

## **Supplementary information**

**First structural characterization of core modified 10,15-meso aryl azuliporphyrins: observation of C-H--- $\pi$  interaction between pyrrole  $\beta$ -CH and mesityl ring**

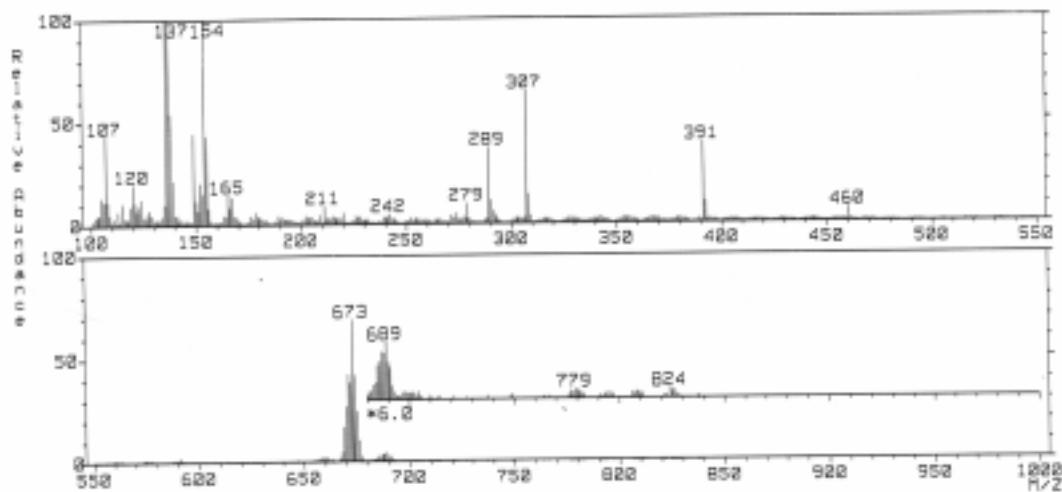
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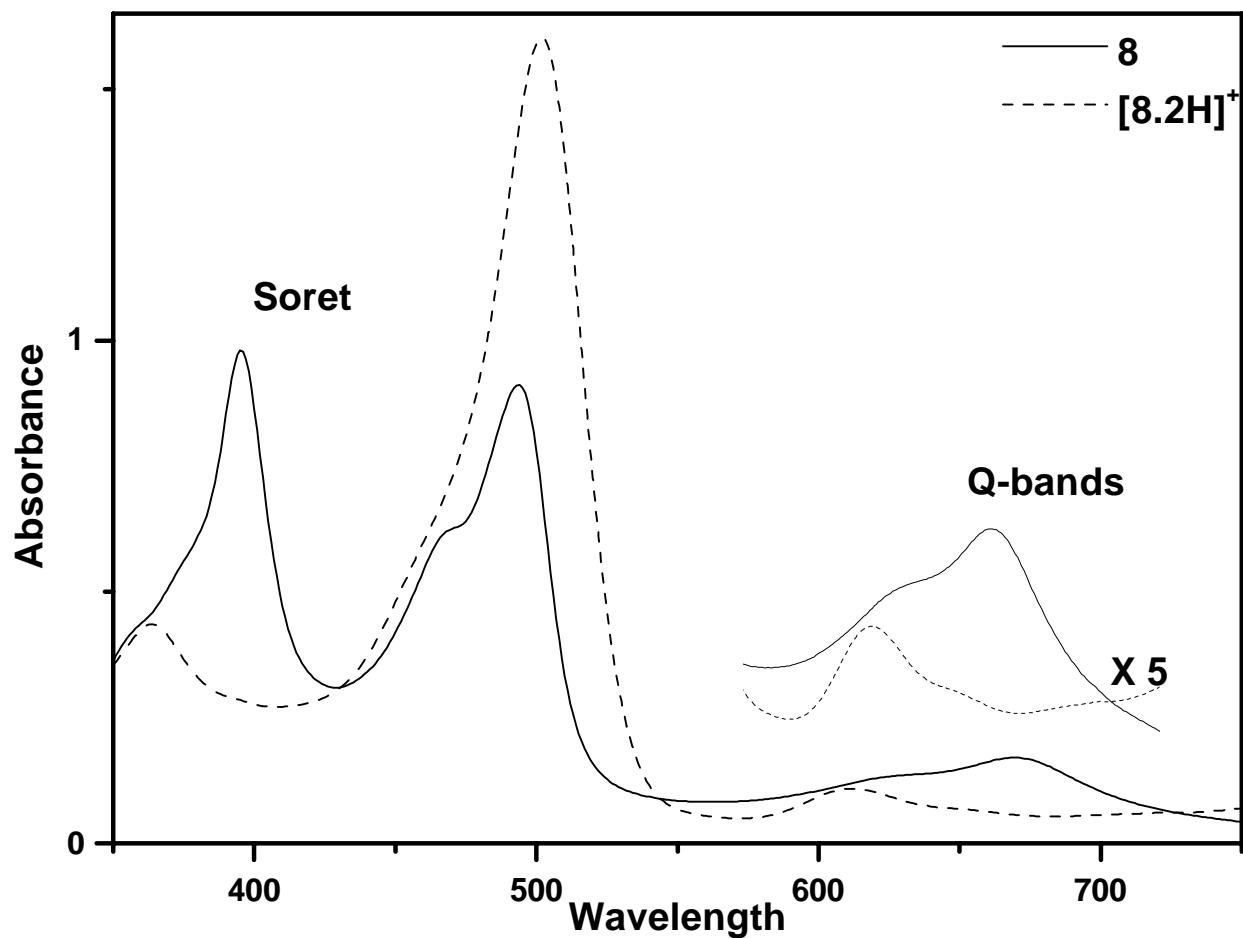
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MASS SPECTRUM Data File: ZIMY13T  
Instrument: FAB(Positive) Date: 9-JUN-1998  
Run Time: 1.40 min BP: m/z 137.0000 Int. 95.4163 Lv 0.00  
Scan# (1)



