Supplementary informations

Breaking azacalix[4]arenes into induline derivatives

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1. NMR spectra

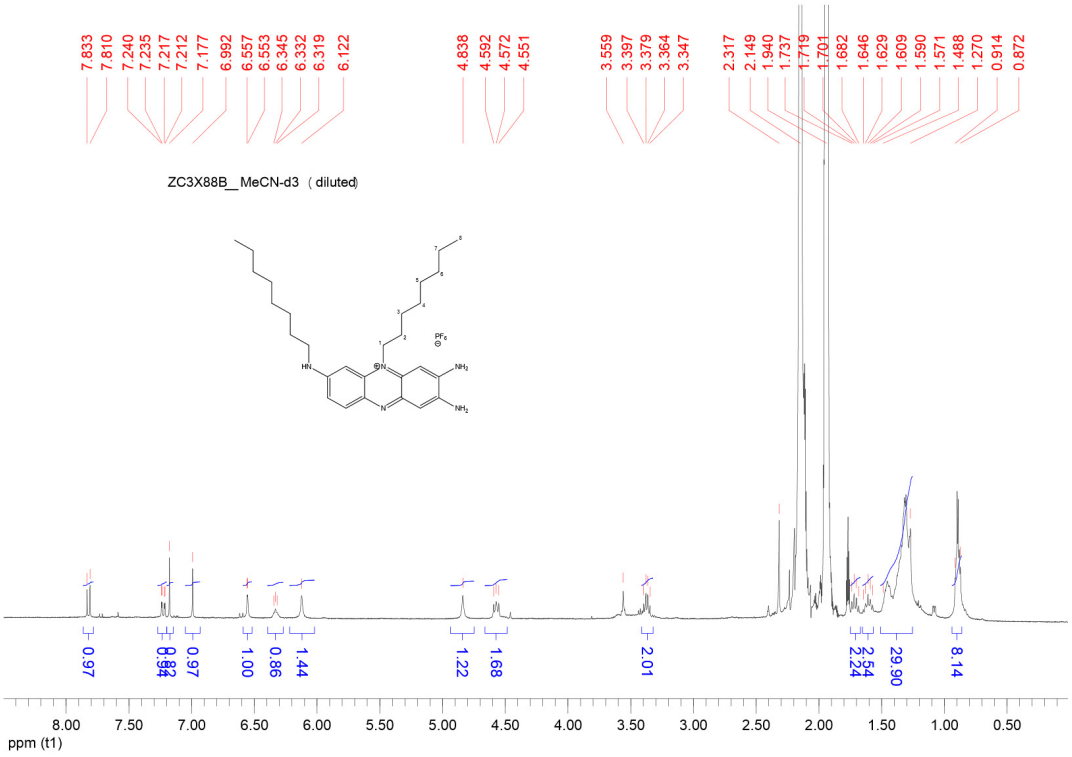


Figure S1. ^{1}H NMR spectrum of **8** in CD_3CN

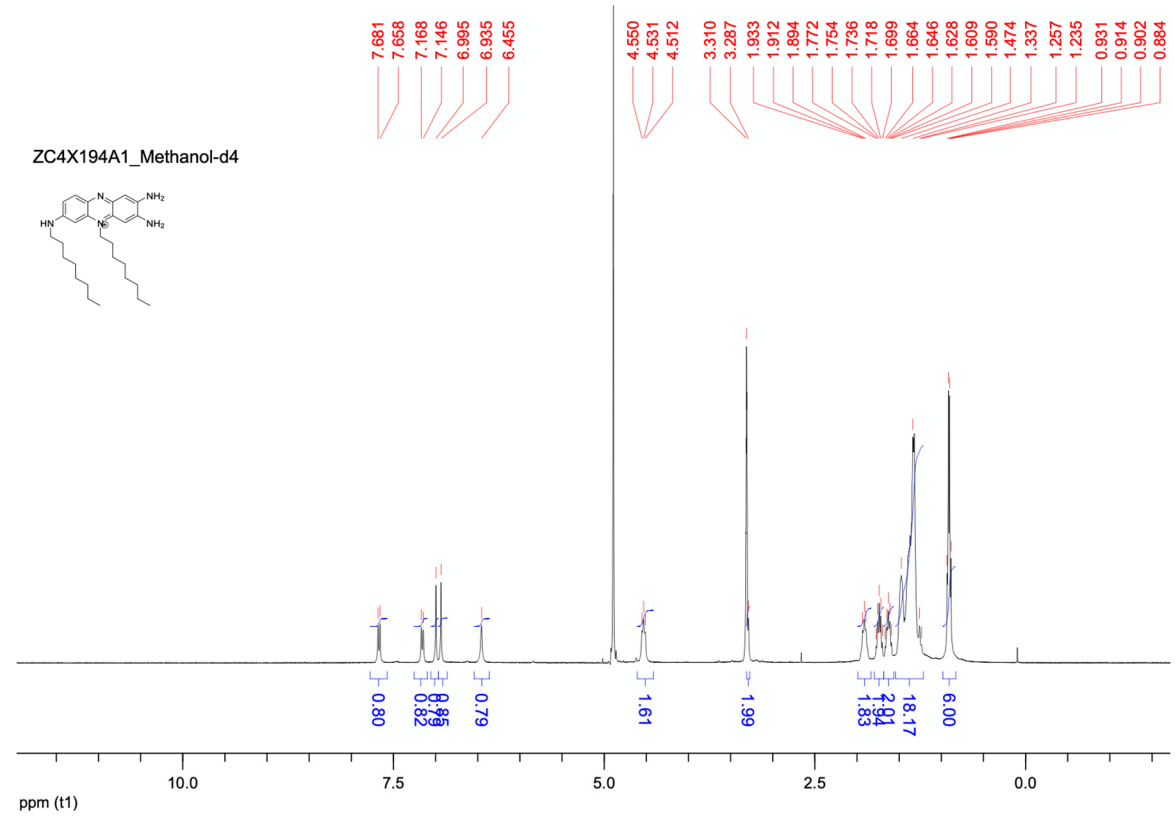


