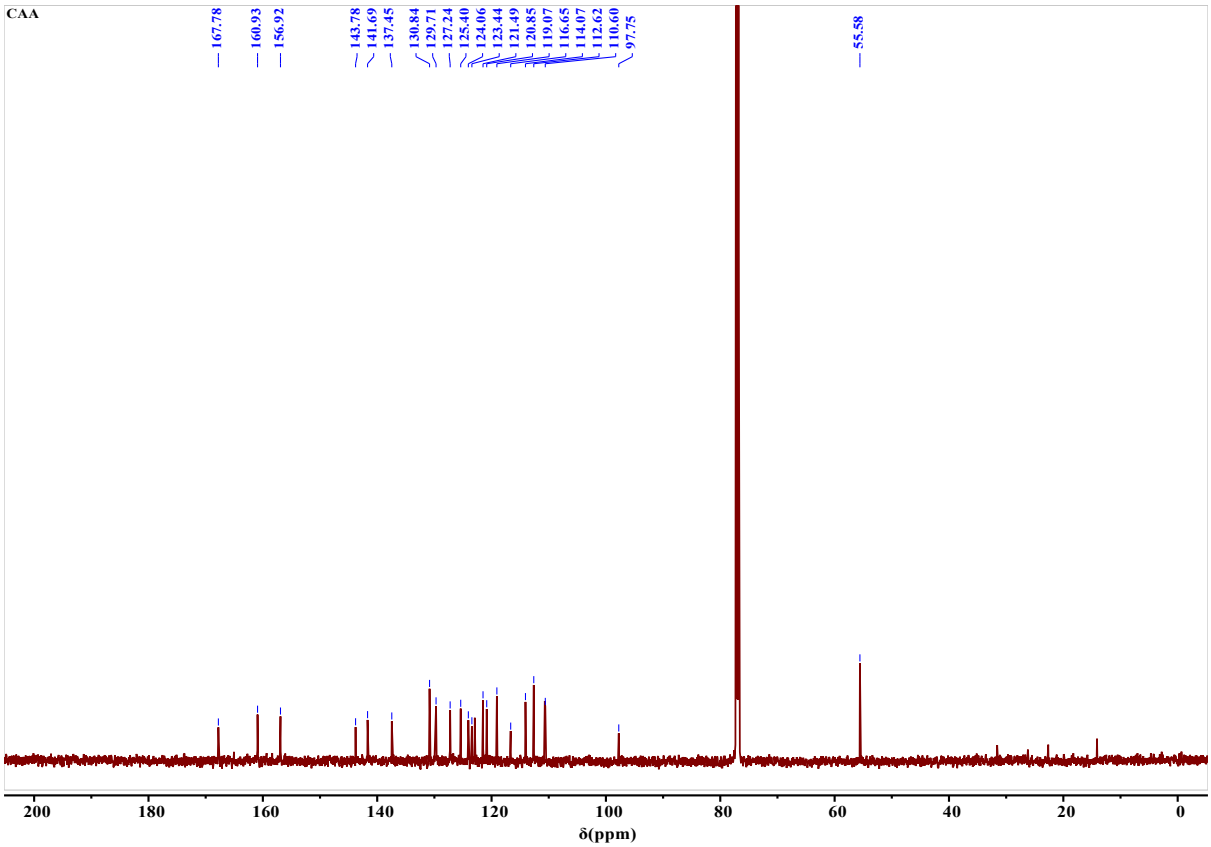
^{1}H and ^{13}C NMR of **Cz-ECA** in $CDCl_3$.