FAB mass m/z (%): 673 [M+1]

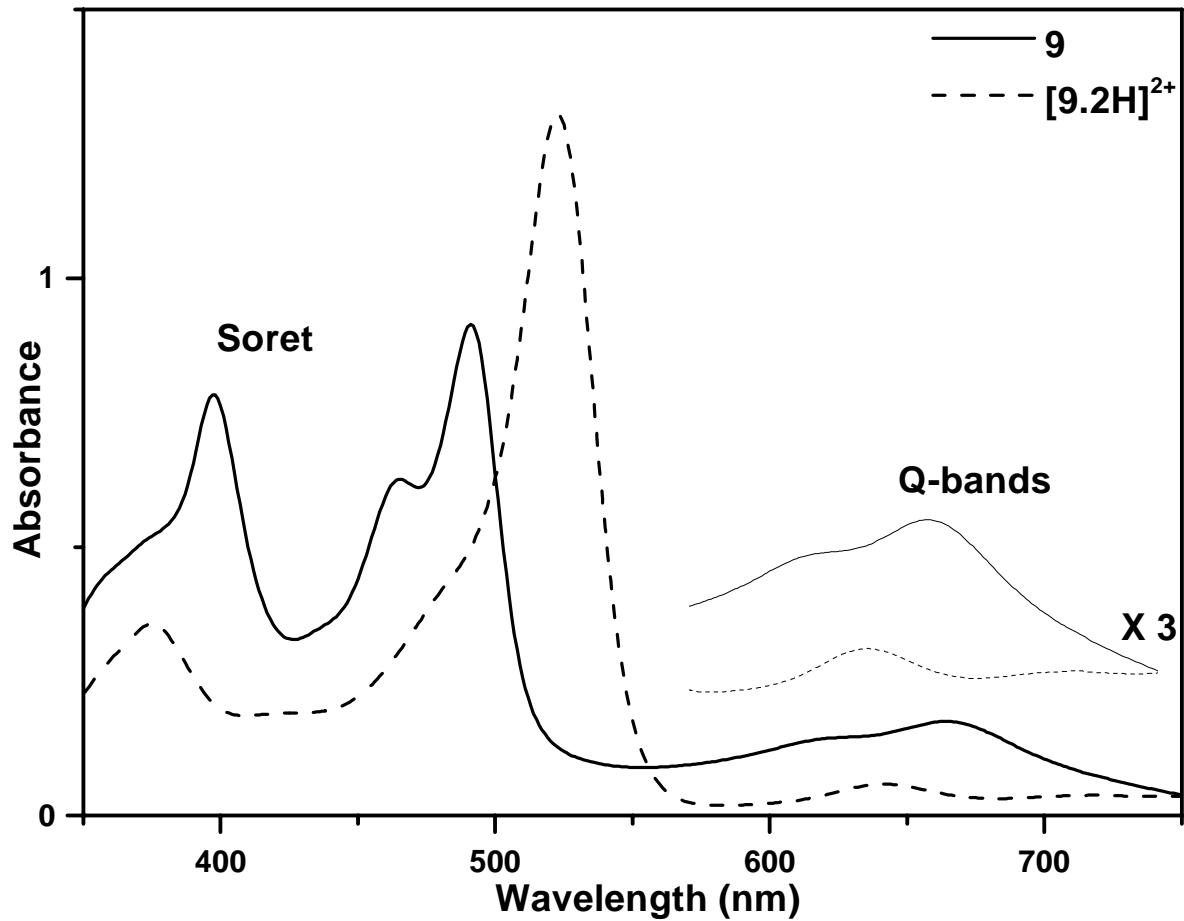
S 1: FAB Mass spectra for **9**



Free base **[8]**: ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  nm ( $\log \epsilon$ ) = 395 (4.99), 477 (sh) (4.7), 494 (4.95), 670 (4.20)

