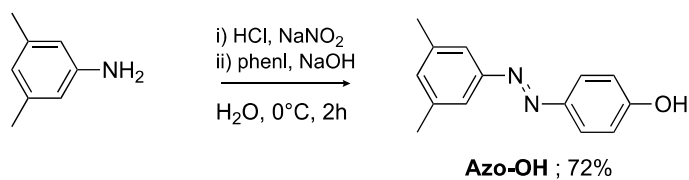


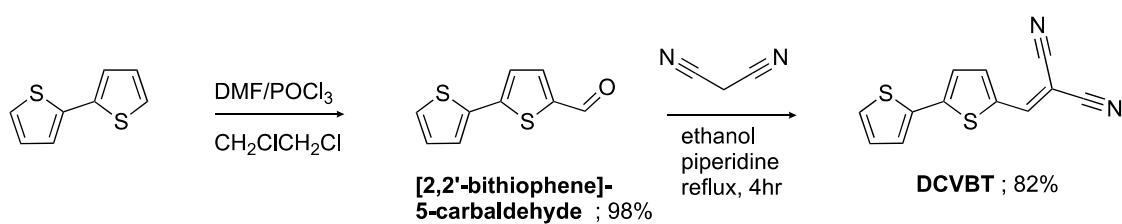
# Supplementary Materials

## Synthetic Schemes

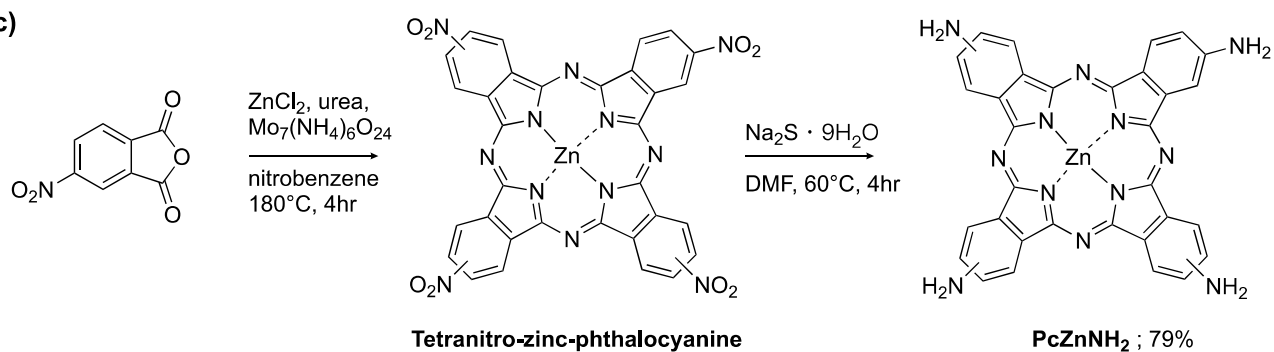
a)



b)



c)



Scheme S1: Synthetic path the of the investigated compounds: **Azo-OH** (a); **DCVTBT** (b); **PcZnNH<sub>2</sub>** (c)

## S1. Raman vibrational modes.

### DCVBT

Vibrational Mode	Frequency (cm <sup>-1</sup> )
$\nu(\text{C}\equiv\text{N})$ of cyano bonds	2220
Symmetric stretching $\nu_s(\text{C}=\text{C})$	1567
Antisymmetric stretching $\nu_a(\text{C}=\text{C})$	1525
C=C/C-C motions	1432, 1414
Bending $\delta(\text{C}-\text{C})$	1336
Stretching of C-C bonds	1235, 1193
Internal bending vibrations $\delta(\text{C}-\text{H})$	1140, 1062
Relative motions among macro structures (e.g., thiophenes or cyano groups)	Below 750cm <sup>-1</sup>

