

Supporting Information

1,3-Bis(pyren-1-yl)imidazolium chloride (IPyr·HCl)

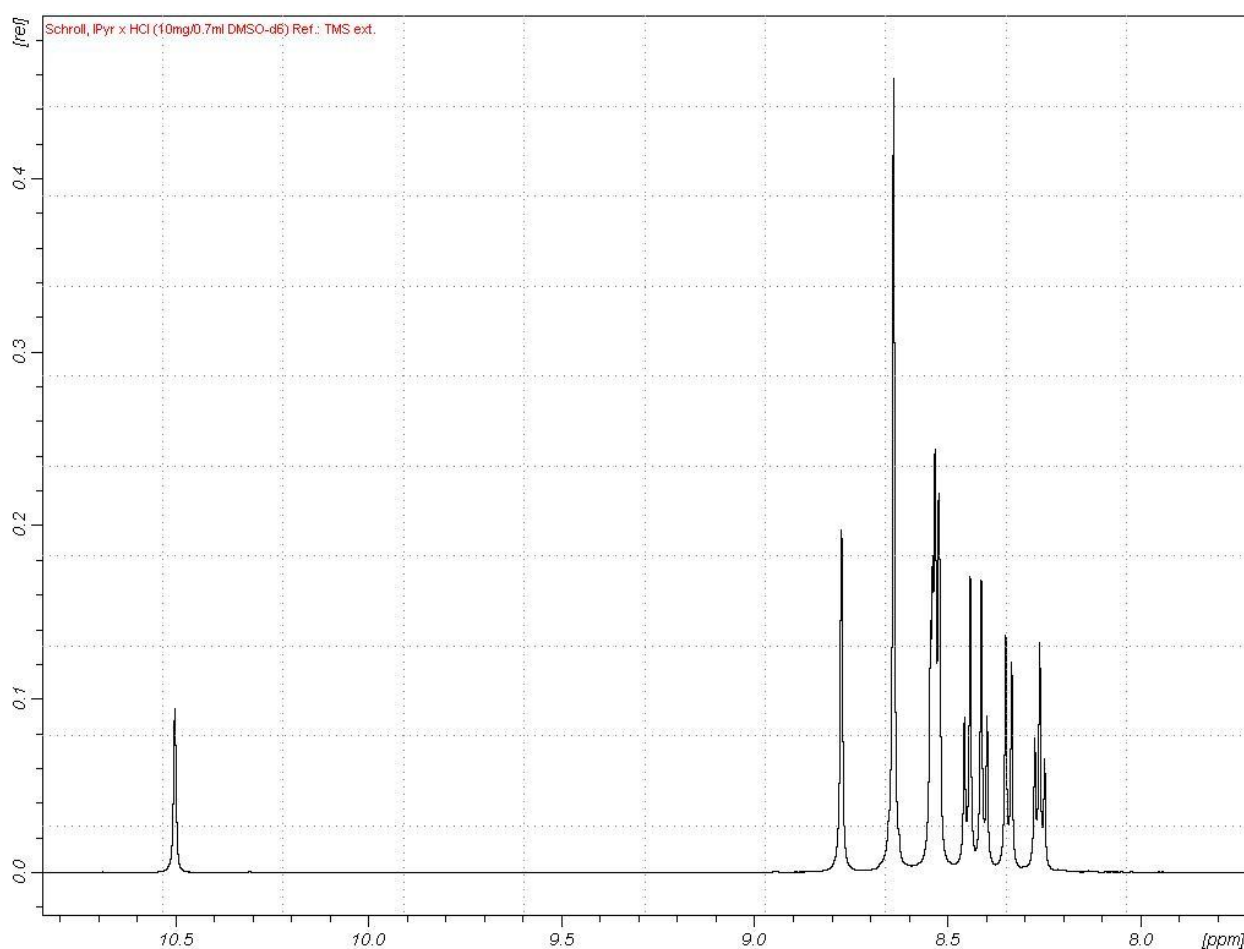