Protonated **[8.2H]<sup>+</sup>** : (5% TFA/  $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  nm ( $\log \epsilon$ ) = 364 (4.6), 502 (5.2), 612 (4.0)

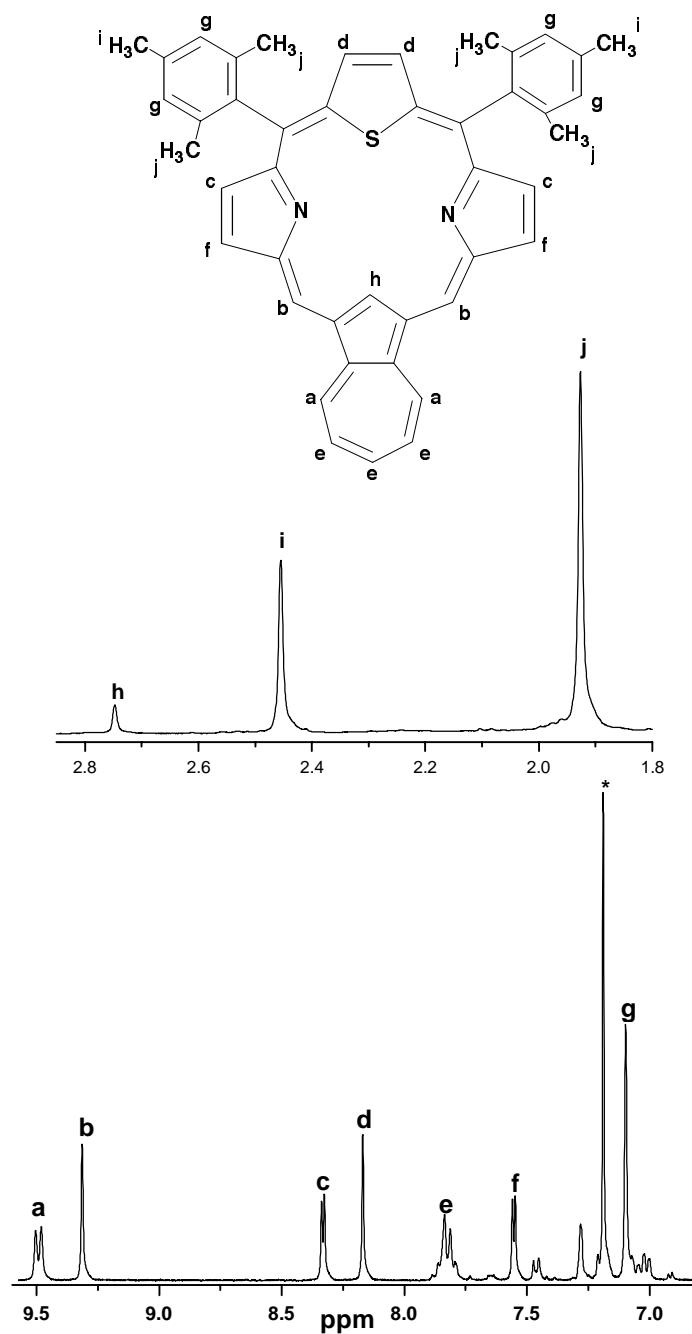
**S2:** Electronic absorption spectra for **8**



