

## Supporting Information for

# Screening Interactions of Zinc Phthalocyanine-PPV Oligomers with Single Wall Carbon Nanotubes – A comparative study

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<i>Index</i>	<i>Page</i>
Experimental details	<b>S3</b>
<sup>1</sup> H-NMR and <sup>13</sup> C-NMR spectra of compound <b>11</b>	<b>S5</b>
MS (EI) spectrum of compound <b>11</b>	<b>S6</b>
<sup>1</sup> H-NMR spectrum of compound <b>9</b>	<b>S7</b>
<sup>13</sup> C-NMR and MS (EI) spectra of compound <b>9</b>	<b>S8</b>
<sup>1</sup> H-NMR and <sup>13</sup> C-NMR spectra of compound <b>8</b>	<b>S9</b>
MS (EI) spectrum of compound <b>8</b>	<b>S10</b>
<sup>1</sup> H-NMR spectrum of compound <b>7</b>	<b>S11</b>
FT-IR and UV-Vis. spectra of compound <b>7</b>	<b>S12</b>
MALDI-TOF spectrum of compound <b>7</b>	<b>S13</b>
<sup>1</sup> H-NMR spectrum of compound <b>6</b>	<b>S14</b>
FT-IR and UV-Vis. spectra of compound <b>6</b>	<b>S15</b>
MALDI-TOF spectrum of compound <b>6</b>	<b>S16</b>
<sup>1</sup> H-NMR and FT-IR spectra of compound <b>2</b>	<b>S17</b>
Figures S1 and S2: Transient absorption spectra of <b>2</b> and SWNT/ <b>2</b> in the visible	<b>S18</b>

## EXPERIMENTAL DETAILS

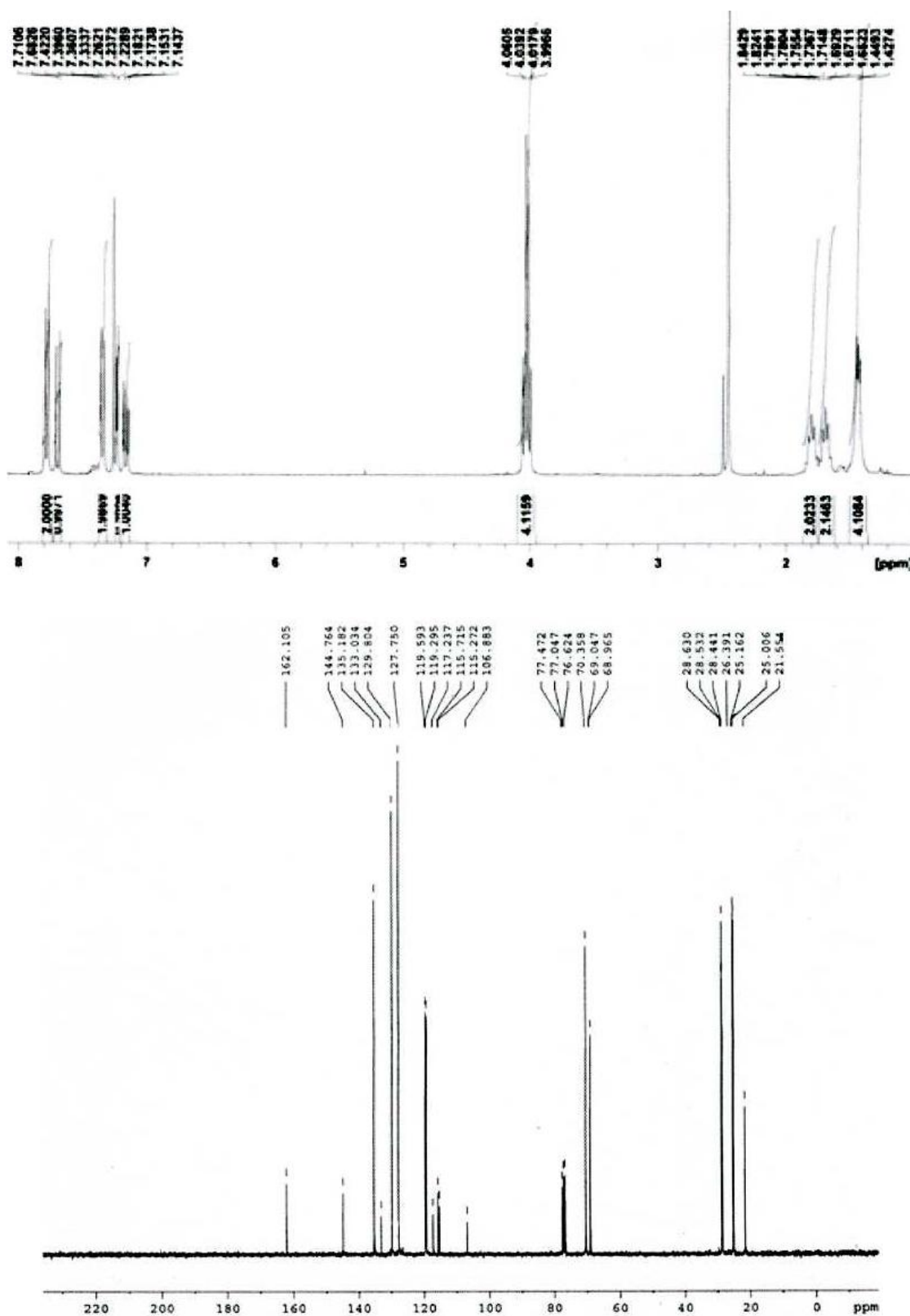
Chemicals employed all over this work were purchased from Aldrich Chemical Co. and used as received without further purification. Dry solvents were purchased from SDS in *anhydrous grade* and dried in addition, over molecular sieves (4Å size) acquired from SDS, as well. Prior to use the molecular sieves were dried in an oven during one night and subsequently activated by microwave oven-assisted irradiations took it in turns with a vacuum pump system. The monitoring of the reactions was carried out by TLC, employing aluminum sheets coated with silica gel 60.