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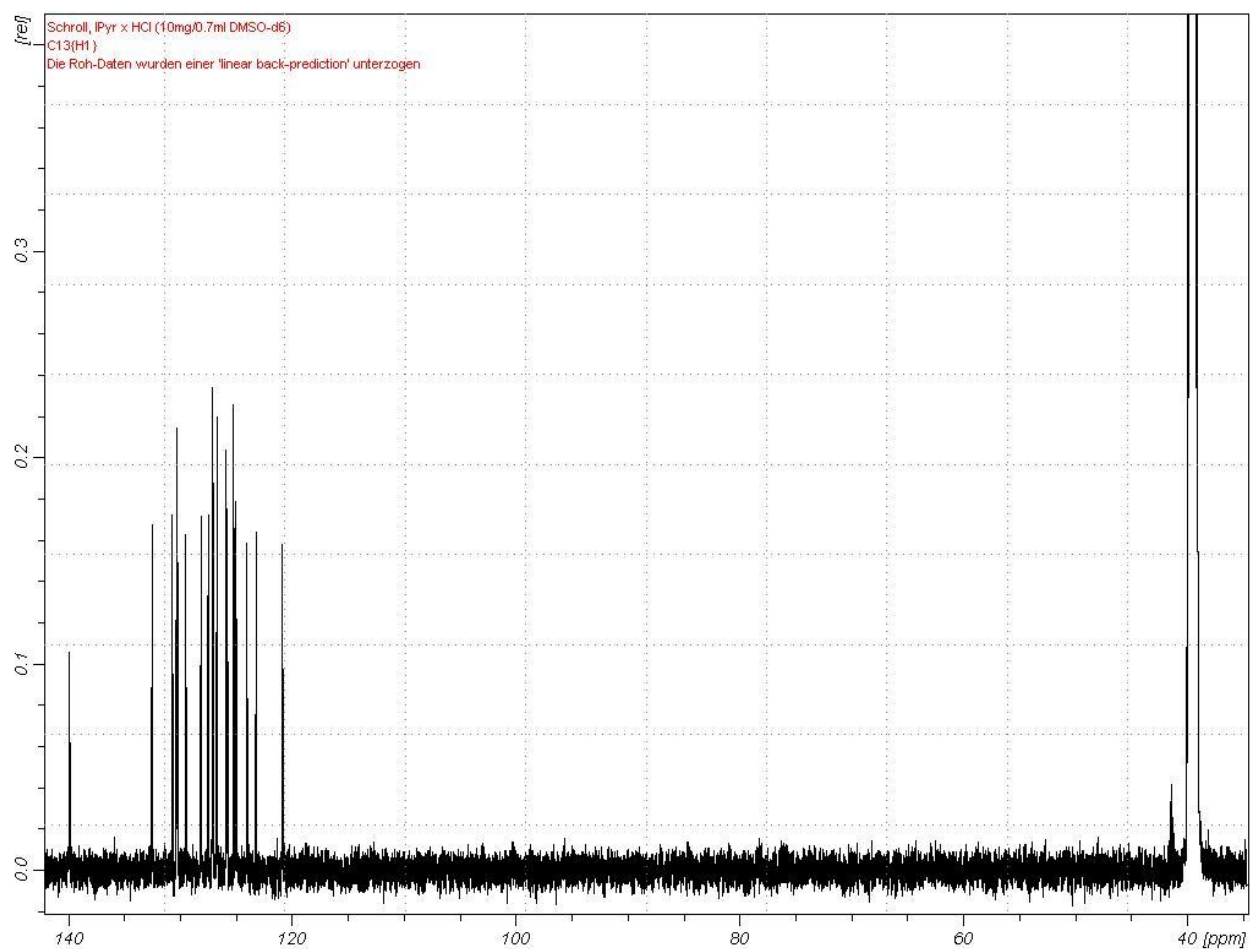
Burkhard.Koenig@chemie.uni-regensburg.de

