

Electronic Supplementary Information (ESI)

Anthracene-naphthylacetonitrile fluorescence isomers and Cl/H substituent dependent molecular packing, solid-state fluorescence and mechanofluorochromism

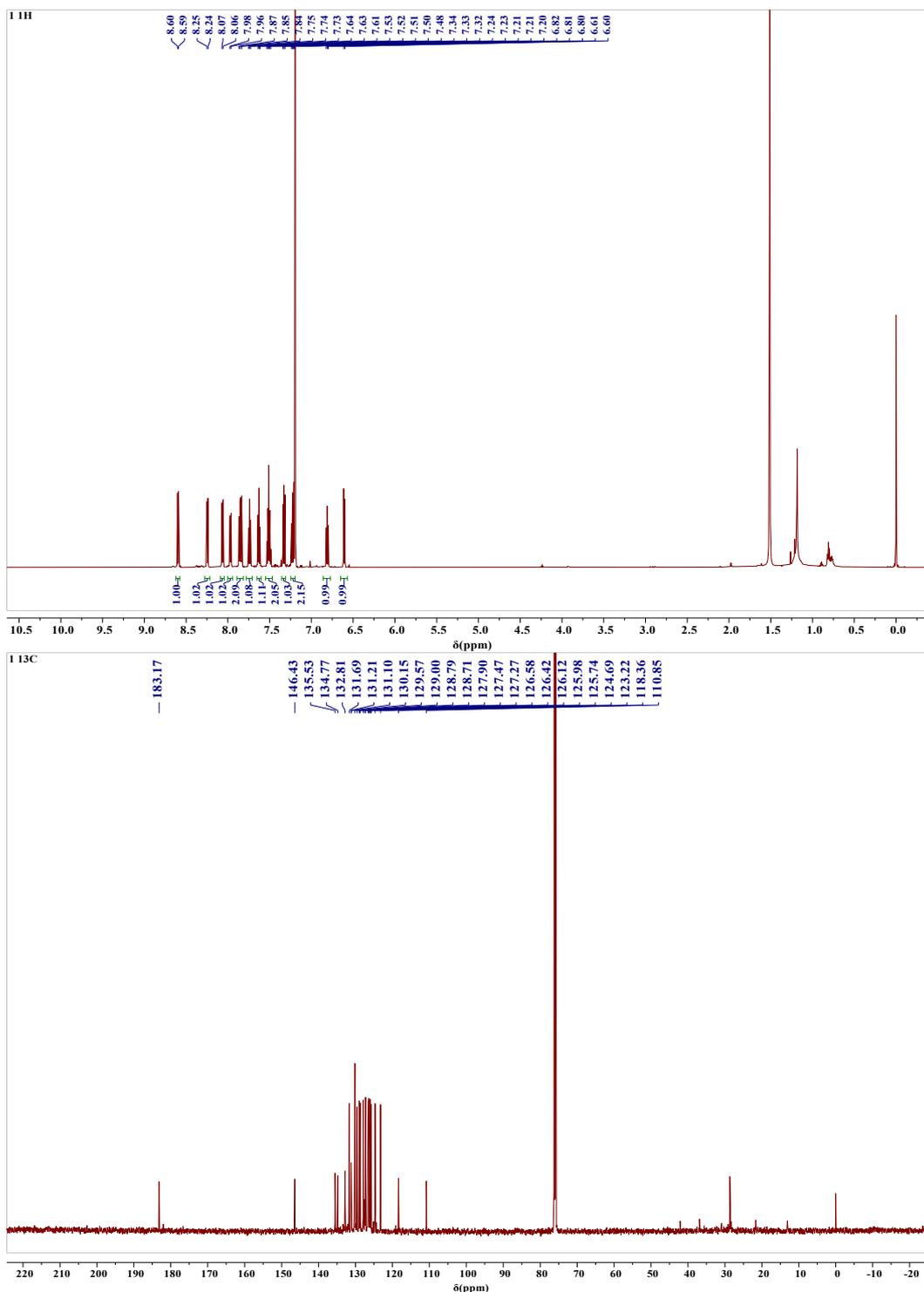


Figure S1. ^1H & ^{13}C NMR spectra for **1**

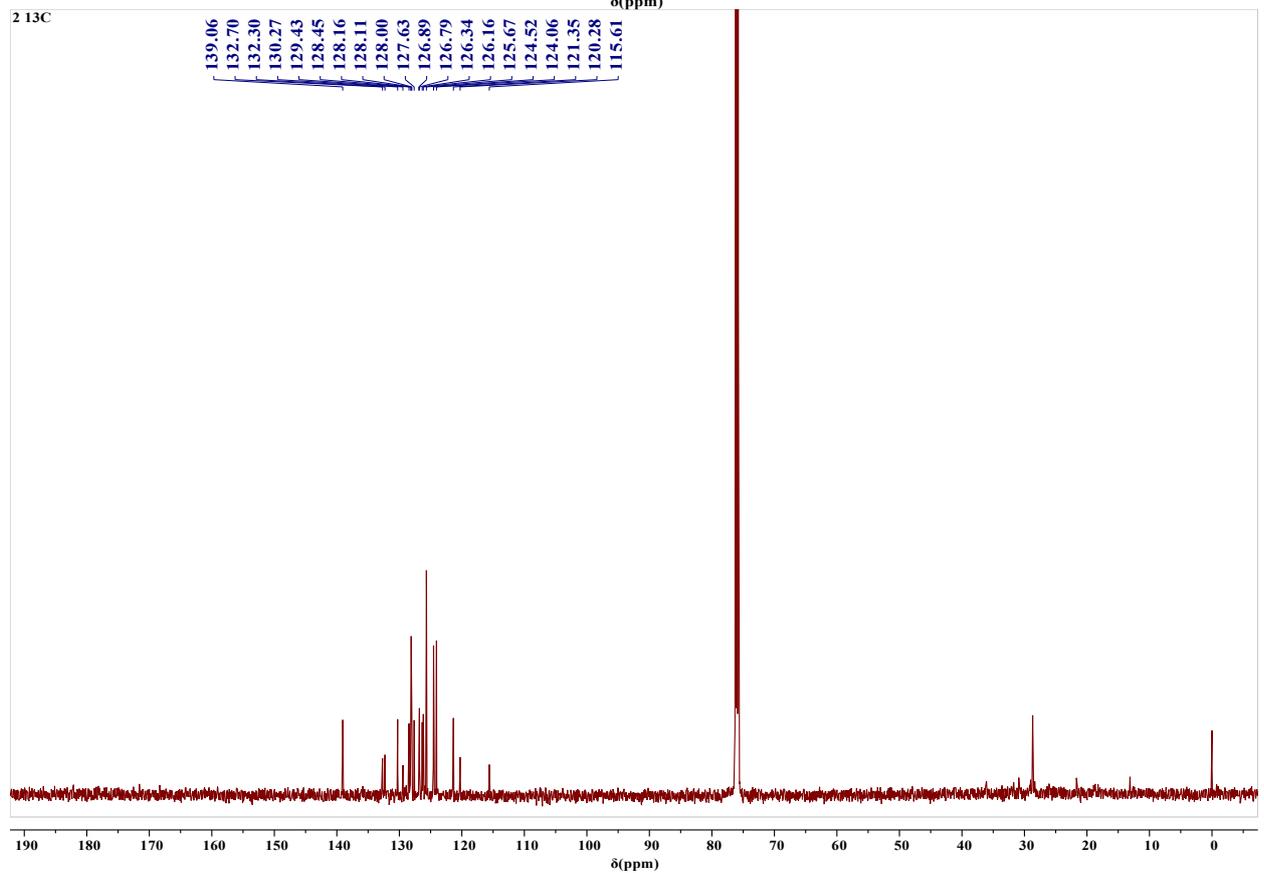
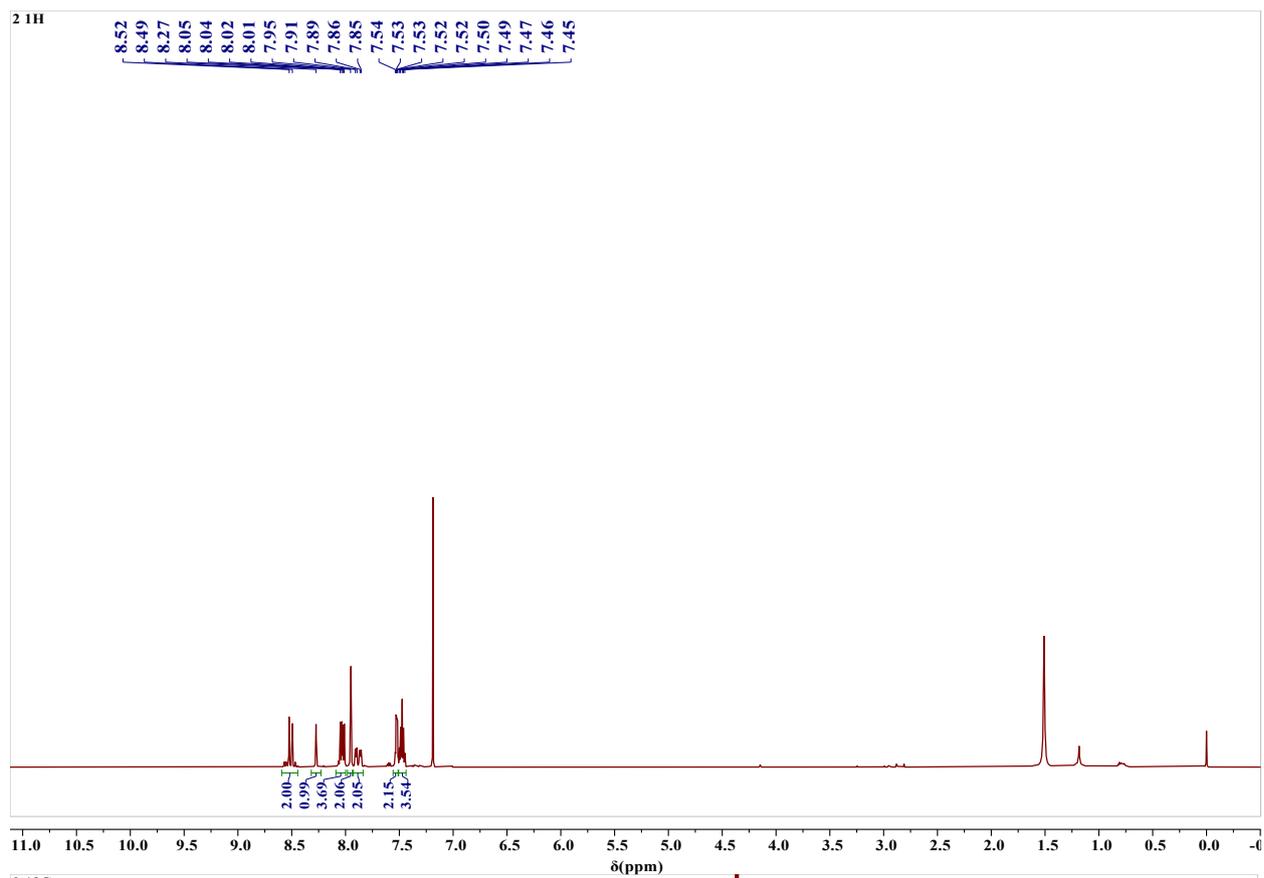