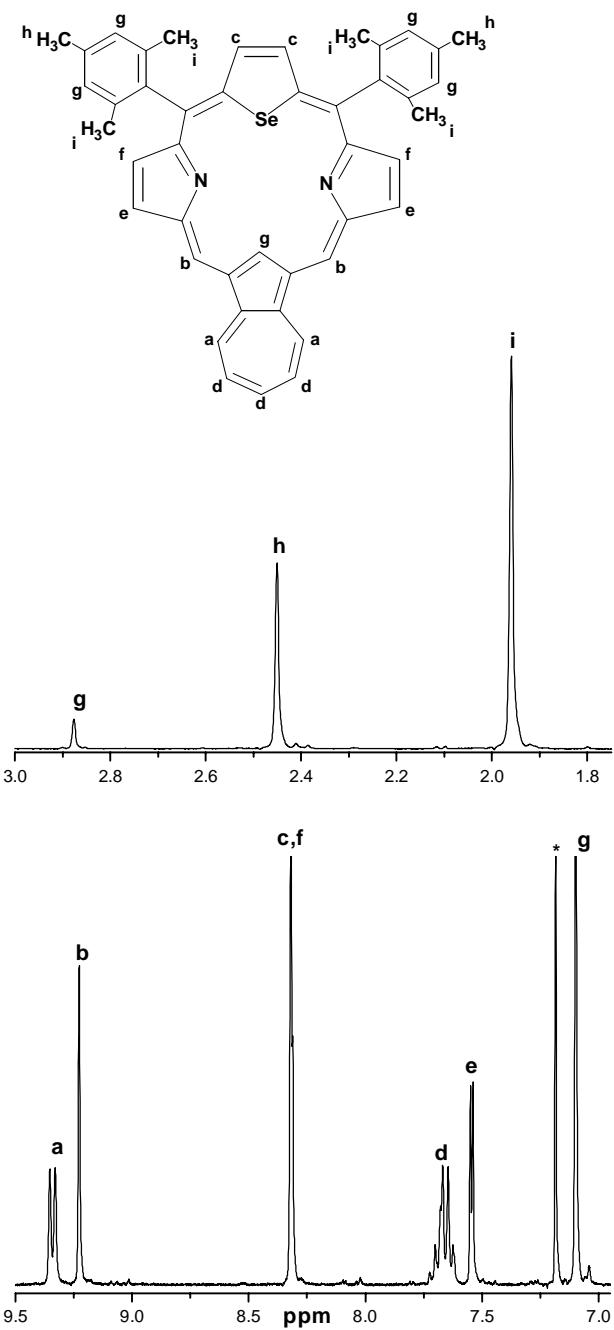
Free base **[9]**: ( $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  nm ( $\log \epsilon$ ) = 397 (4.8), 465 (sh) (4.7), 492 (4.9), 664 (4.2)

Protonated **[9.2H]<sup>+</sup>**: (5% TFA/  $\text{CH}_2\text{Cl}_2$ ):  $\lambda_{\max}$  nm ( $\log \epsilon$ ) = 375 (4.5), 523 (4.11), 642 (3.7)