Figure S2. ^{1}H NMR spectrum of **8** in MeOD

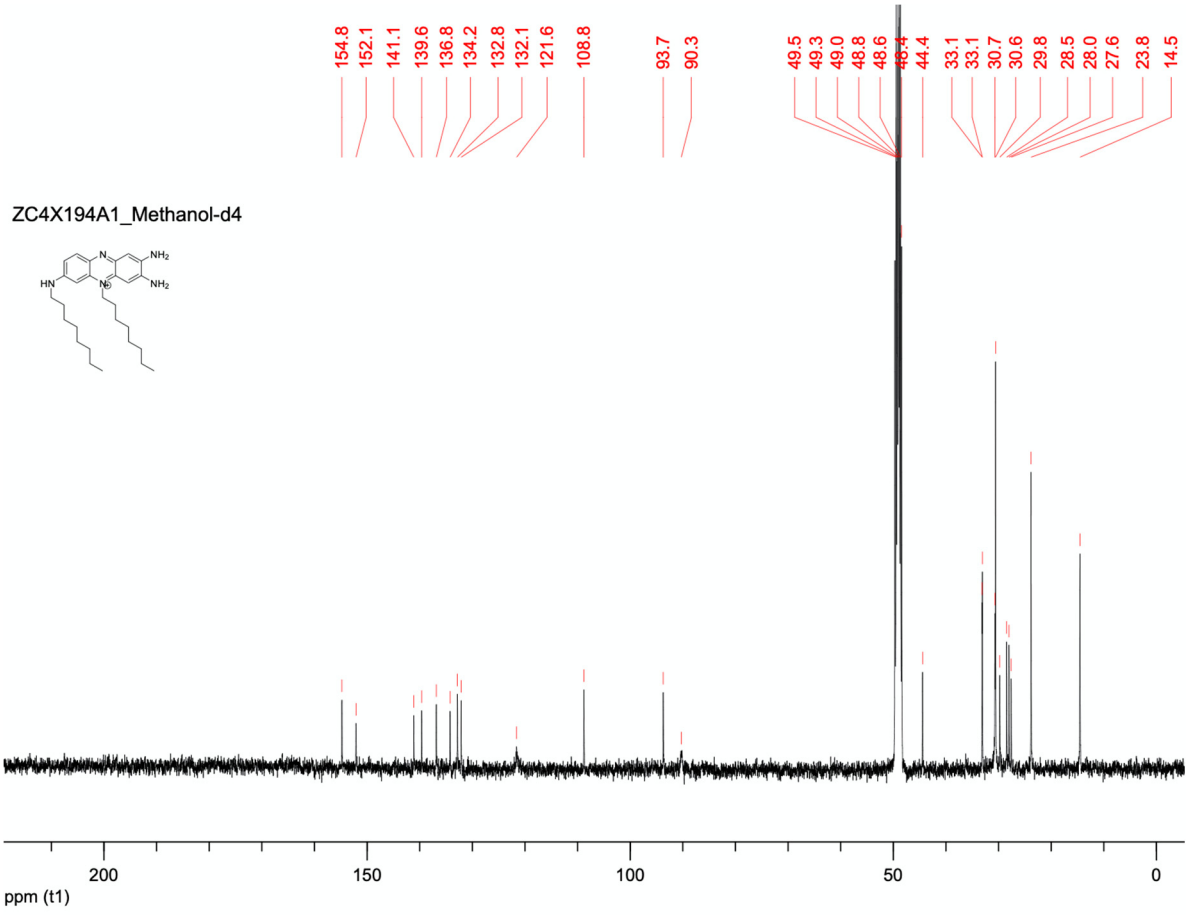


Figure S3. ^{13}C NMR spectrum of **8** in MeOD

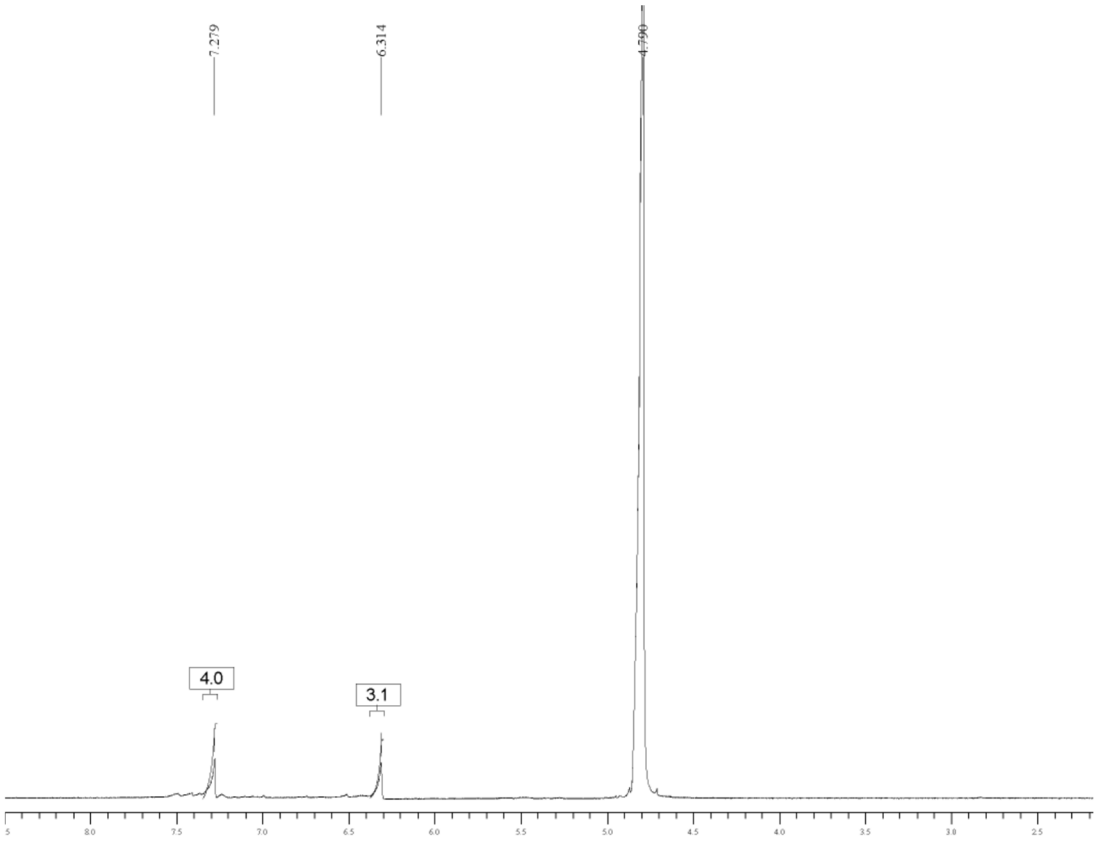


Figure S4. ^{1}H spectrum of **12**•nHCl in D_2O

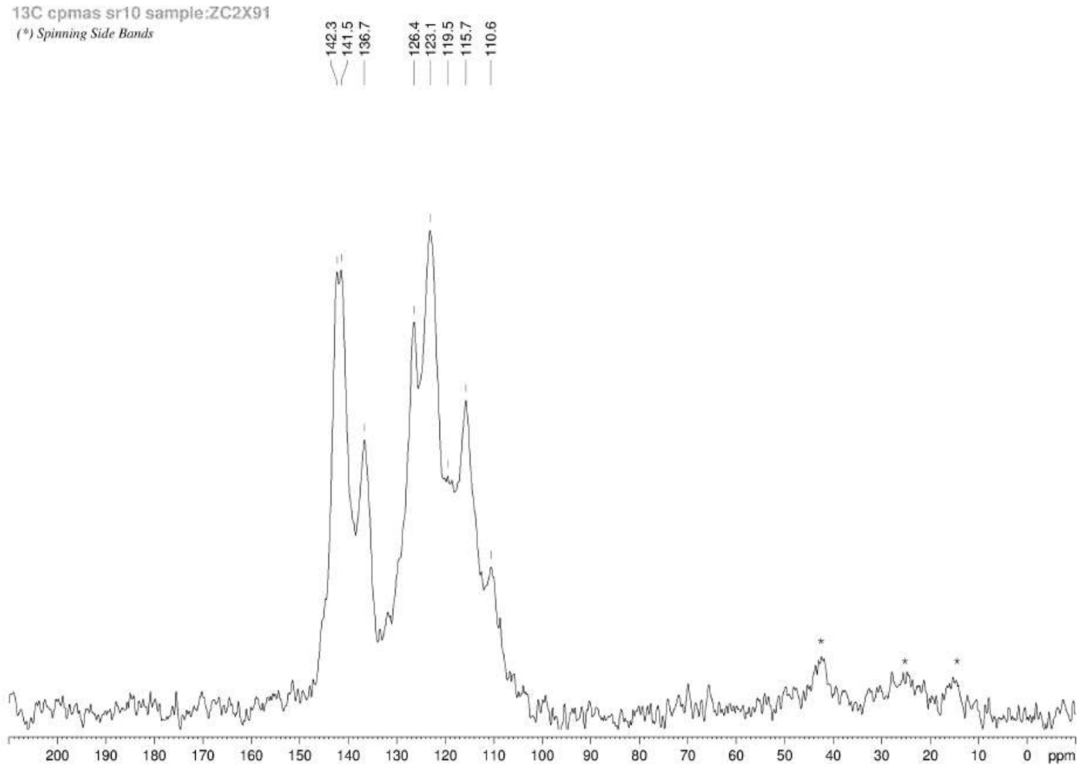