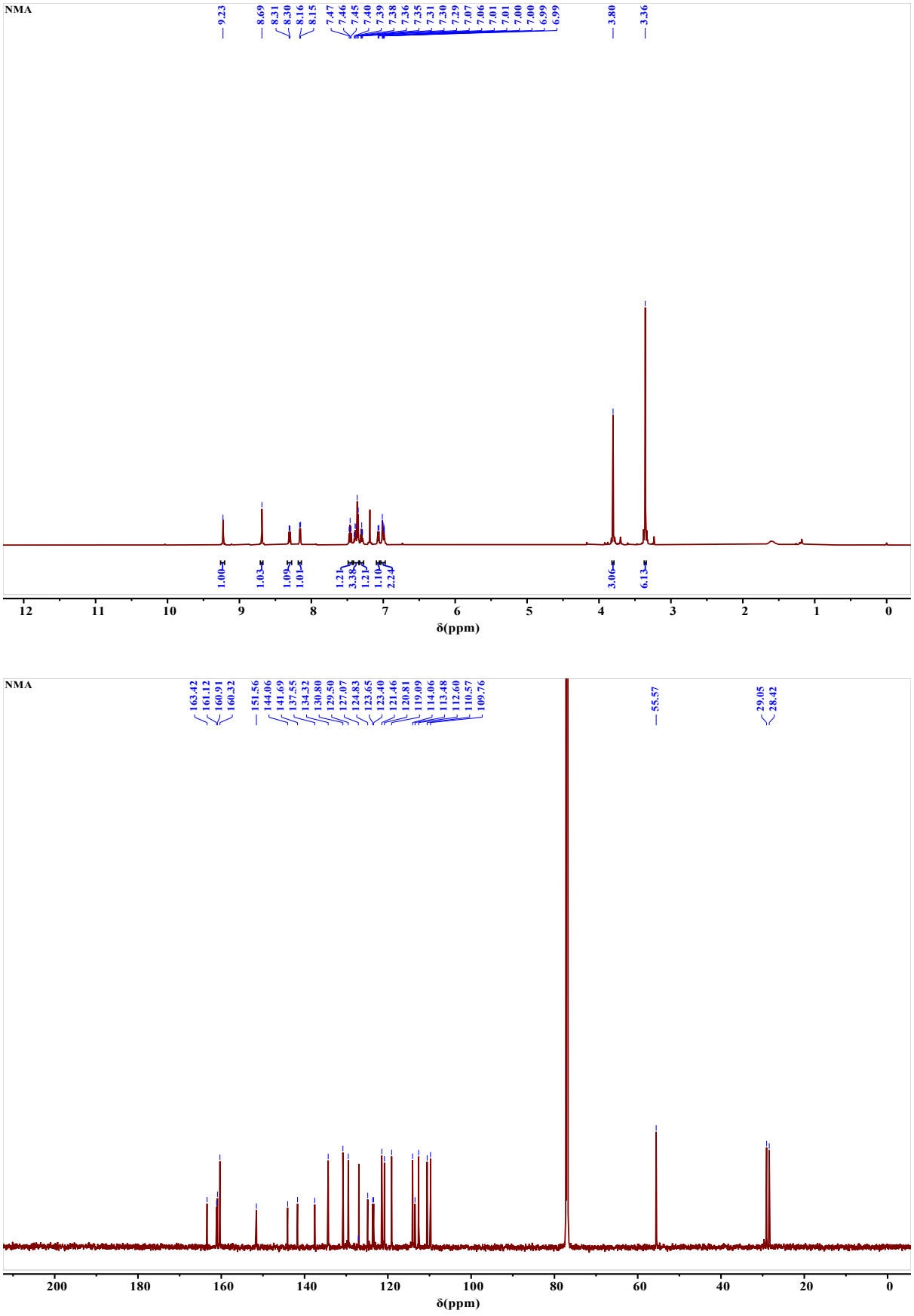


^{1}H and ^{13}C NMR of **Cz-CA** in $CDCl_3$

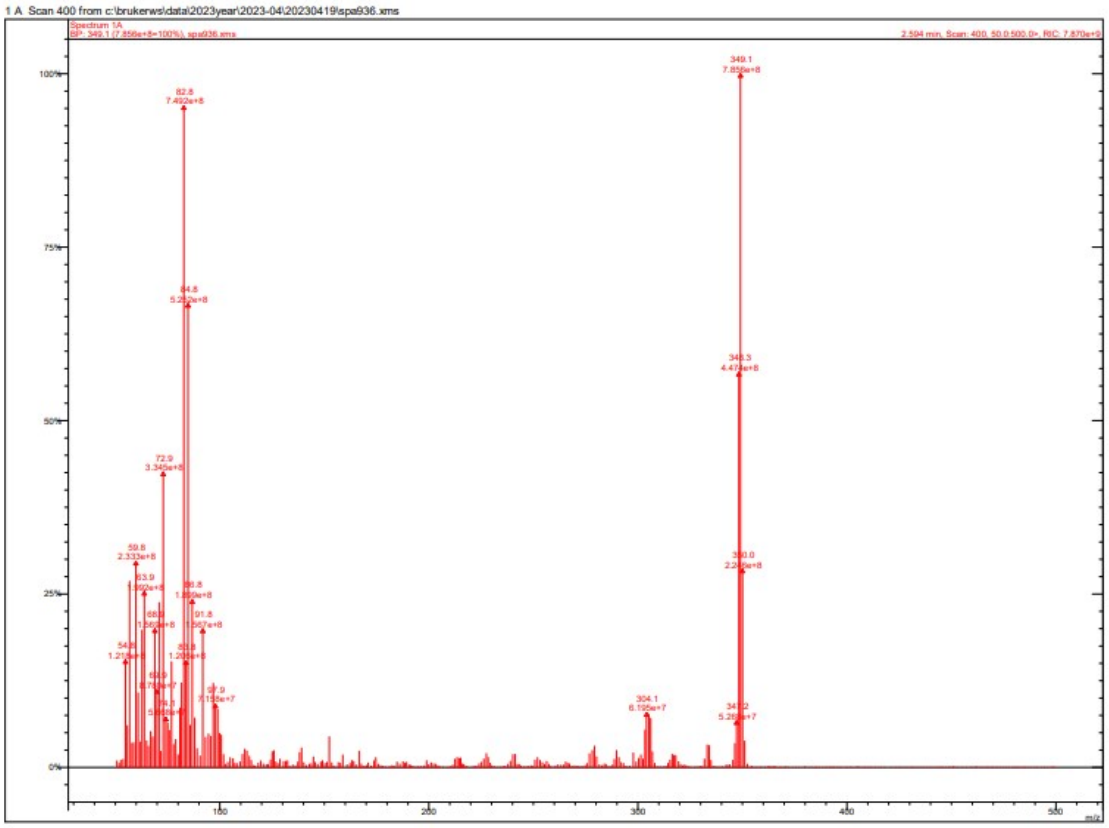




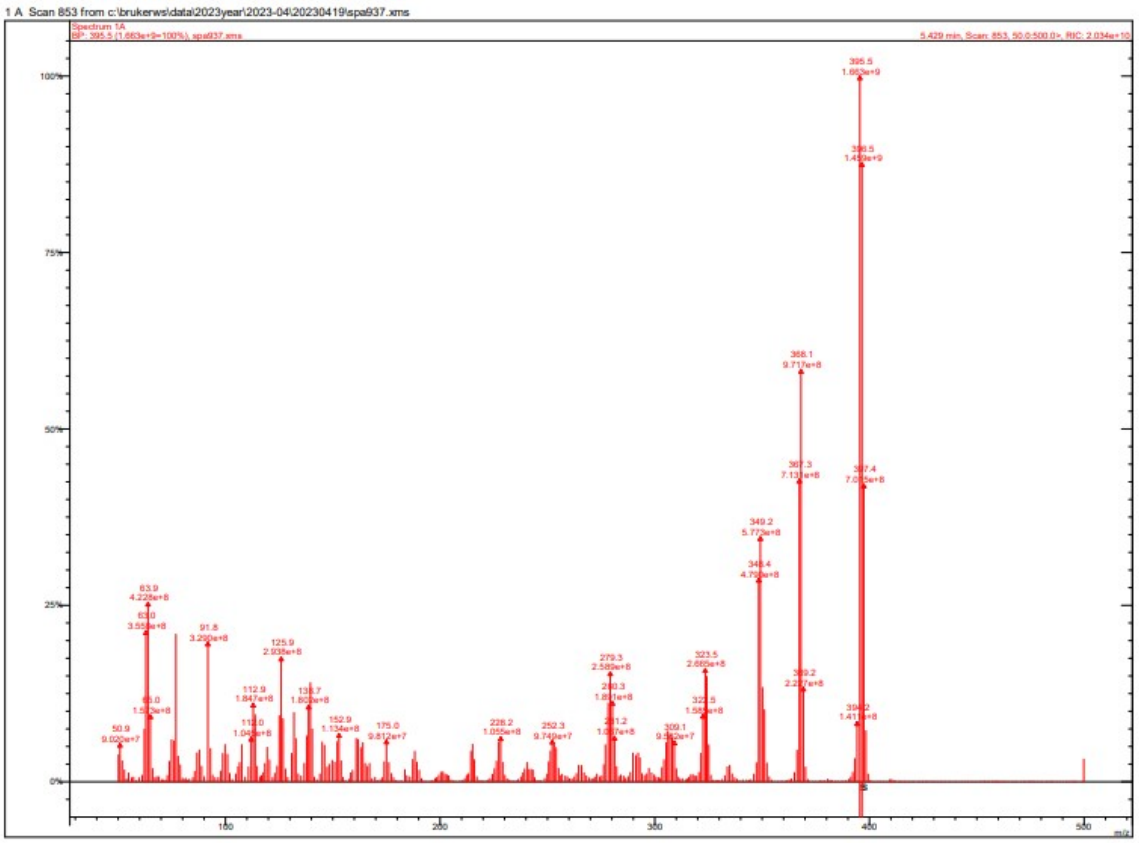