Figure S2. ^1H & ^{13}C NMR spectra for 2

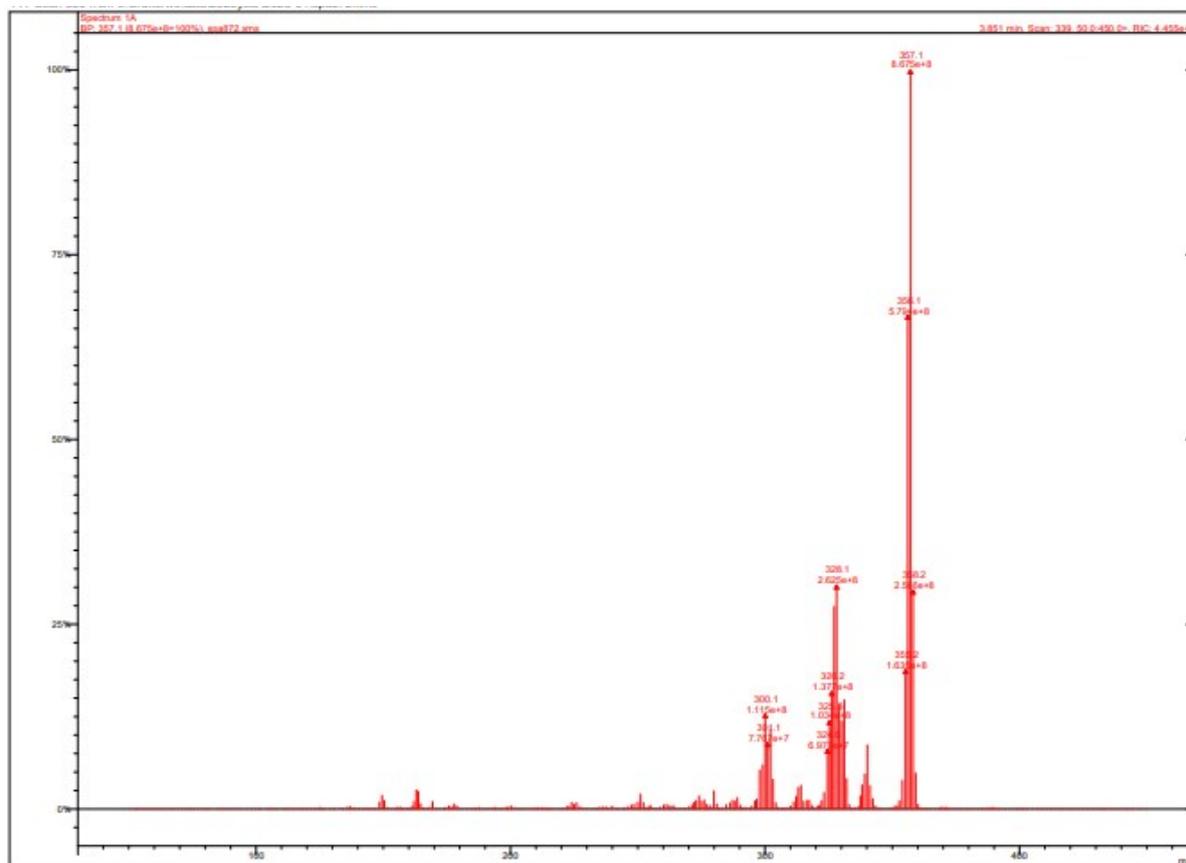


Figure S3. HRMS spectra for 1: m/z calculated: 357.13, Found (M+H): 357.1

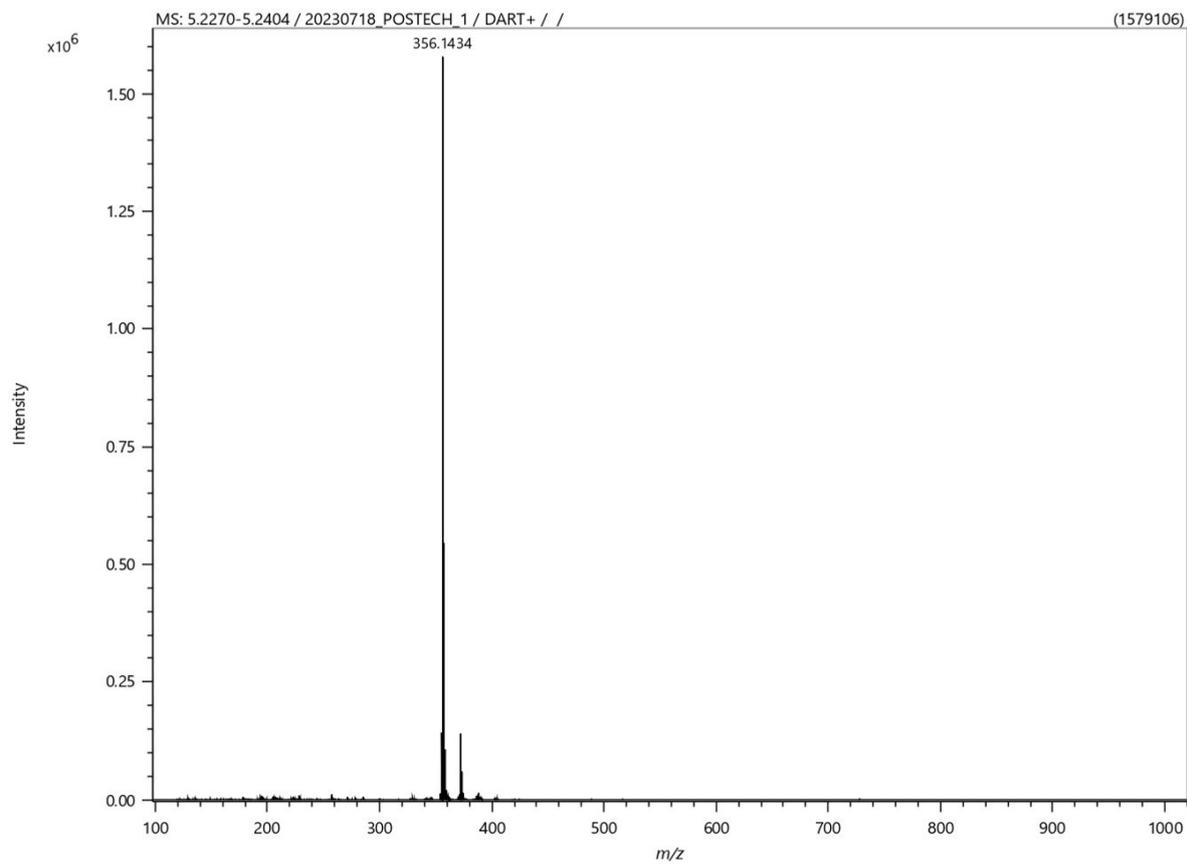


Figure S4. HRMS spectra for **2**: m/z calculated: 355.14, Found (M+H): 356.14.

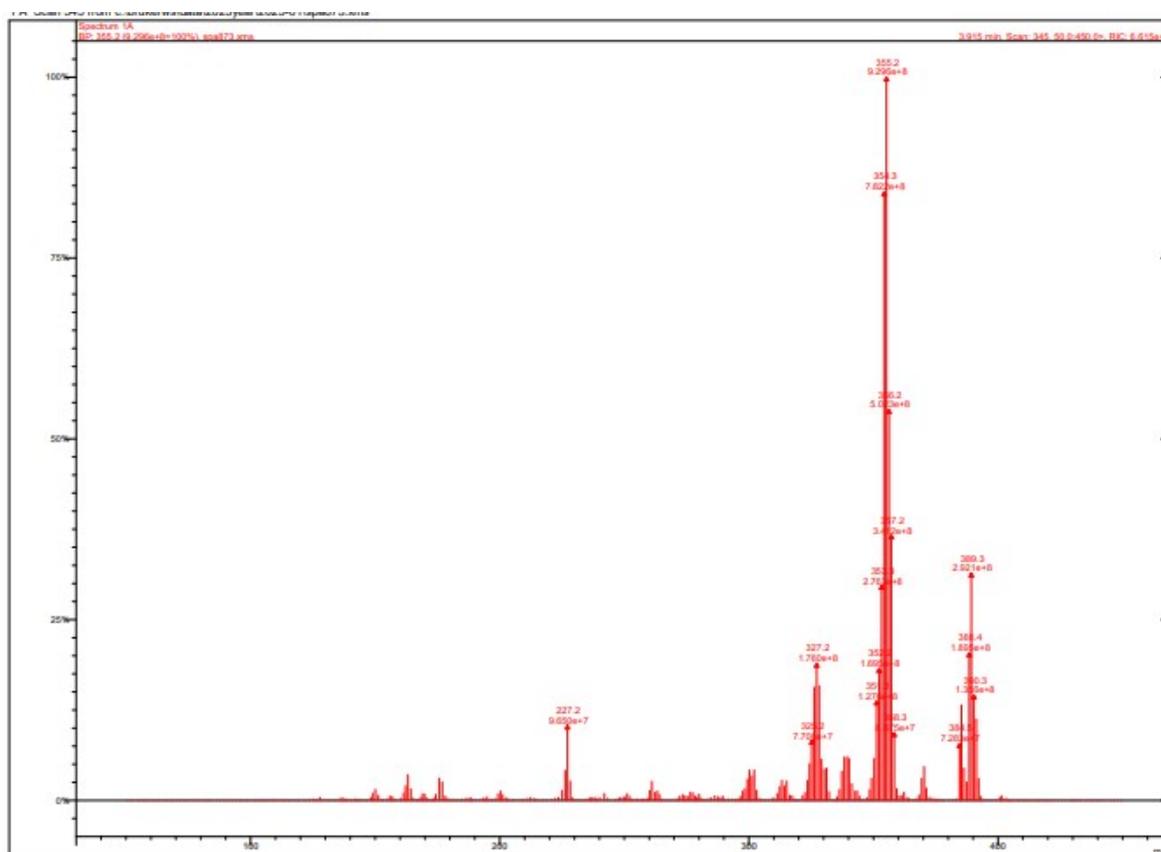


Figure S5. HRMS spectra for 2-Cl: m/z calculated: 355.14, 389.10, Found (M+H): 355.2; (M+Cl): 389.3

Single crystal structural refinement details for disordered 2-Cl:

2-Cl showed a non-centrosymmetric space group in crystal despite the Wilson plot indicating centrosymmetry. The asymmetric unit of 2-Cl contains two molecules with slightly different conformations. However, only about 40% and 60% of the hydrogen present at the C8A and C8B positions (2-Cl), respectively. This was confirmed through in the crystallographic analysis. Then the occupancy of hydrogen and chlorine was adjusted to be approximately 50:50. Crystallographic refinement was performed using the shelx option TWIN/BASF. In the reciprocal space exploration program (XPREP), the systematic absence exception is suggested to be very close between Pna2(1) and Pnma, with CFOM values of 3.92 and 3.68, respectively.