Spectroscopic data of the title compound is reported for ^1H -NMR, ^{13}C -NMR, 2D-NMR experiments and for UV-spectra.

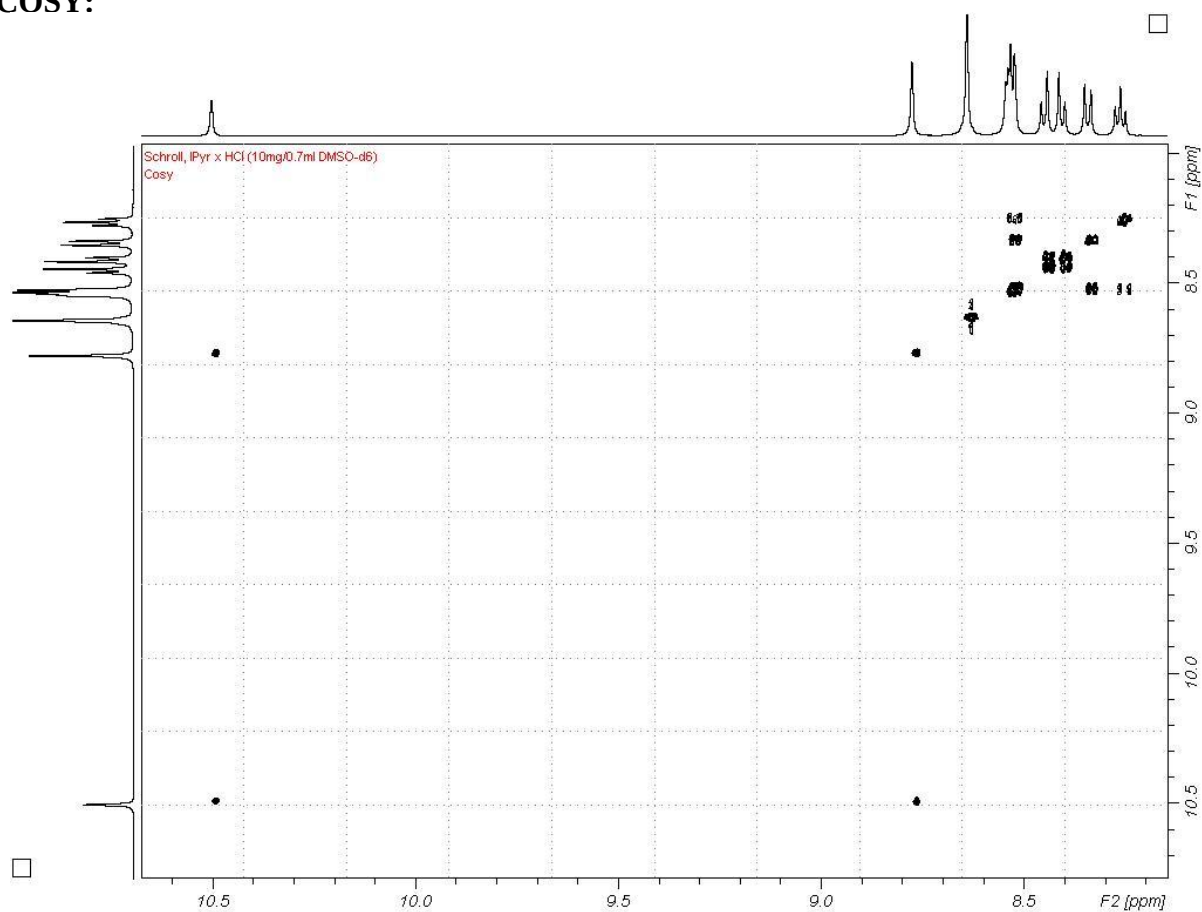
^1H -NMR (600 MHz, DMSO- d_6):