^{1}H and ^{13}C NMR of **Cz-CAA** in $CDCl_3$.



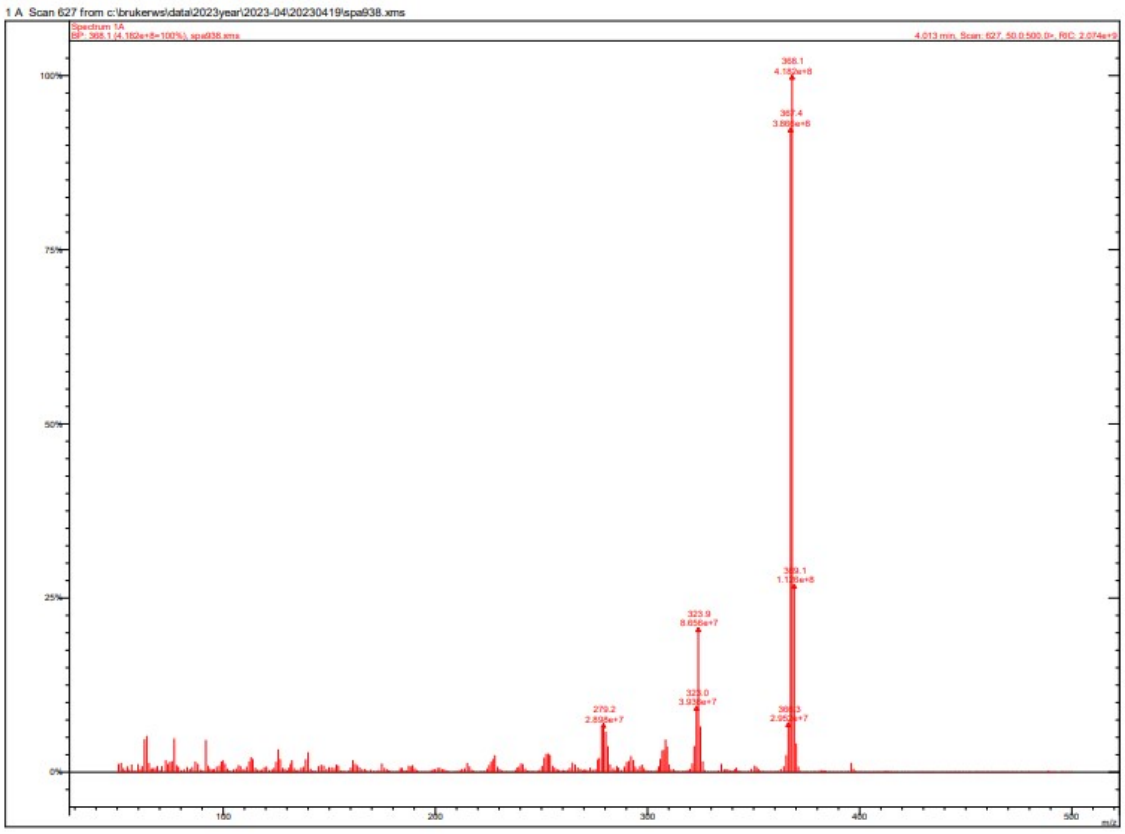
^{1}H and ^{13}C NMR of **Cz-NBA** in $CDCl_3$.