### AZO-OH

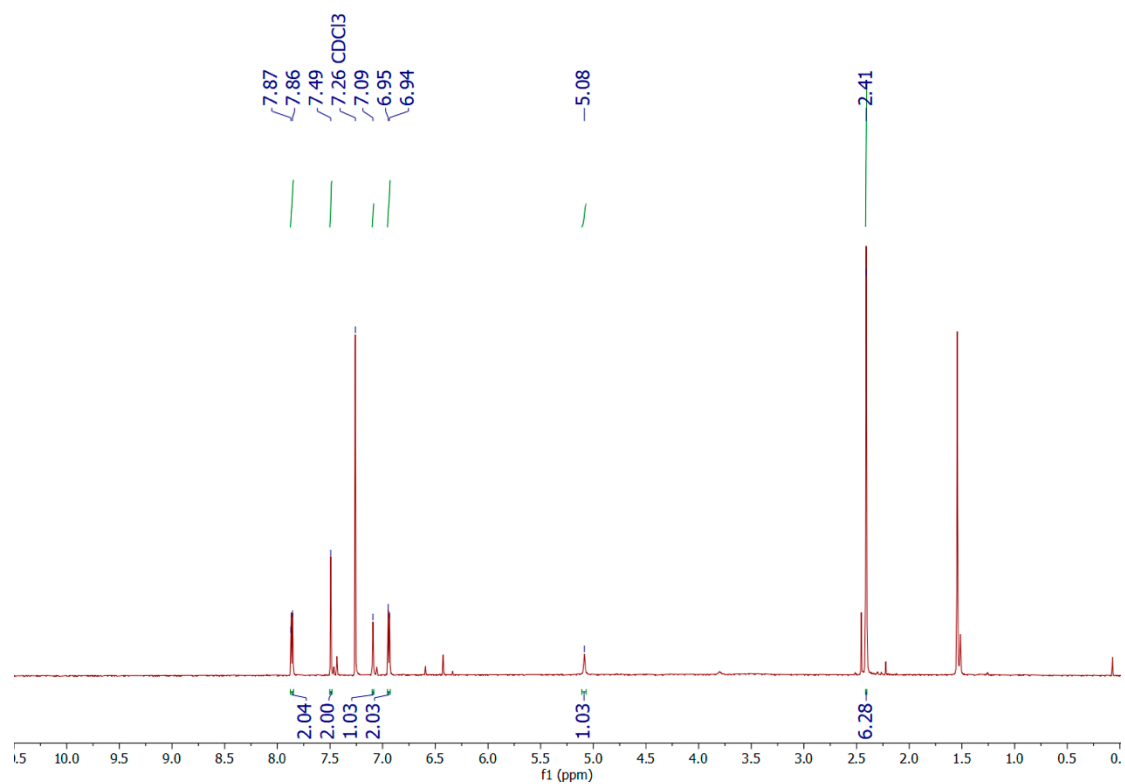
Vibrational Mode	Frequency (cm <sup>-1</sup> )
Symmetric stretching $\nu$ of the ring	1600, 1477, 1430
In-plane bending $\beta$ for rings' CH	1313, 1268, 1211
Symmetric stretching $\nu$ for CO	1286, 1133, 1026, 993
Symmetric stretching $\nu$ for vinylidene CC	1154
Typical vibration modes under for out-of-plane bending for CH (ring), CC, and CO bonds	Below 800 cm <sup>-1</sup>