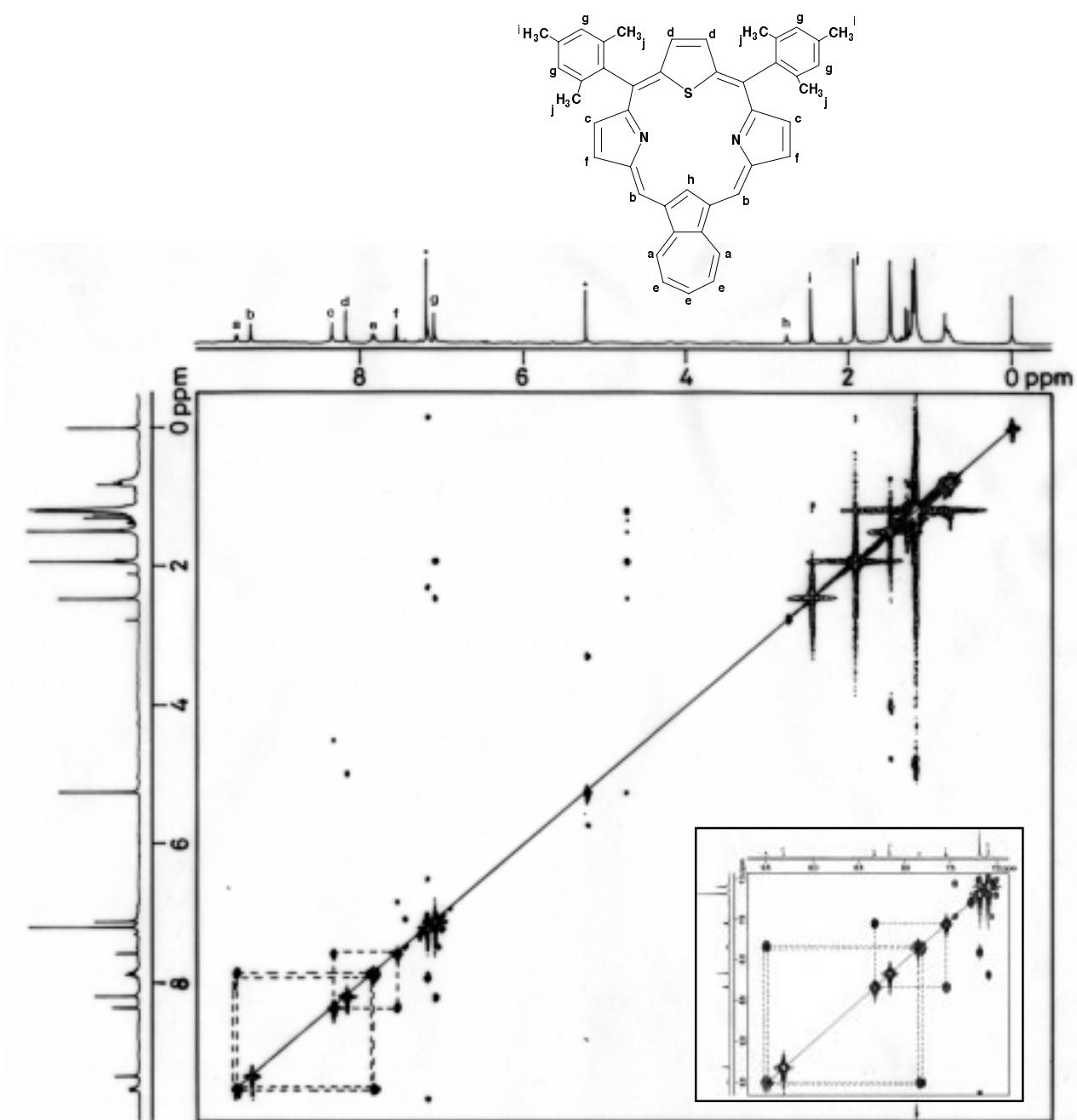
**S3:** Electronic absorption spectra for **9**