Attempts to solve the structure in the centrosymmetric space group $Pnma$ were unsuccessful using SHELXT, SHELXS, and other structure-solving programs that might be due to the disorder of hydrogen and chlorine at the anthracene C8A and C8B position, which prevents the crystallographic centrosymmetric structure and can also cause a pseudo-symmetry in the diffraction pattern, which can lead to an incorrect determination of centrosymmetry.

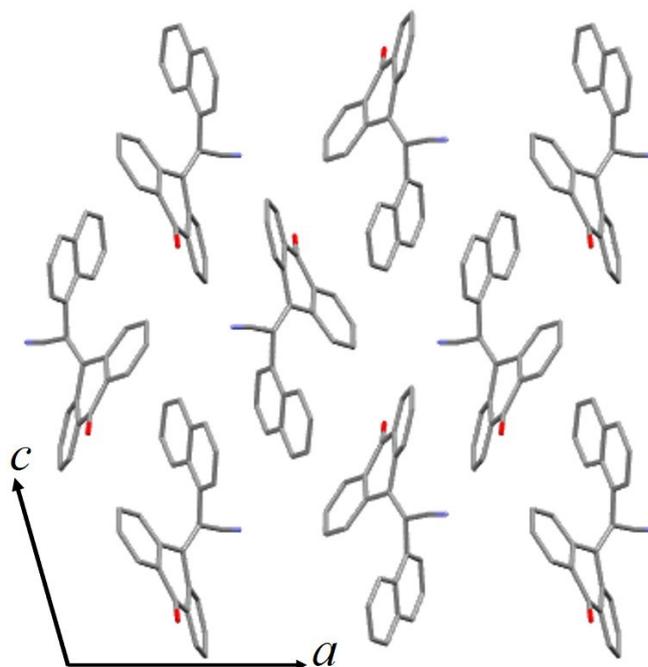


Figure S6. Molecular packing in the crystal lattice of **1**. Hydrogen atoms are omitted for clarity. C (grey), N (blue) and O (red).

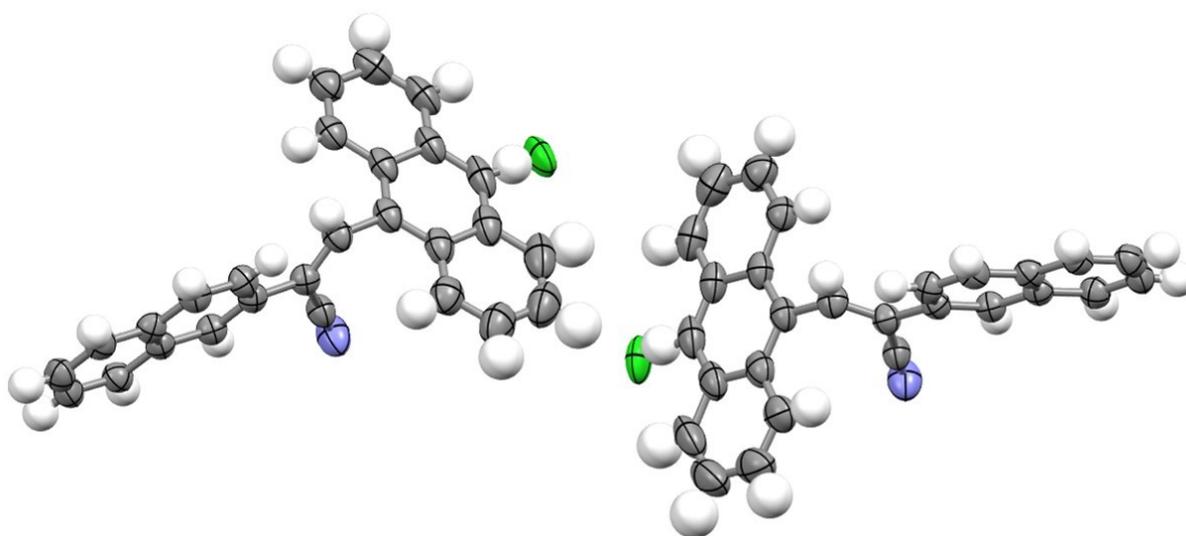


Figure S7. Disordered structure of **2**. C (grey), N (blue), O (red), Cl (green) and H (white).