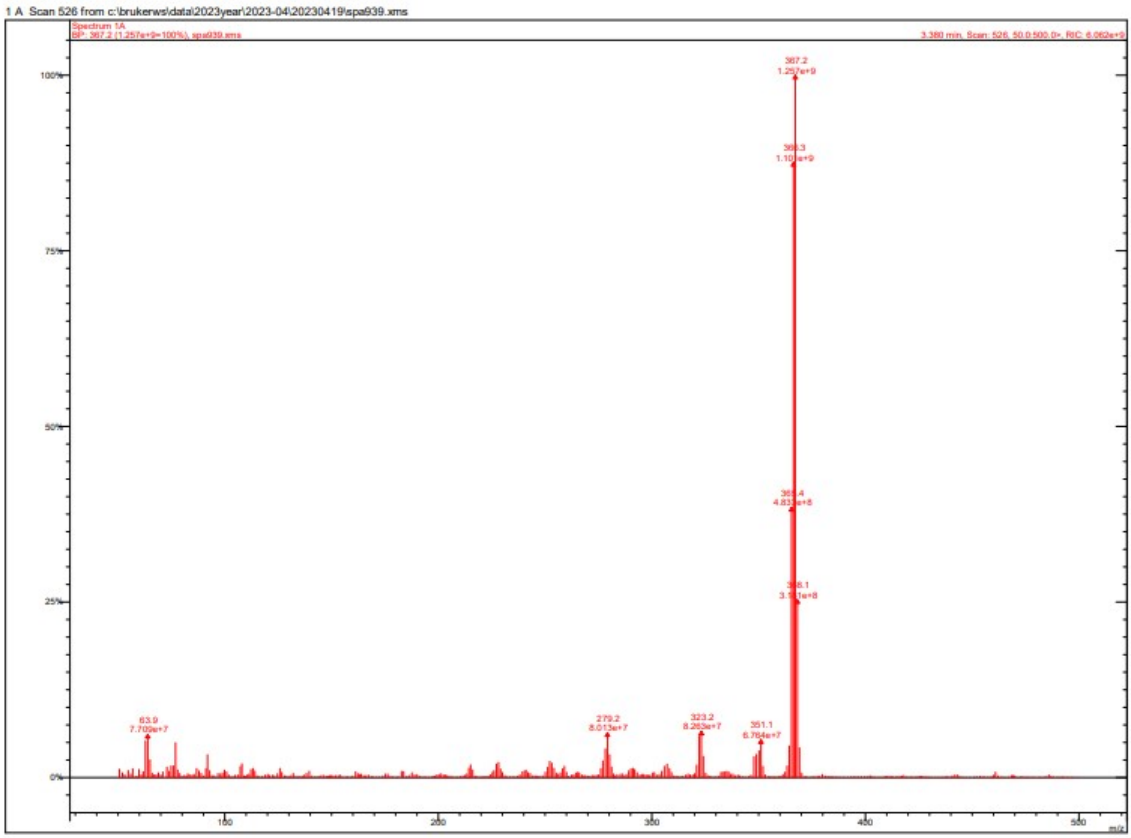
HRMS of **Cz-MN** calculated: 349.1; found 349.1.



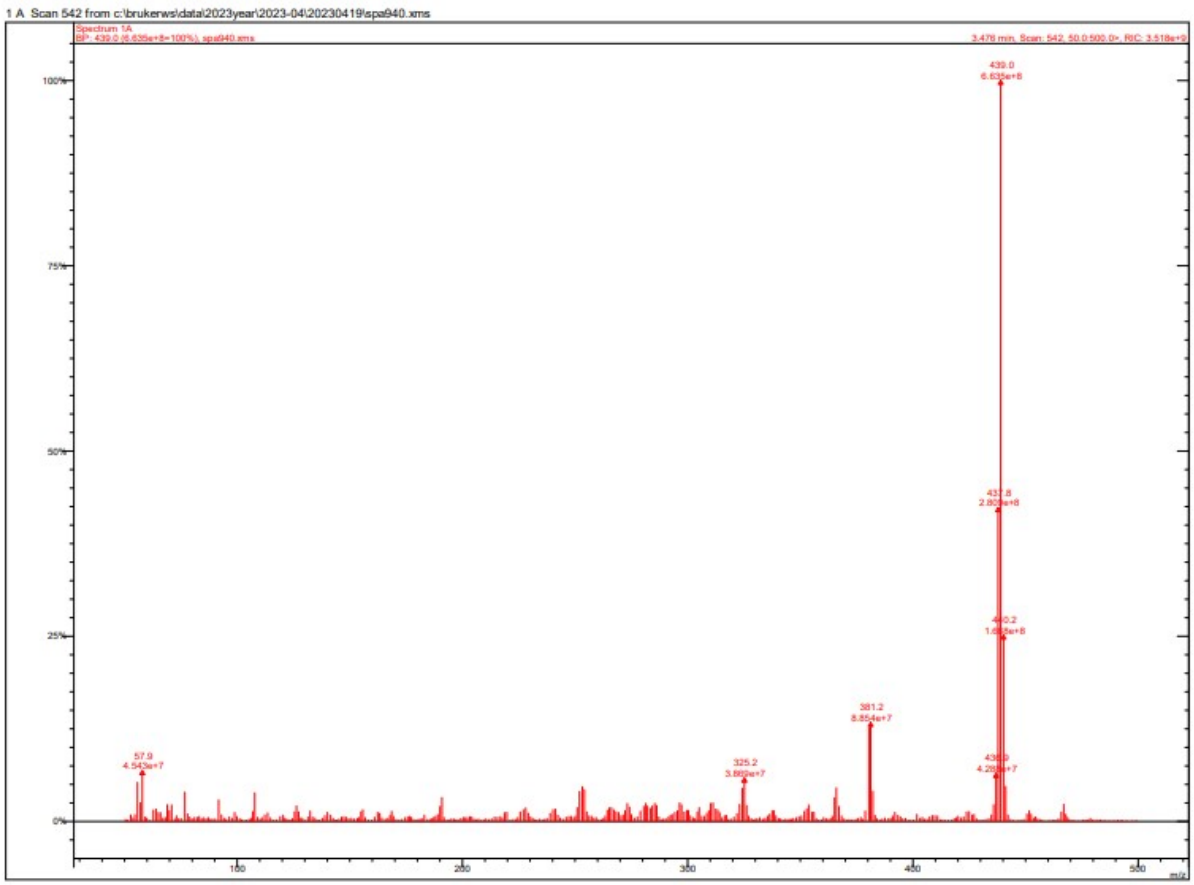
HRMS of **Cz-ECA** calculated: 396.1; found 396.5.