### PcZnNH2

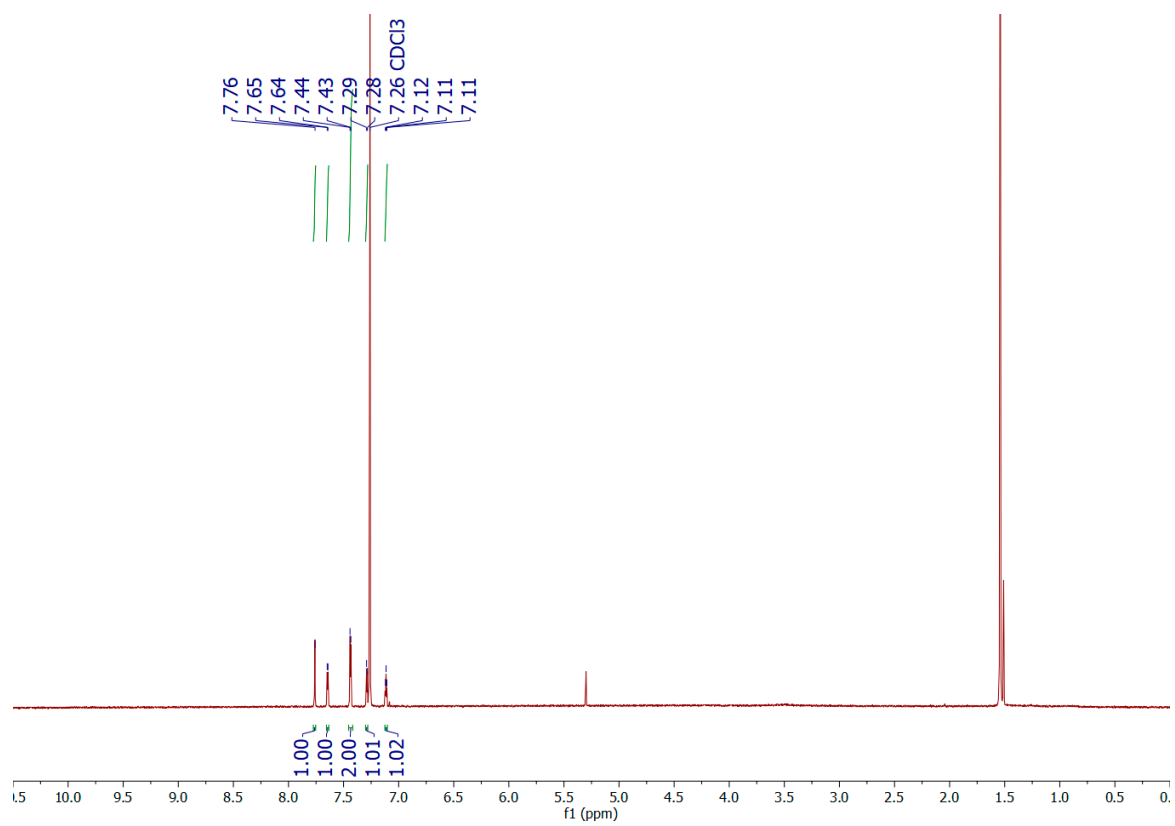
Vibrational Mode	Frequency (cm <sup>-1</sup> )
A <sub>1g</sub> modes	1413, 1317, 830, 687
E modes	1600, 1261, 1044, 781, 745
B <sub>2g</sub> modes	1603, 1115
Relative motions among macro structures	Below 600 cm <sup>-1</sup>