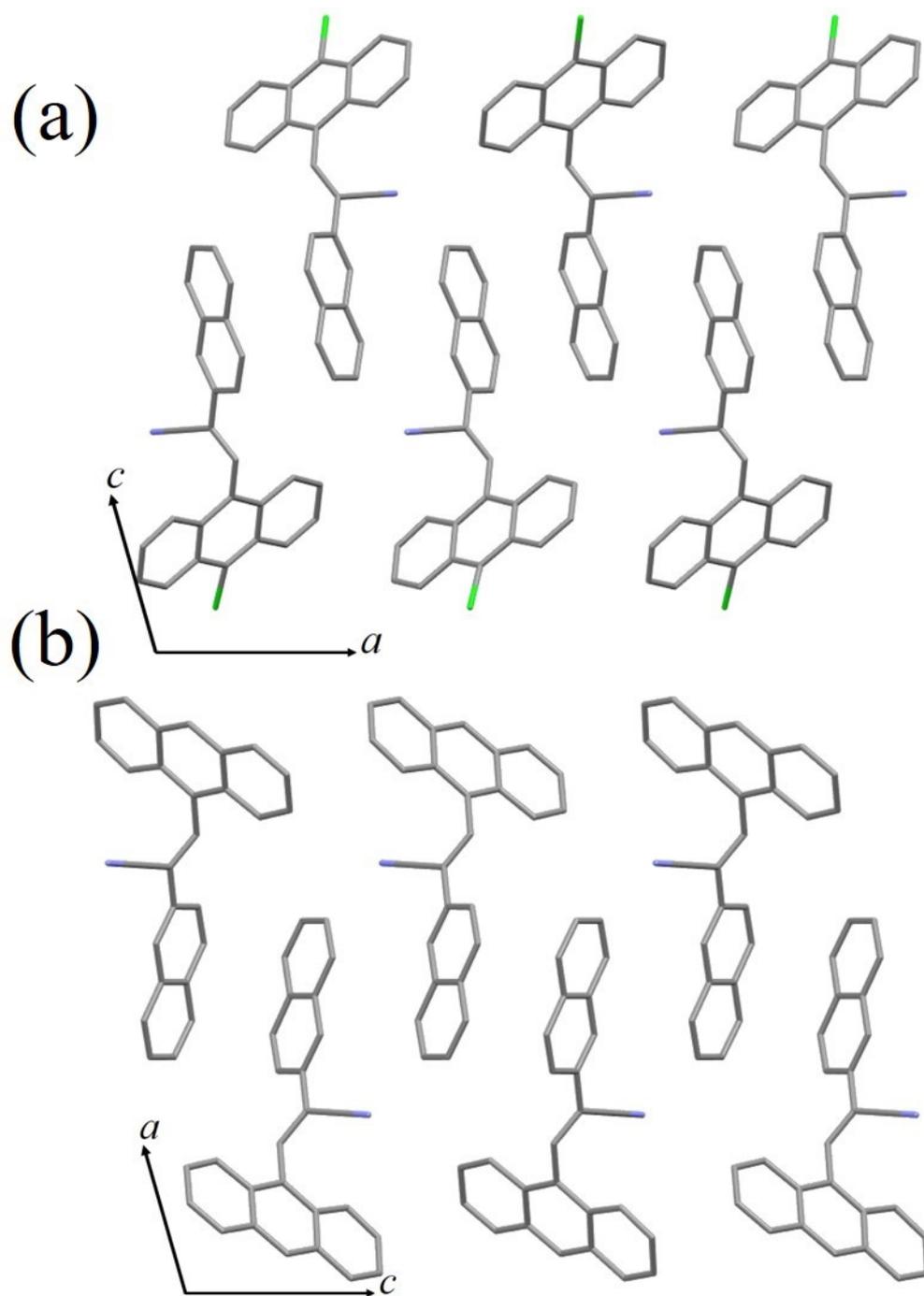
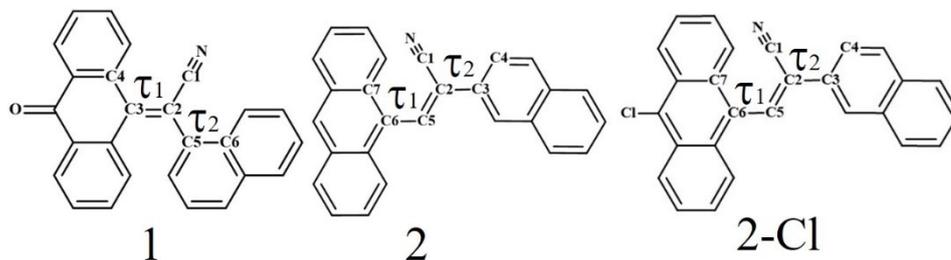


Figure S8. Molecular packing in the crystal lattice of (a) **2-Cl** and (b) **2**. Hydrogen atoms are omitted for clarity. C (grey), N (blue) and Cl (green).

Table S1. The conformation twist observed in the crystal lattice of **1**, **2** and **2-Cl** is expressed using the torsion (τ) angle.



1		2		2-Cl	
τ_1	τ_2	τ_1	τ_2	τ_1	τ_2
8.34	65.11	110.71	20.68	106.41 (I)	20.15 (I)
				109.18 (II)	20.83 (II)

Asymmetric unit of **2-Cl** contains two molecules with different conformation in the crystal lattice and denoted as (I) and (II).