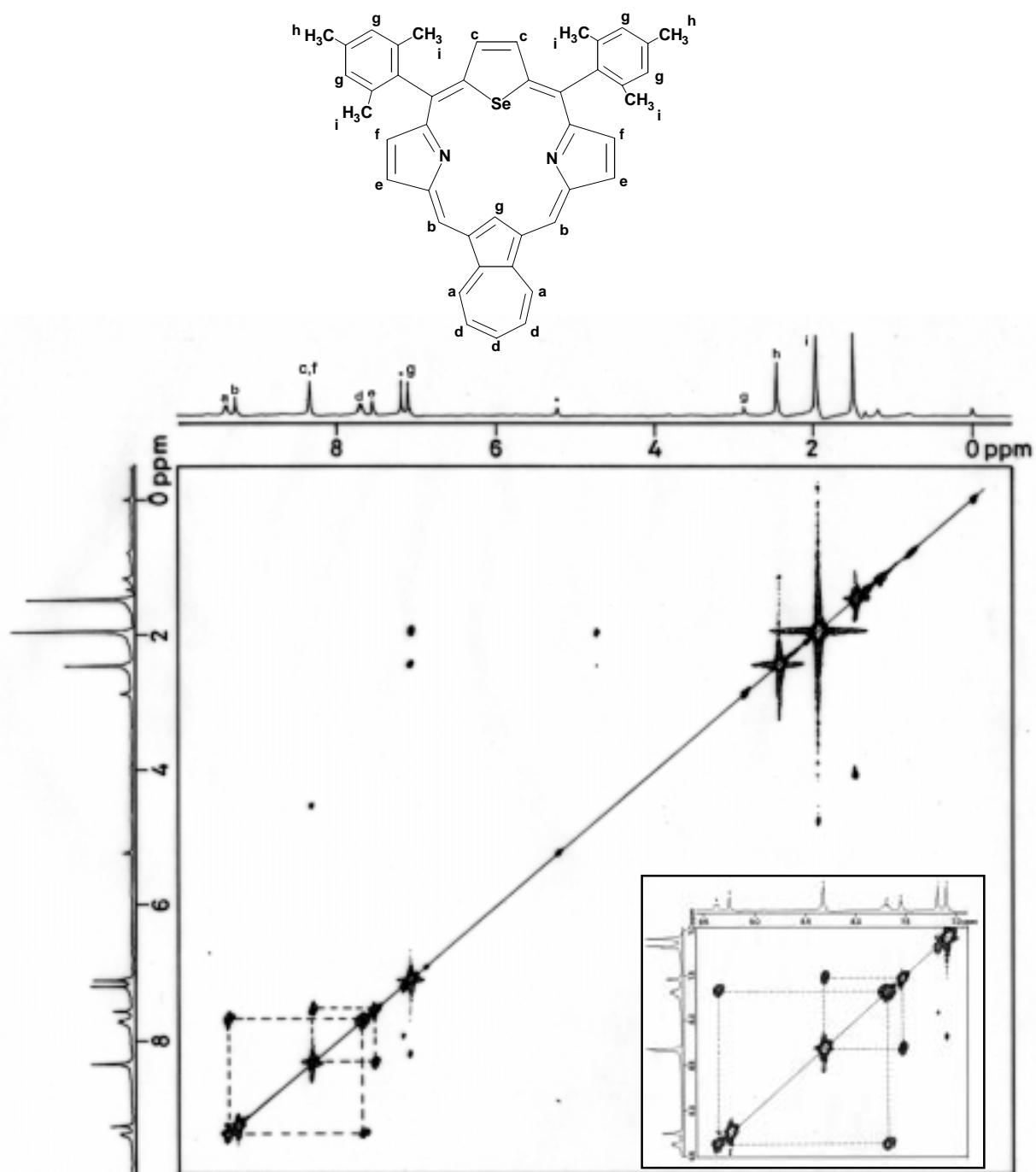
**S4:** <sup>1</sup>H NMR spectra of **8** in CDCl<sub>3</sub>. The assignments are marked