HRMS of **Cz-CAA** calculated: 368.1; found 368.1.



HRMS of **Cz-CA** calculated: 367.1; found 367.2.



HRMS of **Cz-NBA** calculated: 439.1; found 439.0.

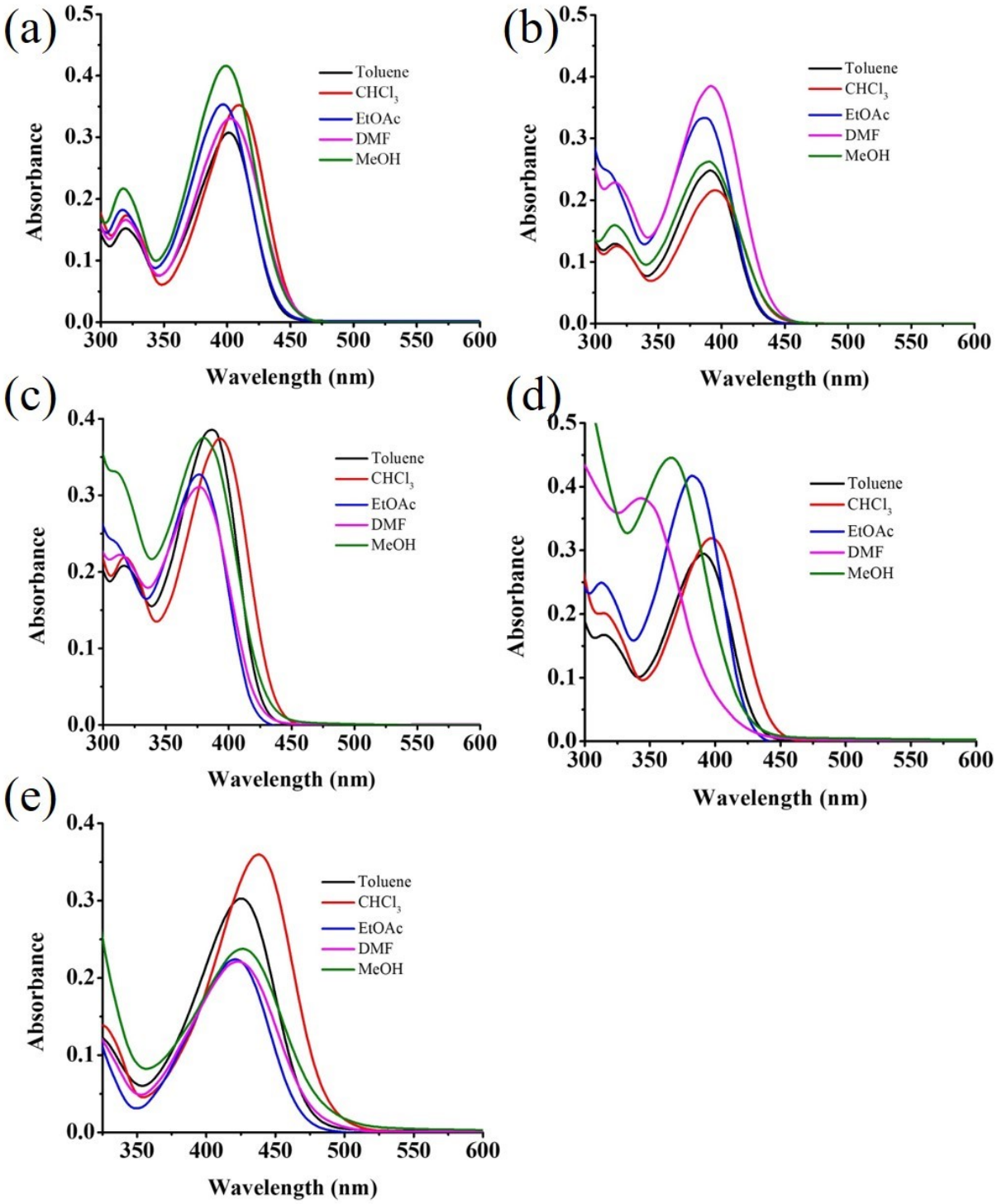


Fig. S1. Absorption spectra of (a) **Cz-MN**, (b) **Cz-ECA**, (c) **Cz-CA**, (d) **Cz-CAA** and (e) **Cz-NBA** in different solvents.