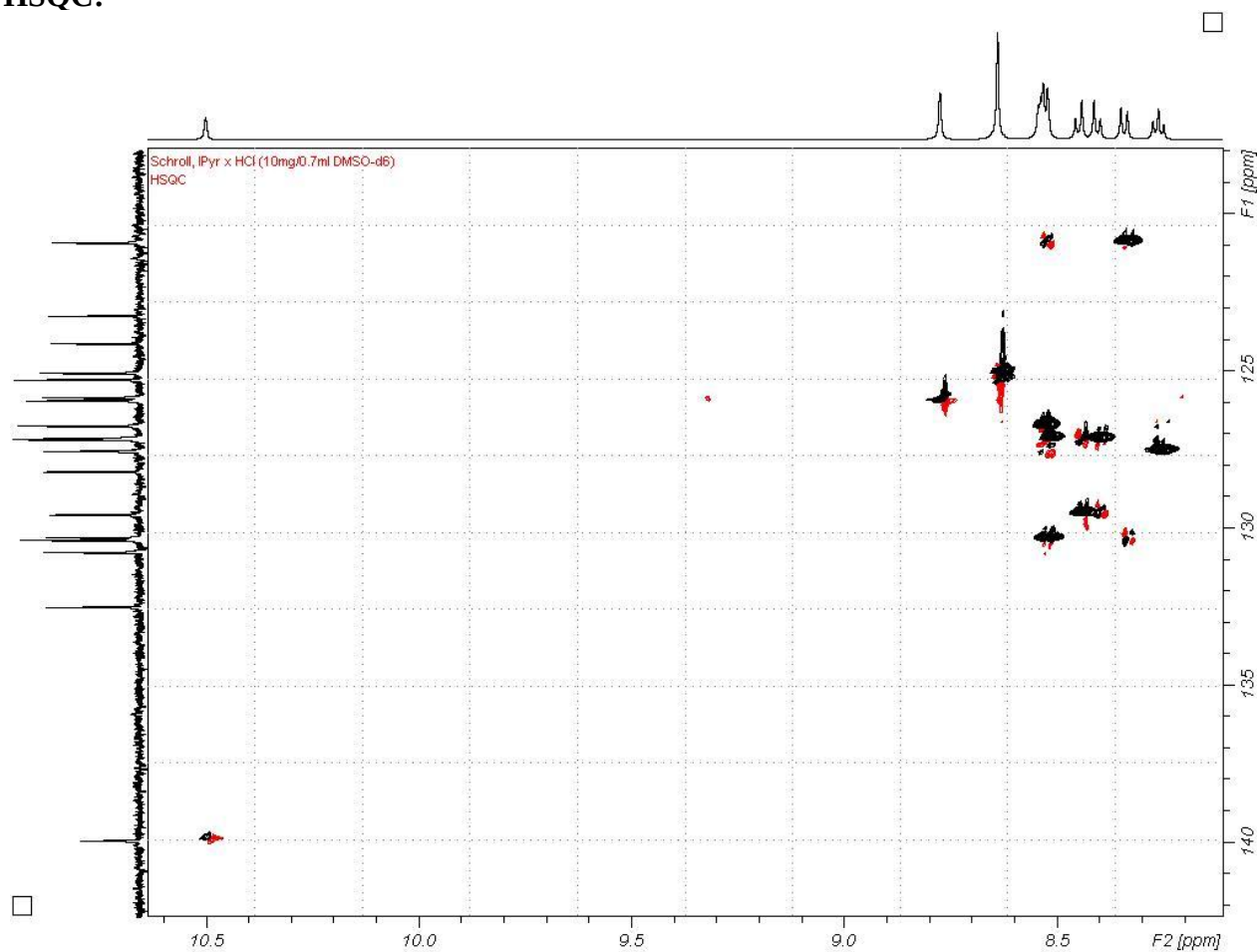
^{13}C -NMR (150 MHz, DMSO- d_6):