## S2. NMR Spectra

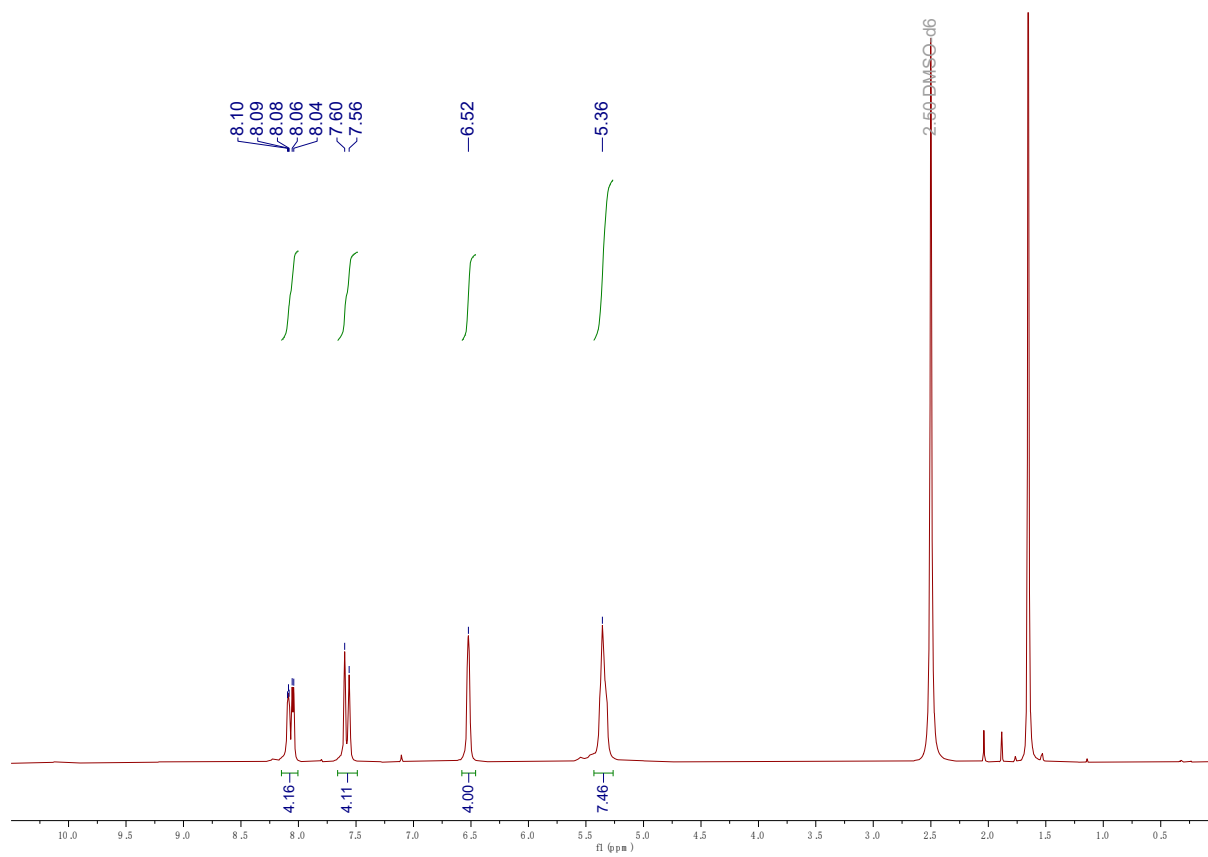
$^1\text{H}$  NMR Compound AZO-OH



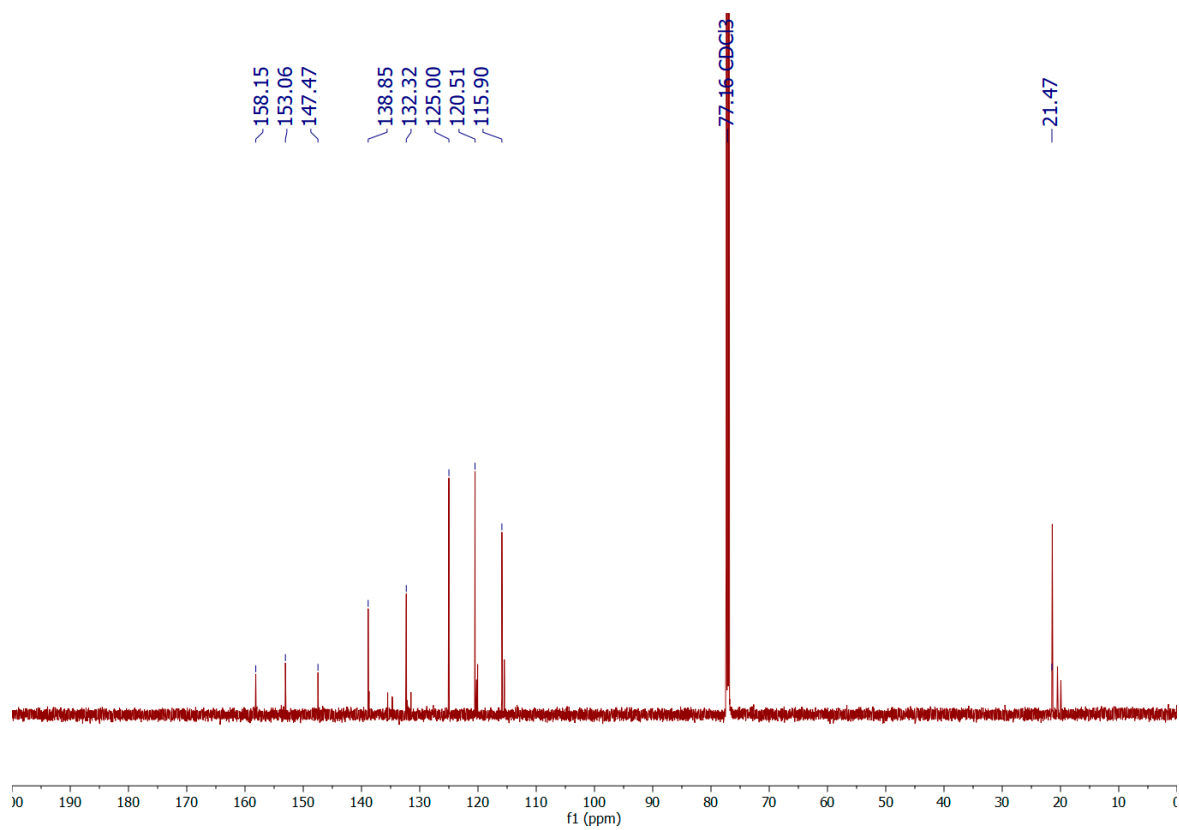