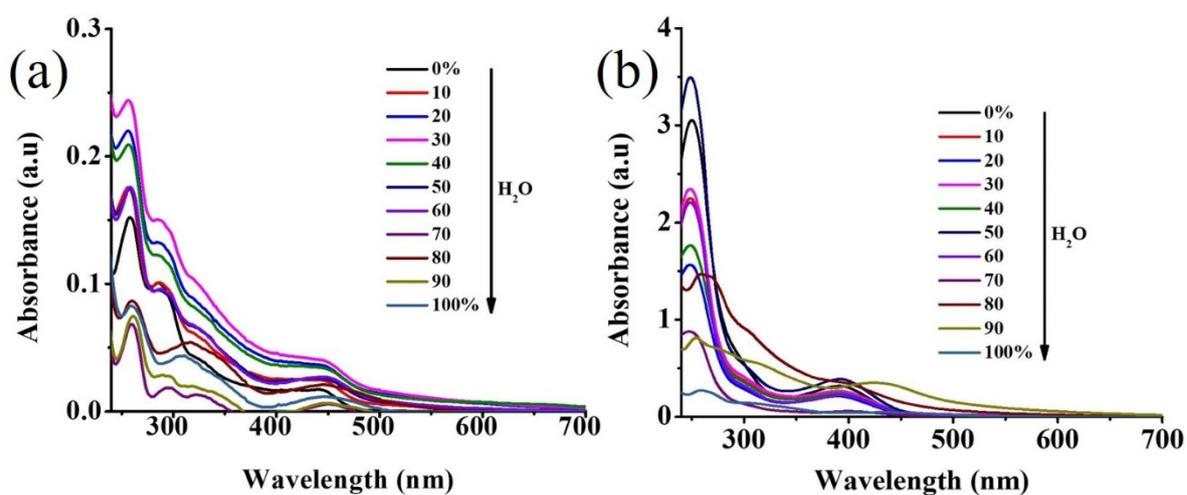


Figure S9. Absorption spectra of (a) **1** and (b) **2** during the AIE studies.

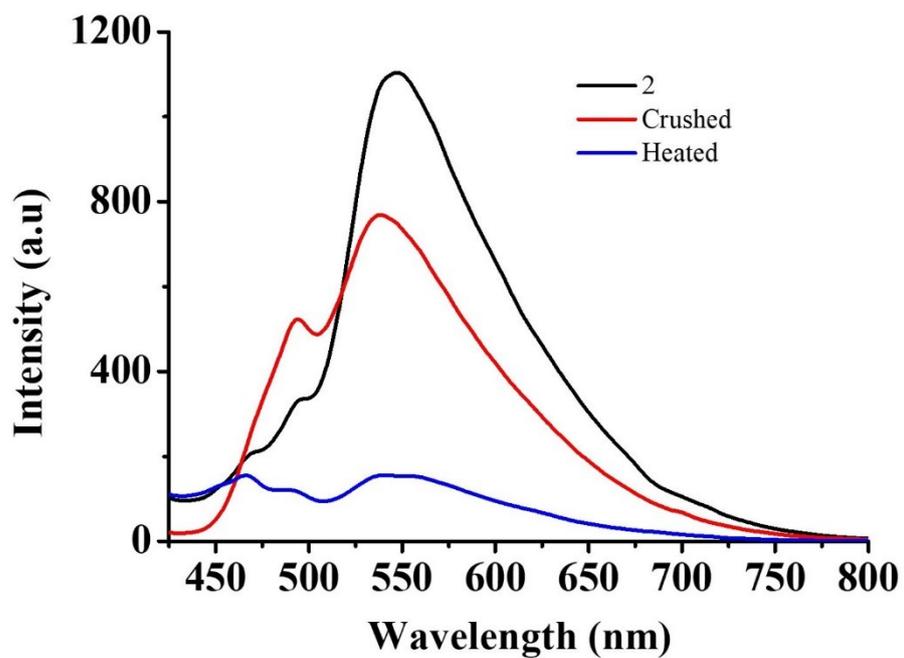


Figure S10. Mechanofluorochromism of **2**.

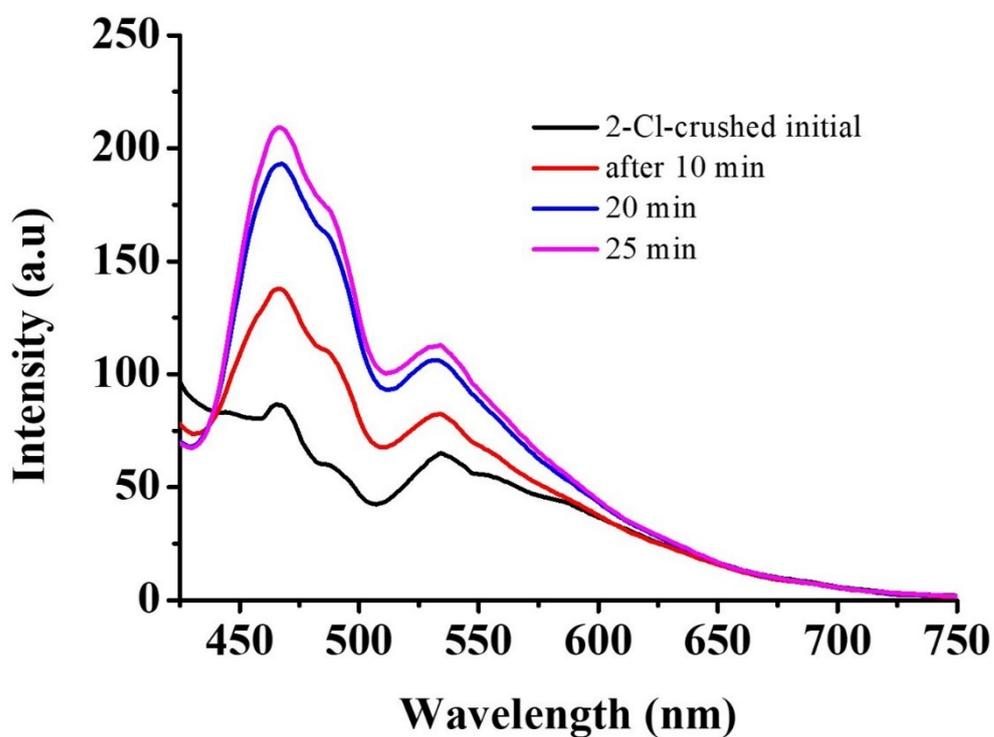


Figure S11. Self-reversible mechanofluorochromism of **2-Cl**.