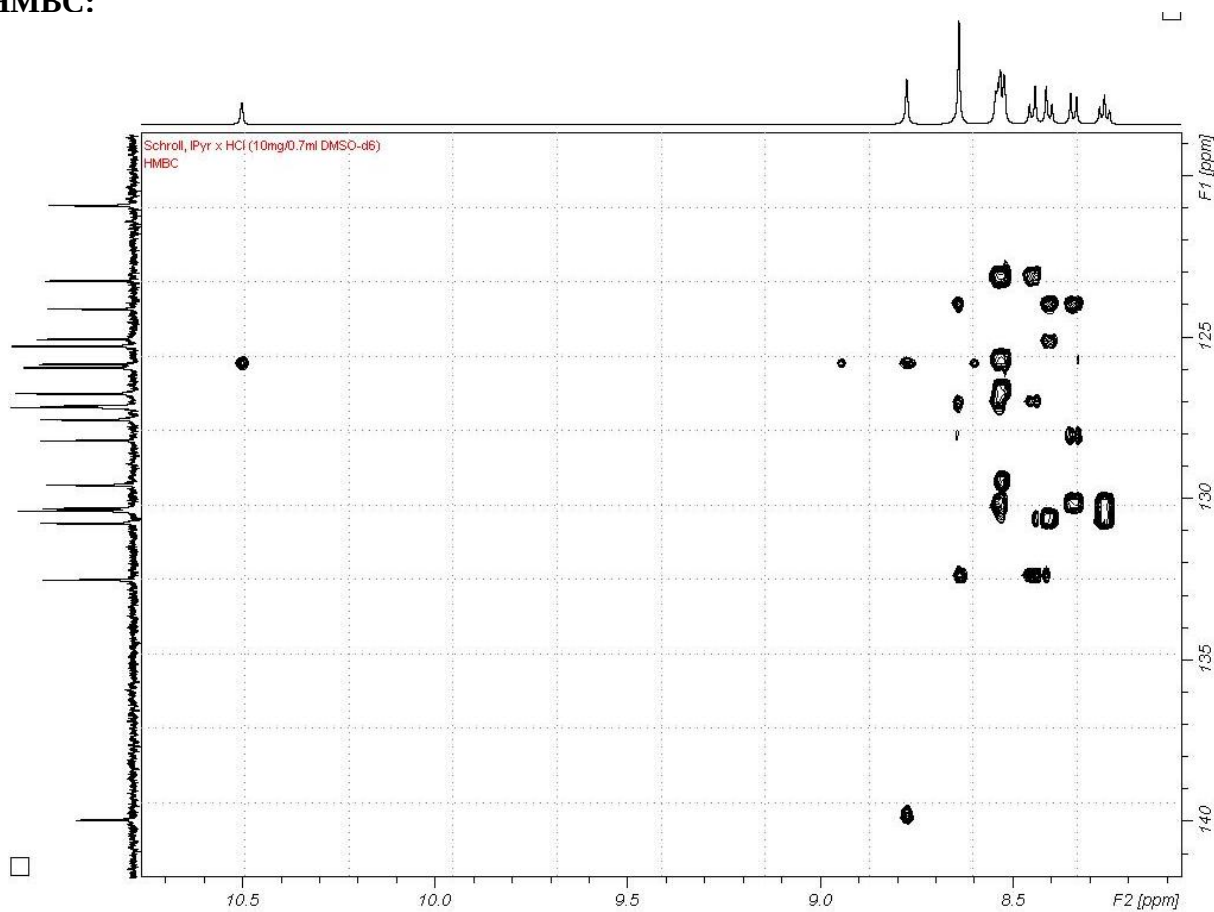
COSY:



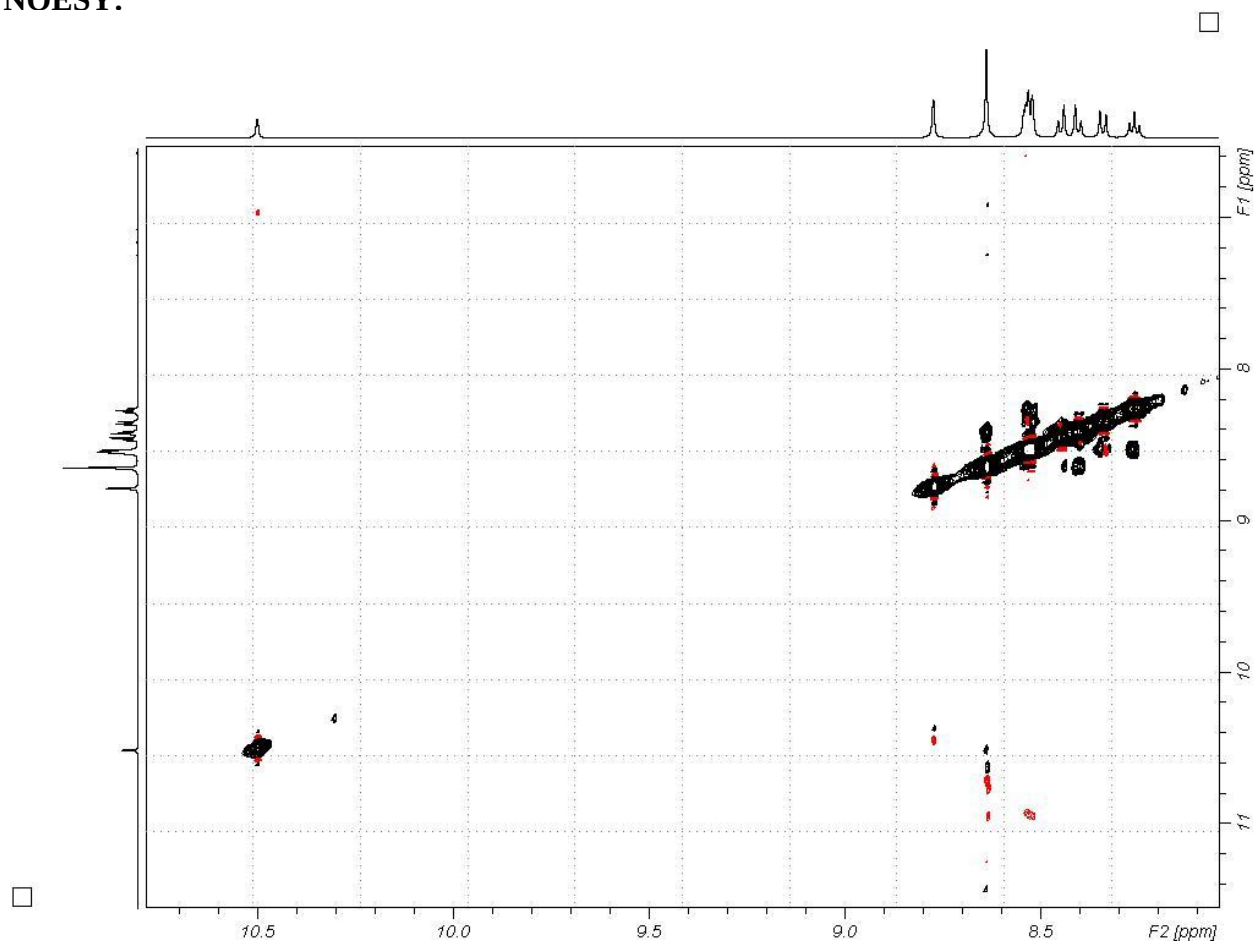
HSQC:



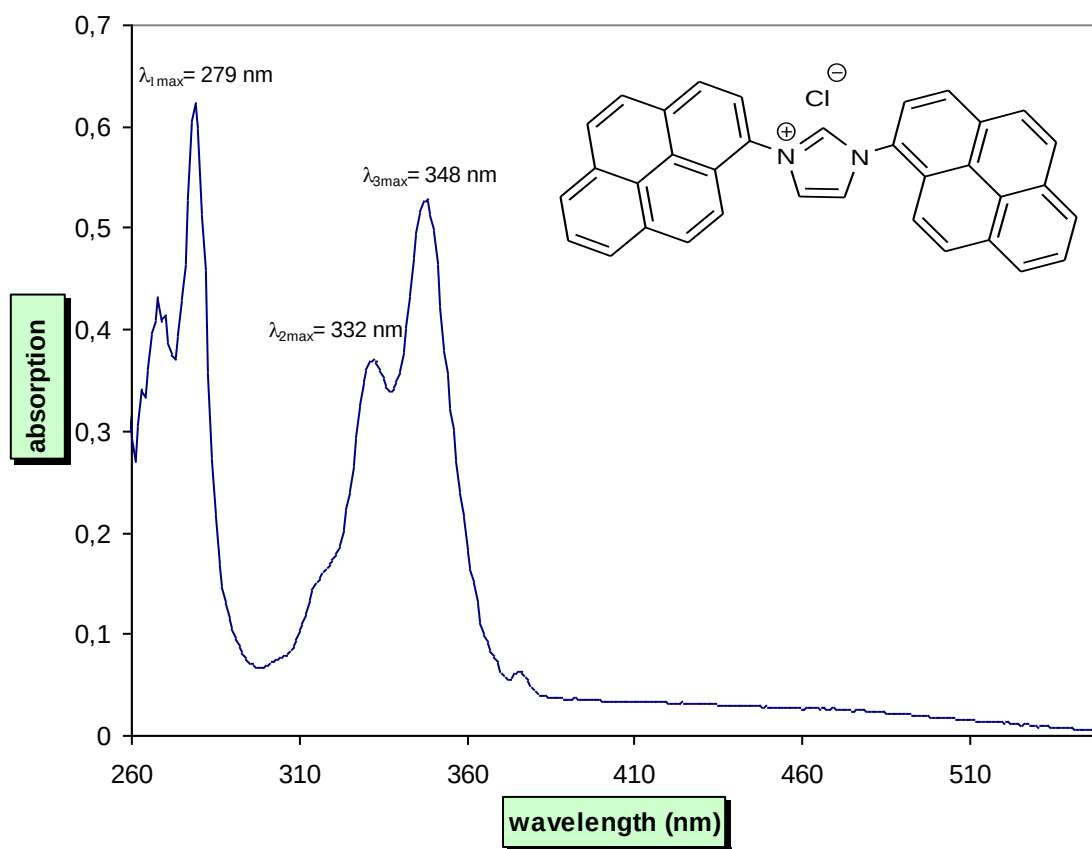
HMBC:



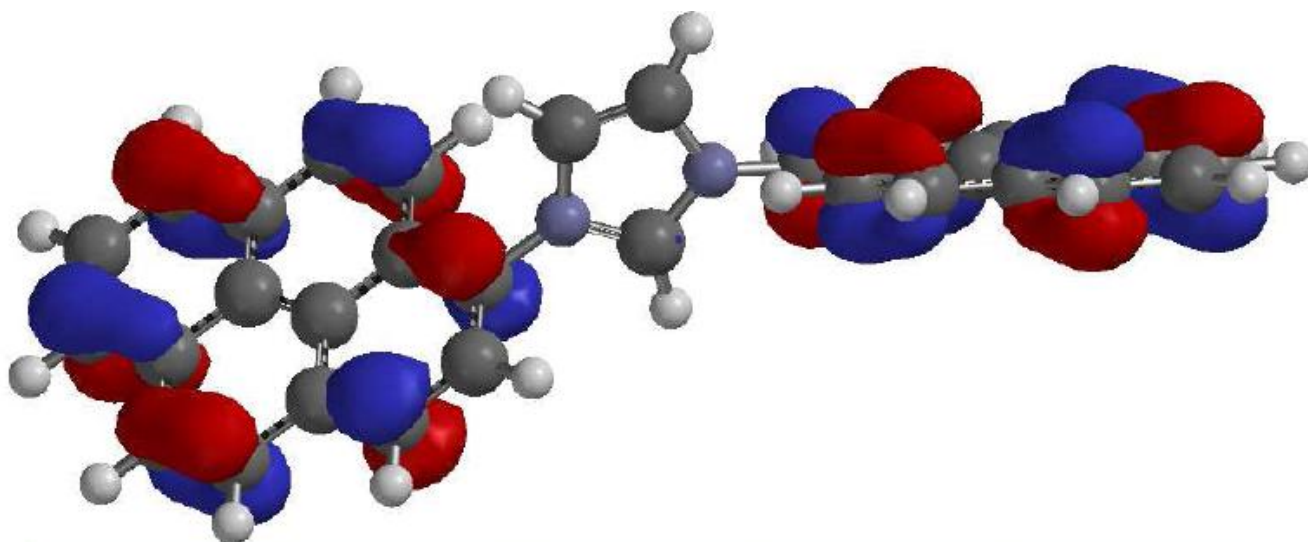
NOESY:



UV/VIS (IPyr·HCl in DMSO; $c = 10^{-5} \text{ mol L}^{-1}$):



Calculated lowest energy conformation and HOMO



The lowest energy conformation of the title compound in the gas phase was calculated using DFT methods (B3LYP, 6-31G*) in the program package SPARTAN'06. The HOMO (highest occupied molecular orbital) of the pyrene residues is shown in red and blue.