**<sup>1</sup>H NMR Compound DCVBT**



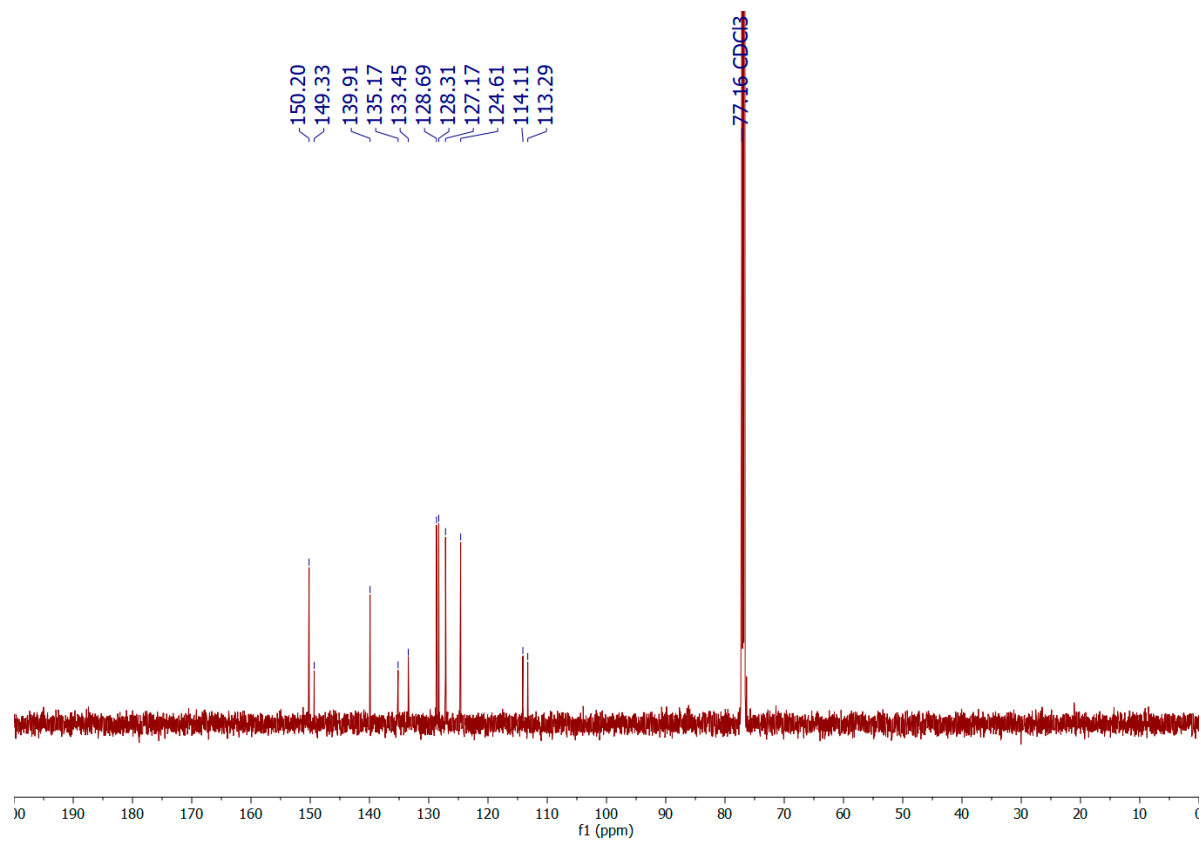
**$^1\text{H}$  NMR Compound  $\text{PcZnNH}_2$**