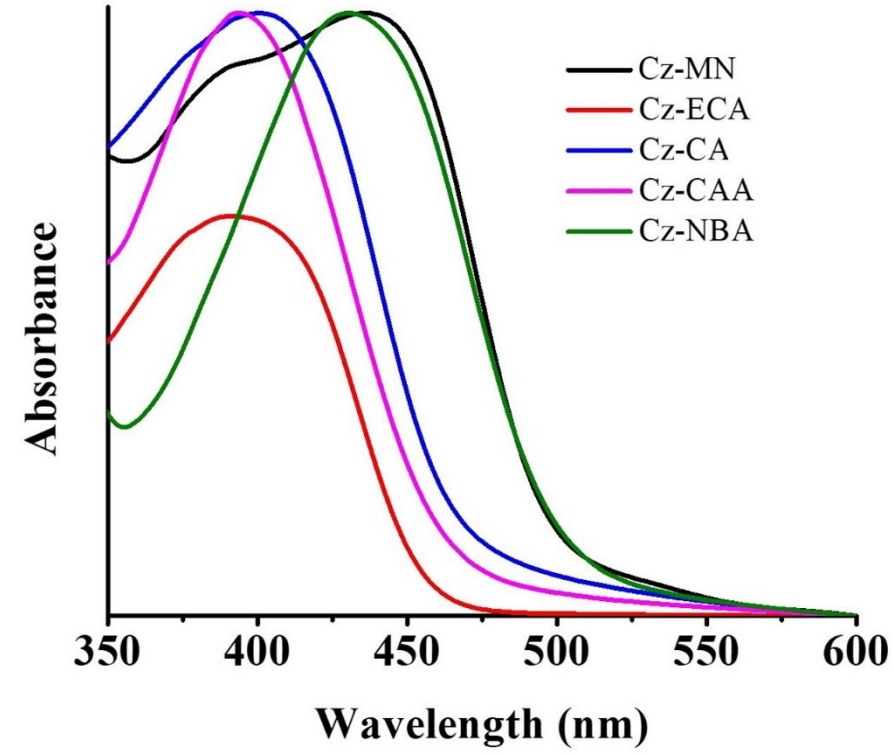


Fig. S2. Solid-state absorption spectra.

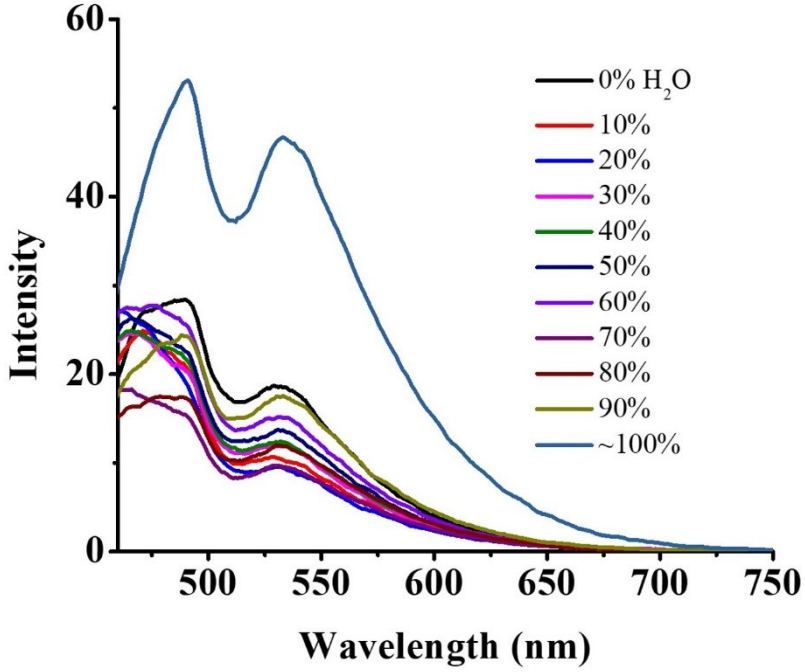


Fig. S3. AIE studies of **Cz-CAA**.

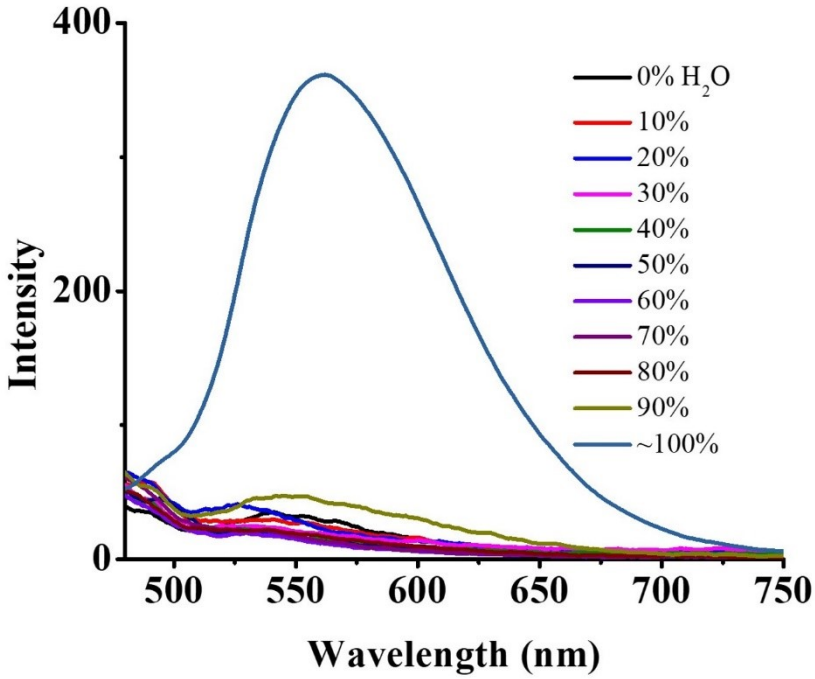


Fig. S4. AIE studies of **Cz-NBA**.

Table S1. Optical band gap of carbazole derivatives obtained from the theoretical calculation.