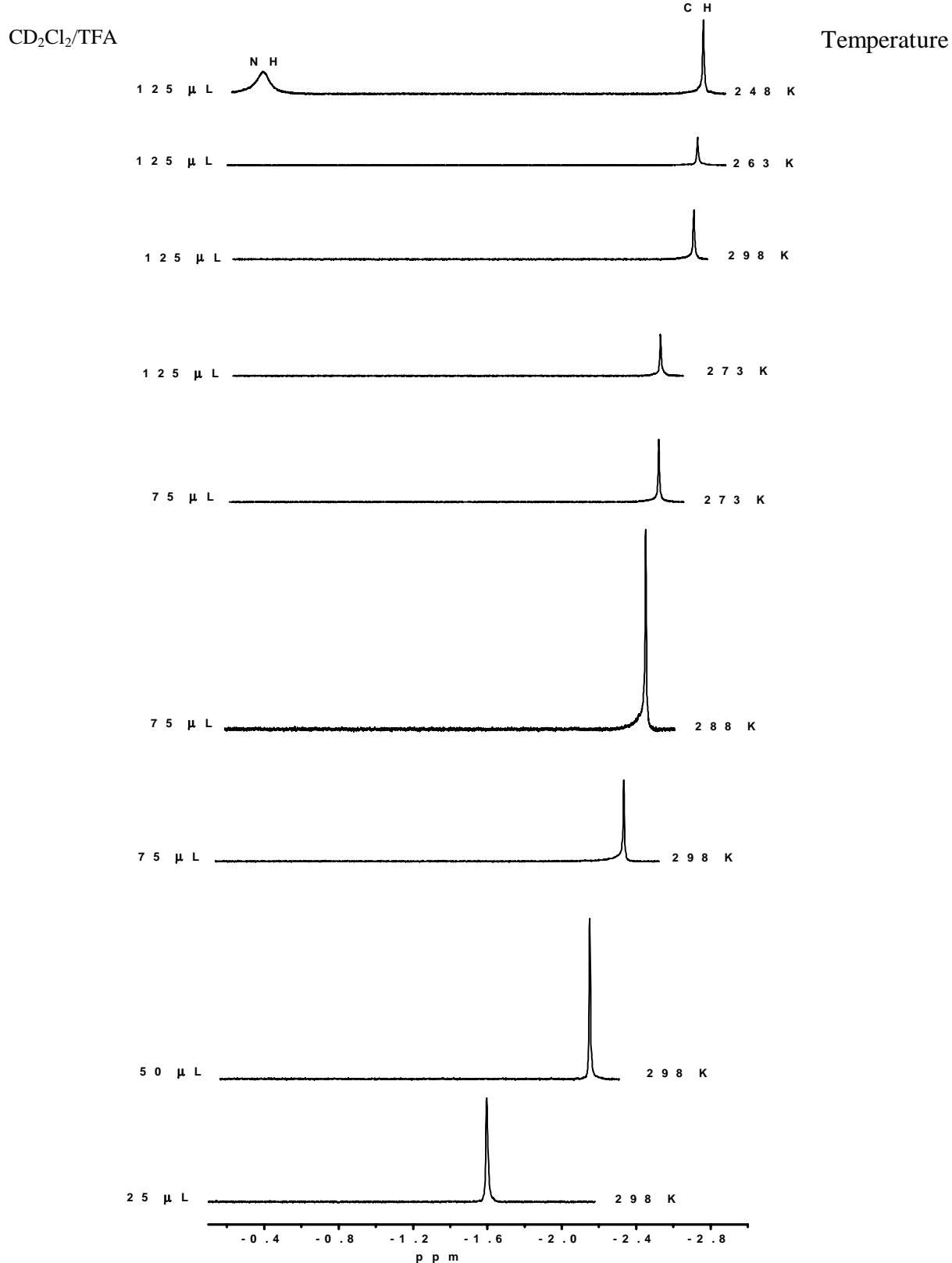
S5: <sup>1</sup>H NMR spectra of **9** in CDCl<sub>3</sub>. The assignments are marked



**S6:** 2D COSY NMR spectra of **8**: observed correlations are marked



**S7:** 2D COSY NMR spectra of **9**: observed correlations are marked



**S8:** Dependence of chemical shift of azulene inner CH proton on the concentration of TFA and the temperature. From a stock solution of 10% v/v TFA in CD<sub>2</sub>Cl<sub>2</sub>, the titrations were carried out using indicated amount of this solution. The protonated pyrrole proton (NH) is also shown.