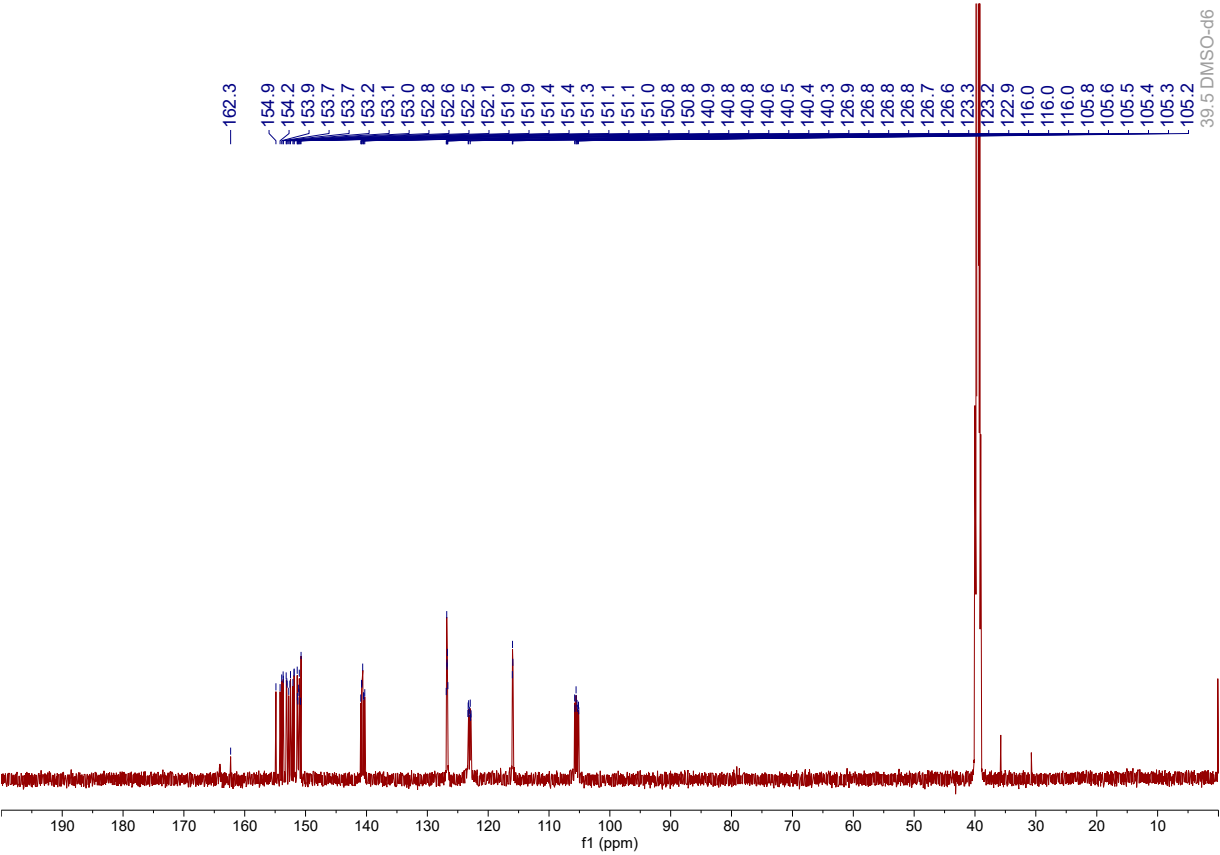
**$^{13}\text{C}$  NMR Compound AZO-OH**