Compound	**HOMO**	**LUMO**	**band gap(eV)**
Cz-MN	-6.16	-2.64	3.52
Cz-ECA	-5.89	-2.33	3.56
Cz-CA	-5.90	-2.22	3.68
Cz-CAA	-5.96	-2.46	3.50
Cz-NBA	-5.92	-2.70	3.22

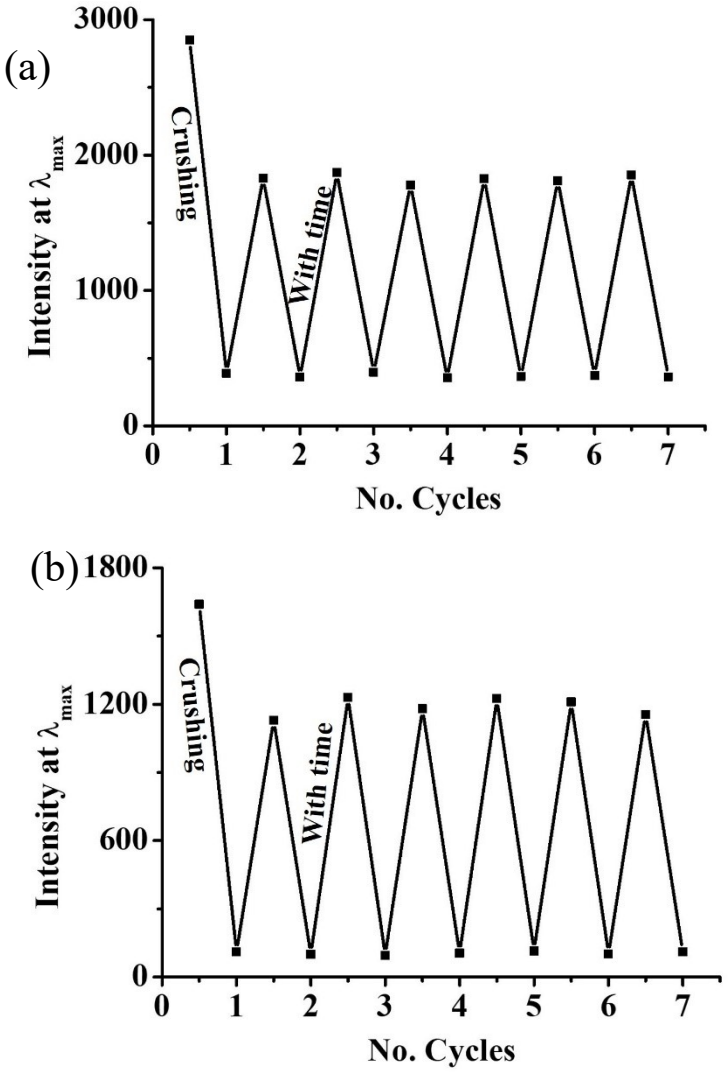


Fig. S5. Self-reversible fluorescence switching cycle of (a) **Cz-MN** and (b) **Cz-ECA**.

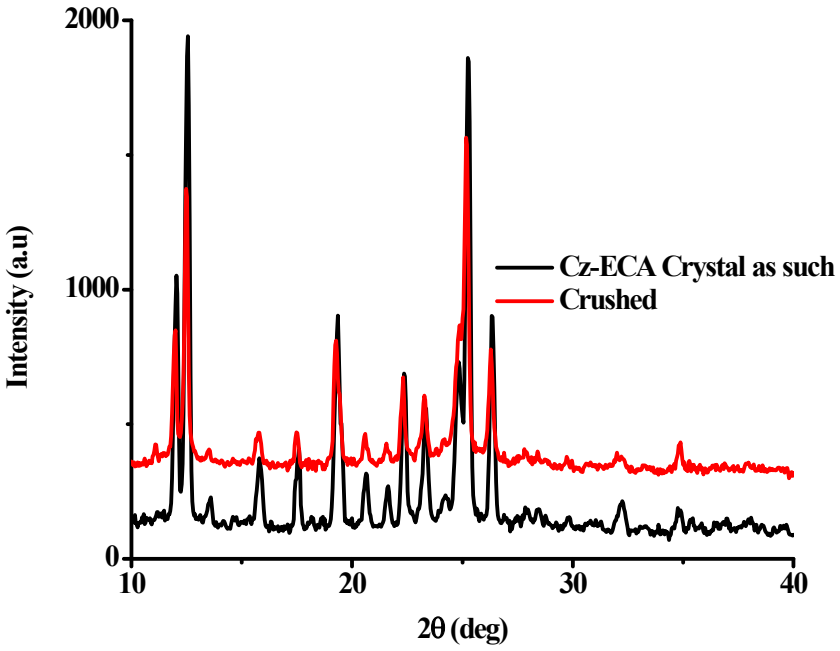


Fig. S6. PXRD of **Cz-ECA** before and after crushing.