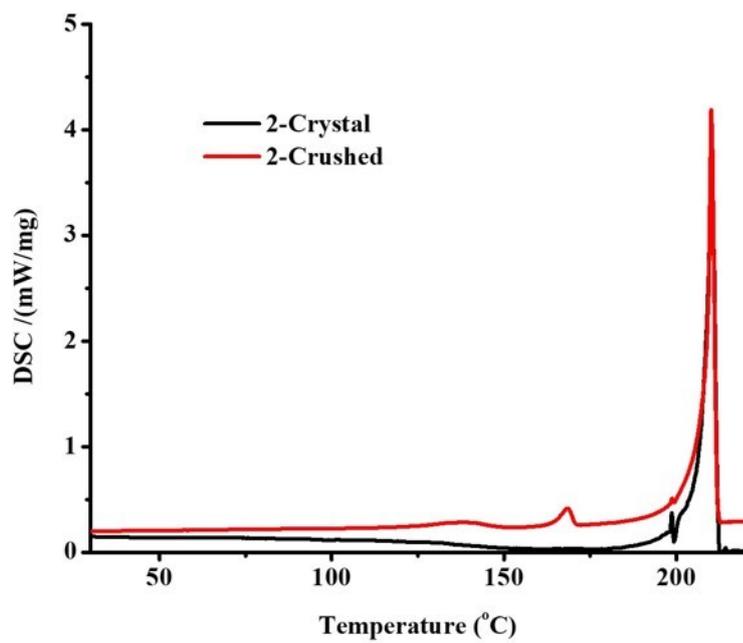
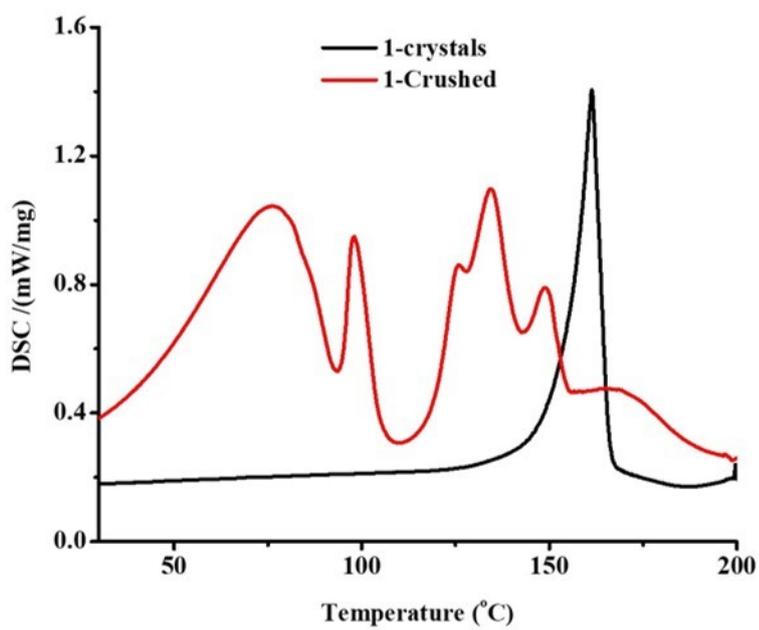


Figure S12. DSC of 1 and 2.

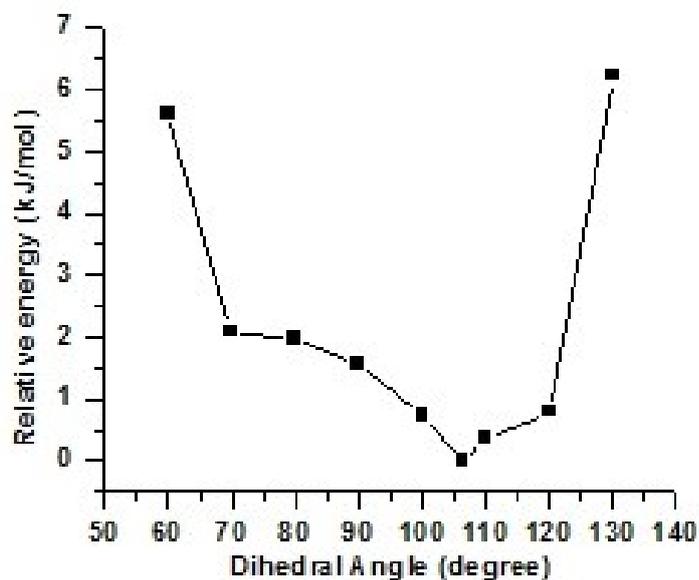


Figure S13. Potential energy was calculated for different dihedral angle using B3PW91/6-31G* level of theory. We plotted relative energy against dihedral angle. From the graph, it can be concluded that theoretically most stable structure (dihedral angle 106°) was good agreement with experimental one (dihedral angle 106°).