Figure S5. solid state ^{13}C NMR spectrum of **12**•nHCl

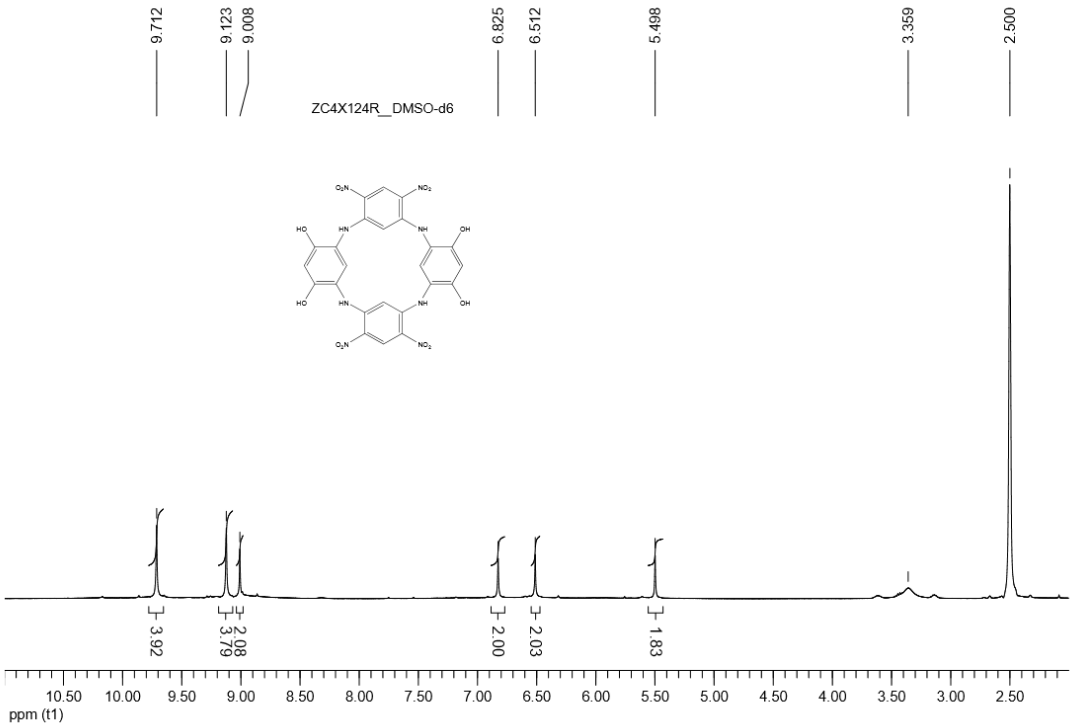


Figure S6. ^{1}H NMR spectrum of **15** in DMSO

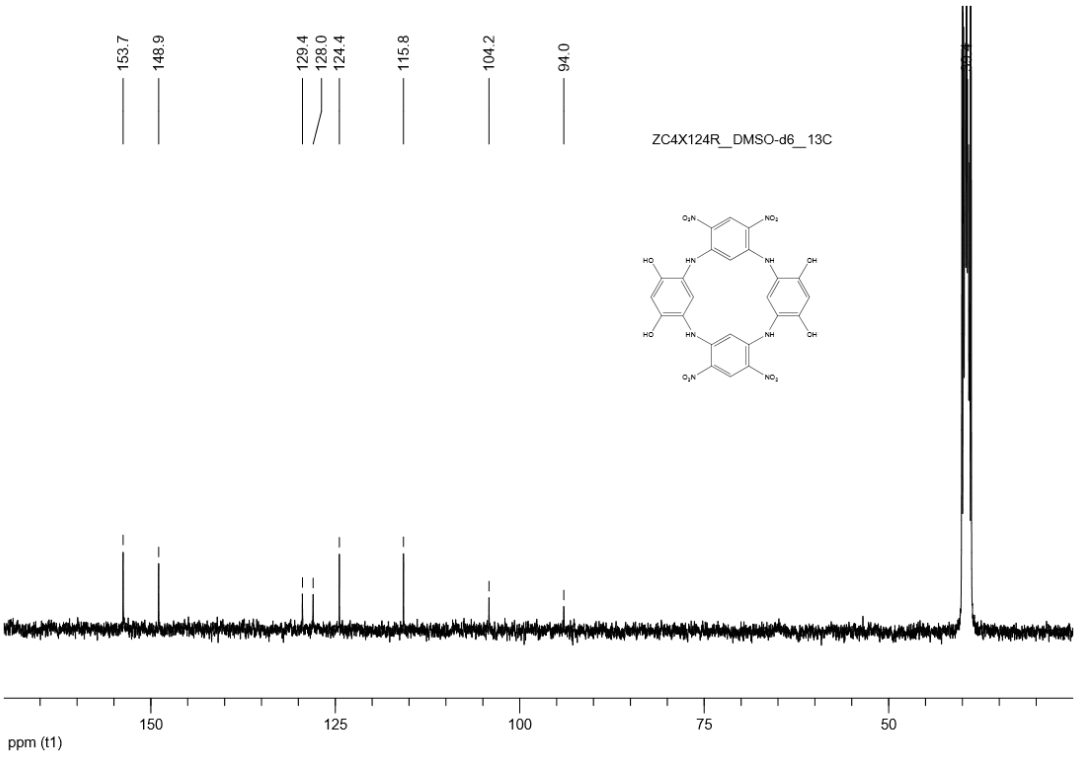


Figure S7. ^{13}C NMR spectrum of **15** in DMSO

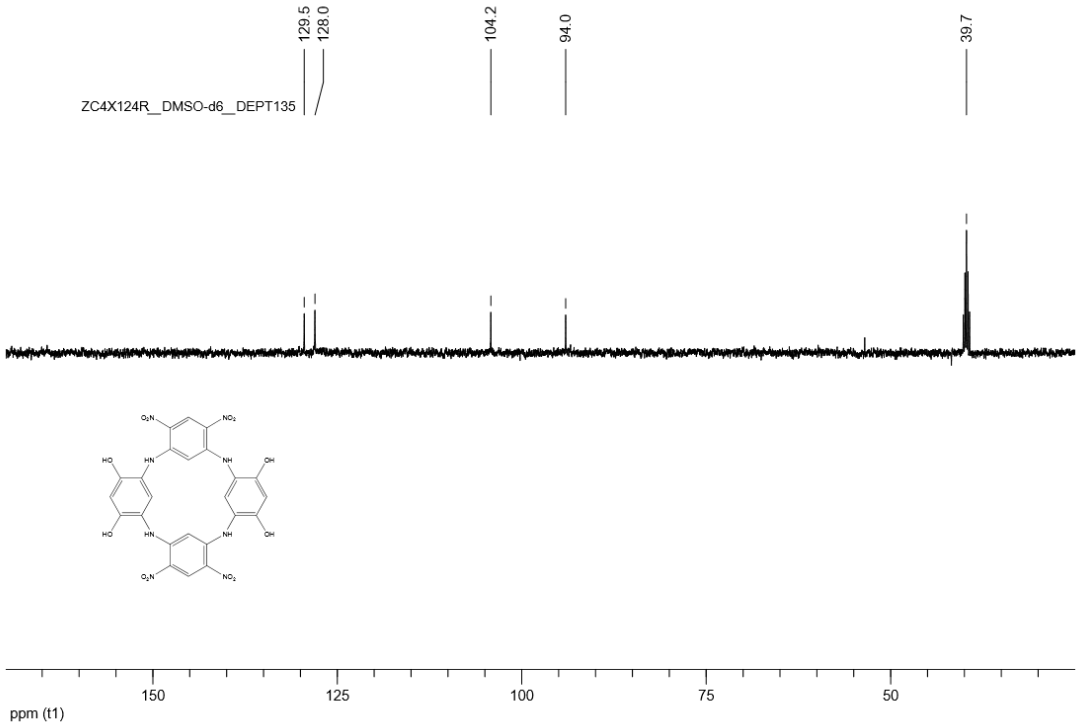


Figure S8. ^{13}C NMR spectrum of **15** (DEPT) in DMSO