**$^{13}\text{C}$  NMR Compound DCVBT**

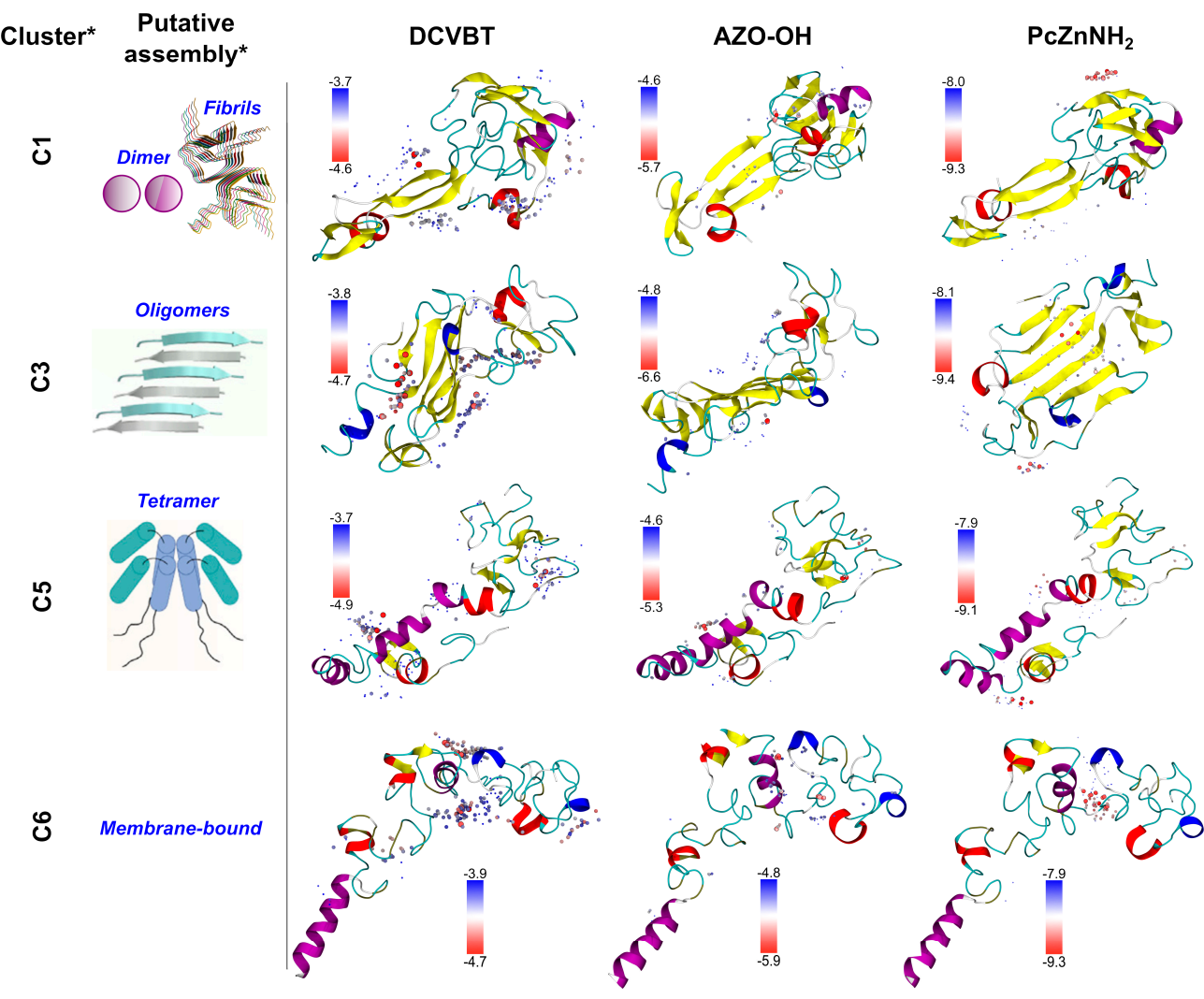


<sup>13</sup>C NMR Compound PcZnNH2

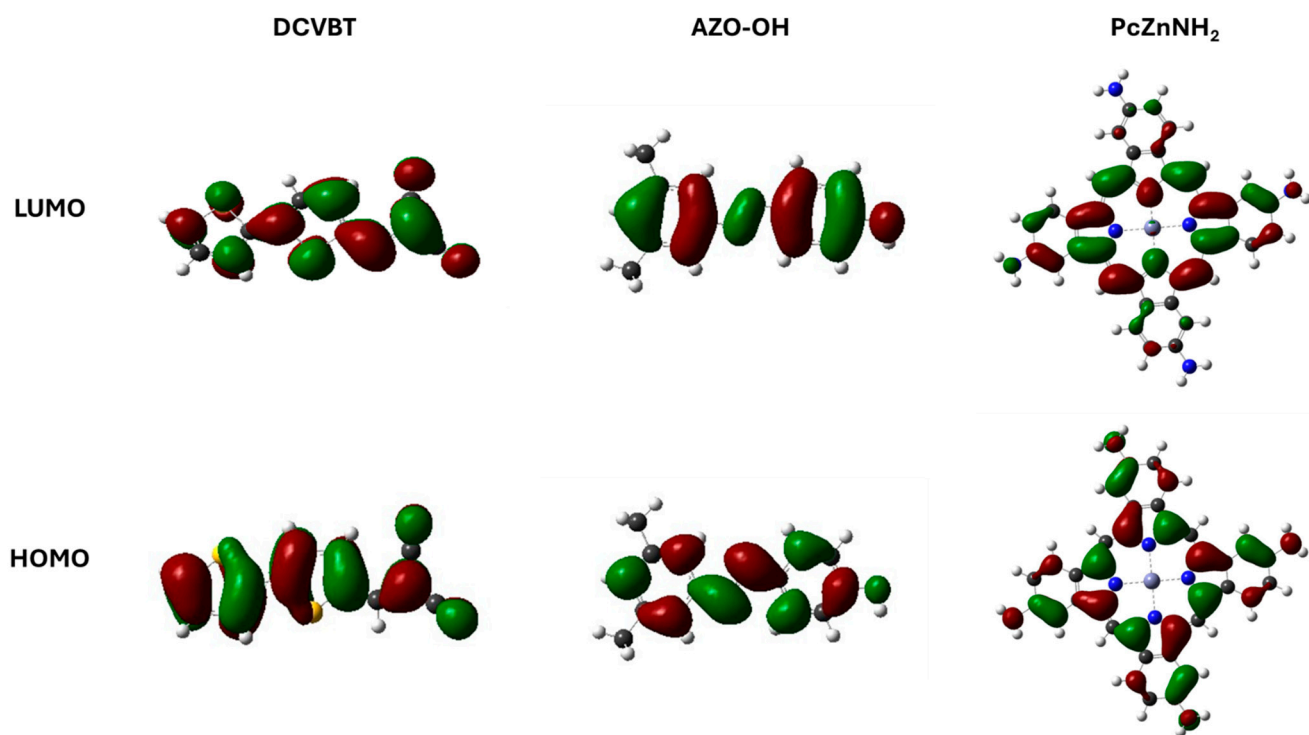




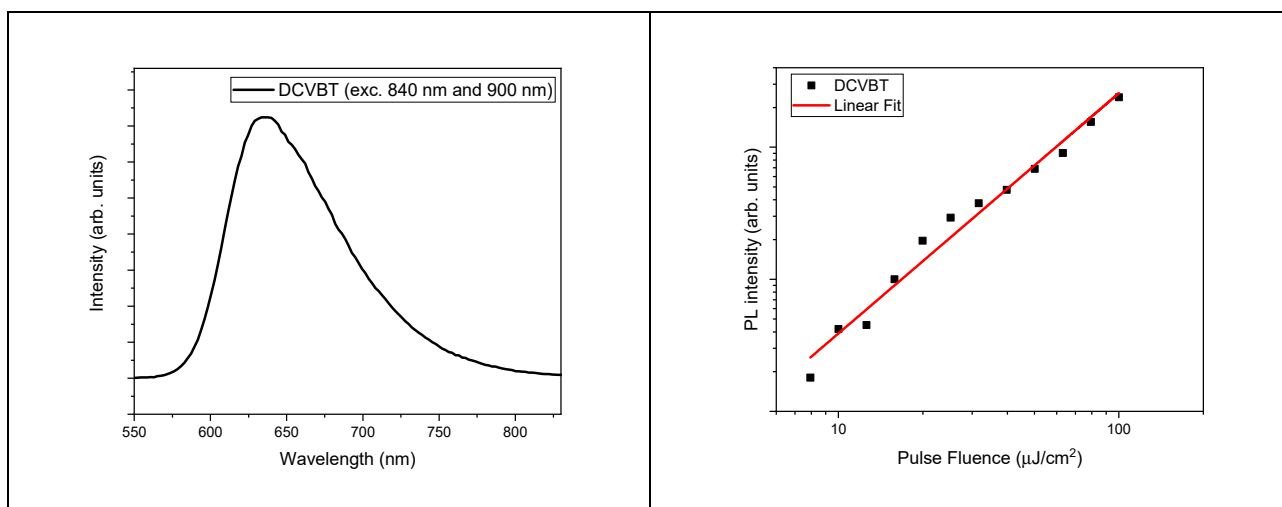
**S3. Distribution of docking poses of the three molecules investigated in this work on the surface of a-syn.** The centers of mass of each pose are shown as spheres of size and color proportional to the docking score (in kcal/mol in the color bars accompanying each picture). The protein is shown using the cartoon representation and colored by secondary structure.[1]



S4. HOMO-LUMO orbitals for DCVBT, AZO-OH, PcZnNH<sub>2</sub>. The isocontour value is 0.02 au.



## S5. Two-Photon emission of DCVBT under excitation at 840 nm and 900 nm



## References

- [1] J. Chen, S. Zaer, P. Drori, J. Zamel, K. Joron, N. Kalisman, E. Lerner, N. V. Dokholyan, Structure 29 (2021) 1048-1064.e6.