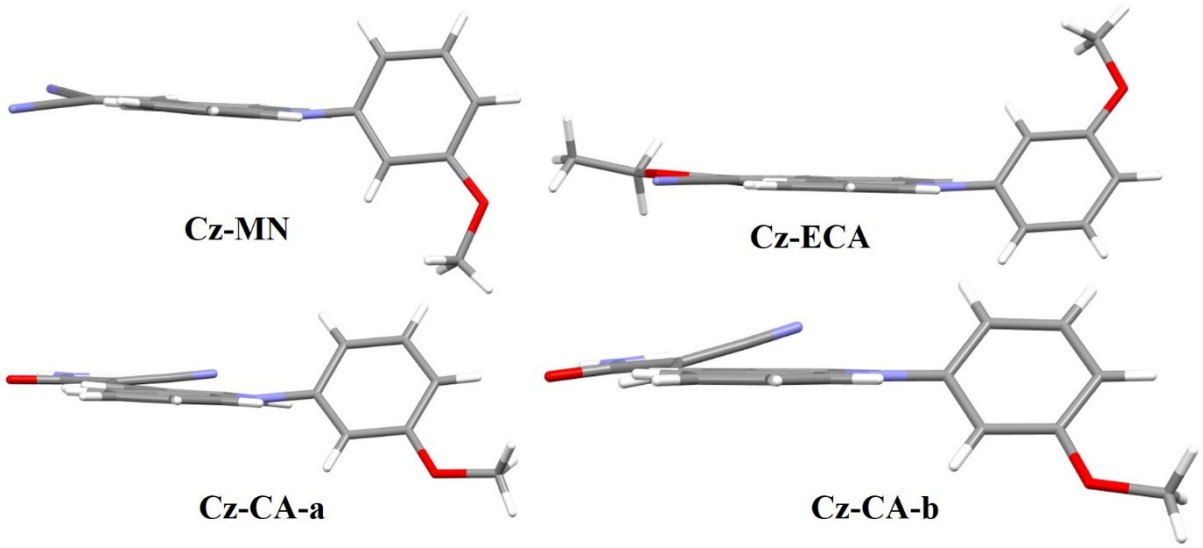
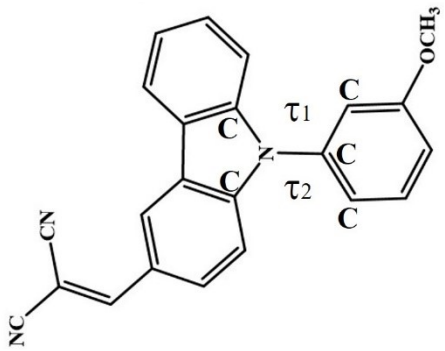


Fig. S7. Molecular confroamtion of **Cz-MN, Cz-ECA and Cz-CA** in the crystal lattice.

Table S2. Moelcular twist between the methoxy phenyl and carbazole in the crystal lattice. measured by torsion angle (τ) in the



Compound	τ1	τ2
Cz-MN	107.08	95.15
Cz-ECA	55.00	56.89
Cz-CA-a	54.11	51.07
Cz-CA-b	63.75	52.19

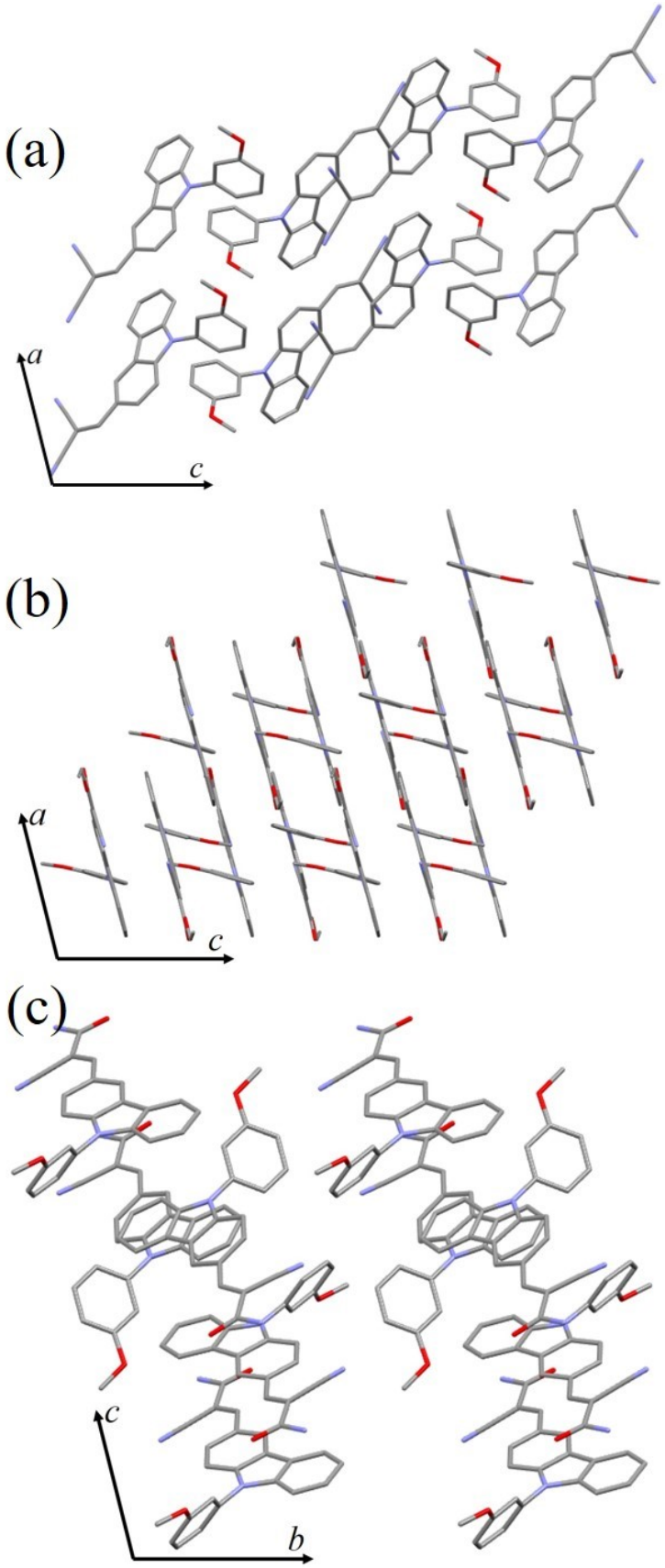


Fig. S8. Molecular packing in the crystal lattice of (a) **Cz-MN**, (b) **Cz-ECA** and (c) **Cz-CA**.