2. X-ray Structure of molecule **15**

Alert level B in checkcif:

Alert level B

```
          Crystal system given = triclinic
PLAT430_ALERT_2_B Short Inter D...A Contact  S1B
O10      ..       2.82 Ang.
```

Comment on this alert:

If we look at the structure by extending the molecule a little towards its neighbors, we see that the NO_2 bearing the oxygen O(10) is the only one of the 4 out of the plane.

What's more, the DMSO involved in the interaction defined as short by the check-cif is disordered on 2 sites, with the S(1B) sulfur on one of the two sites interacting with O(10) on this NO_2. The two observations combined show quite clearly that there is a particular interaction at this level.

Hence the short distance observed by the check-cif.

3. SEM analysis

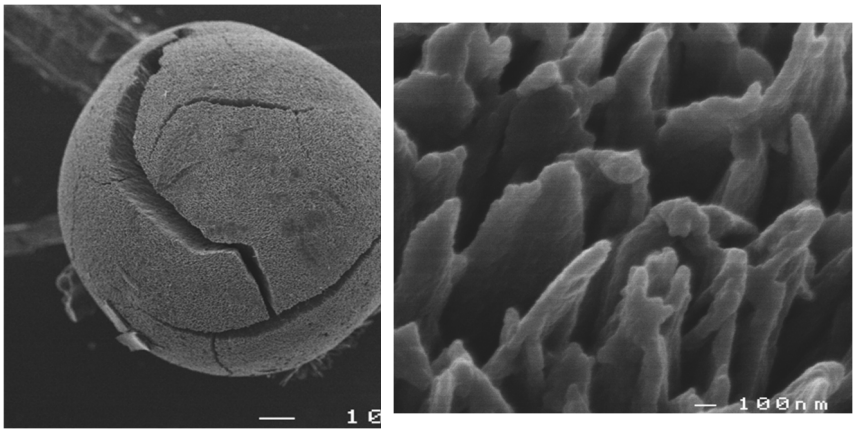


Figure S9. SEM images of **12**•nHCl-aggregates.