Purification of compounds was performed by flash column chromatography using silica gel Merck-60 (230-400 mesh, 0.040-0.063 mm). Organic eluents were purchased from SDS in a *synthesis grade*.

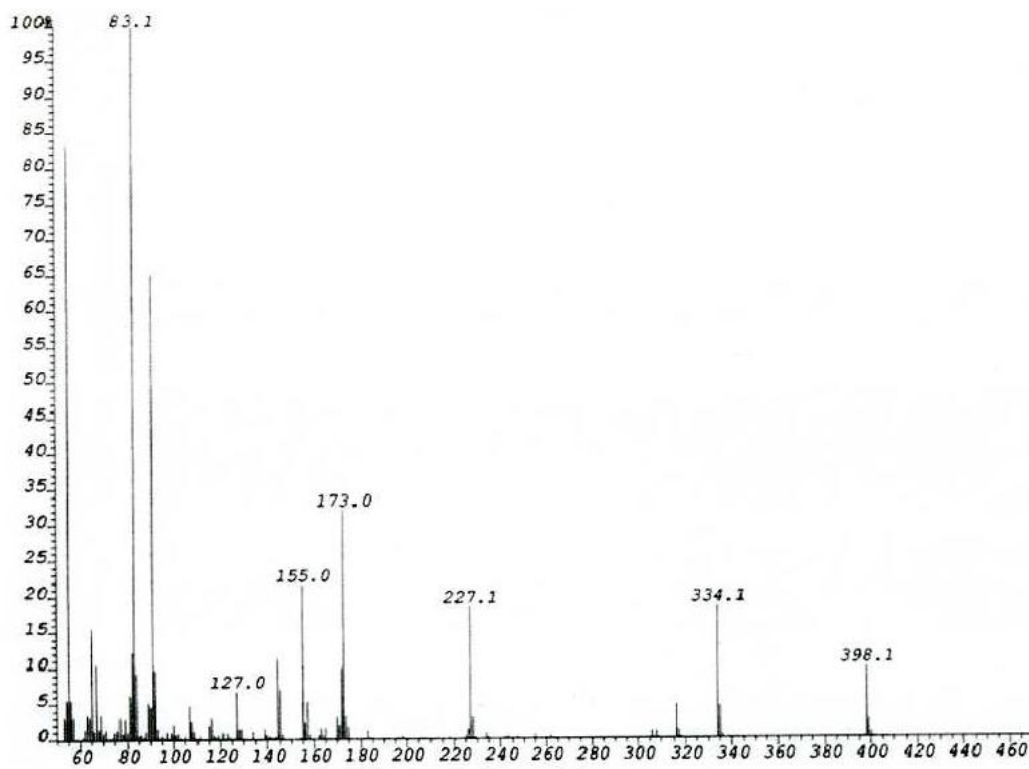
Melting points were determined in a Büchi 504392-S equipment and are uncorrected. NMR spectra were recorded with a BRUKER AC-300 and a BRUKER AC-500 apparatus. Deuterated solvent employed is indicated in brackets for each case. Chemical shift values ( $\delta$ ) are referred to tetramethylsilane (TMS), utilized as internal reference. UV/Vis. spectra were recorded in solution using solvents purchased from Fluka Chemie in *spectroscopic grade* on a Hewlett-Packard 8453 spectrophotometer. The logarithm of the absorption coefficient ( $\epsilon$ ) is indicated in brackets for each maximum. FT-IR spectra were recorded on a Bruker Vector 22 spectrophotometer, employing for all cases, solid samples embedded in pressed disks of KBr. MS (Electronic Impact or Matrix-Assisted Laser Desorption Ionization Time-Of-Flight) and HR-MS were performed in a REFLEX-III apparatus with a laser beam operating at 337 nm. Dithranol (1,8,9-anthracenetriol) and PEGNa1000 poly(ethylenglycol)-1000 were used as matrix and internal reference, respectively.

All spectroscopic data presented in the results and discussion section were obtained using the following instruments and materials. THF was of spectrophotometric grade (99.5%) and was purchased from Sigma-Aldrich. SWNTs (HiPCO Batch Nr.: R0510C) were purchased from CNI. The experiments were performed at room temperature and ambient conditions. Steady-state absorption spectra were measured by a Cary5000 (Varian) two beam spectrometer. Emission spectra were recorded by using a FluoroMax-P (HORIBA). NIR emission spectra were measured by a Fluorolog spectrometer (HORIBA Jobin Yvon). Here, the optical detection was performed by a Symphony InGaAs array in combination with an iHR320 imaging spectrometer. The samples were excited by a 450 W Xenon lamp or the SHG (532 nm) of a Nd/YAG laser. Femtosecond transient absorption studies were performed using 387 nm laser pulses with a 150 fs pulse width (1 kHz, ~200 nJ), from an amplified Ti:sapphire laser system (SHG, CPA 2001, Clark-MXR Inc.) For the detection we used a Helios TAPPS from Ultrafast Inc..

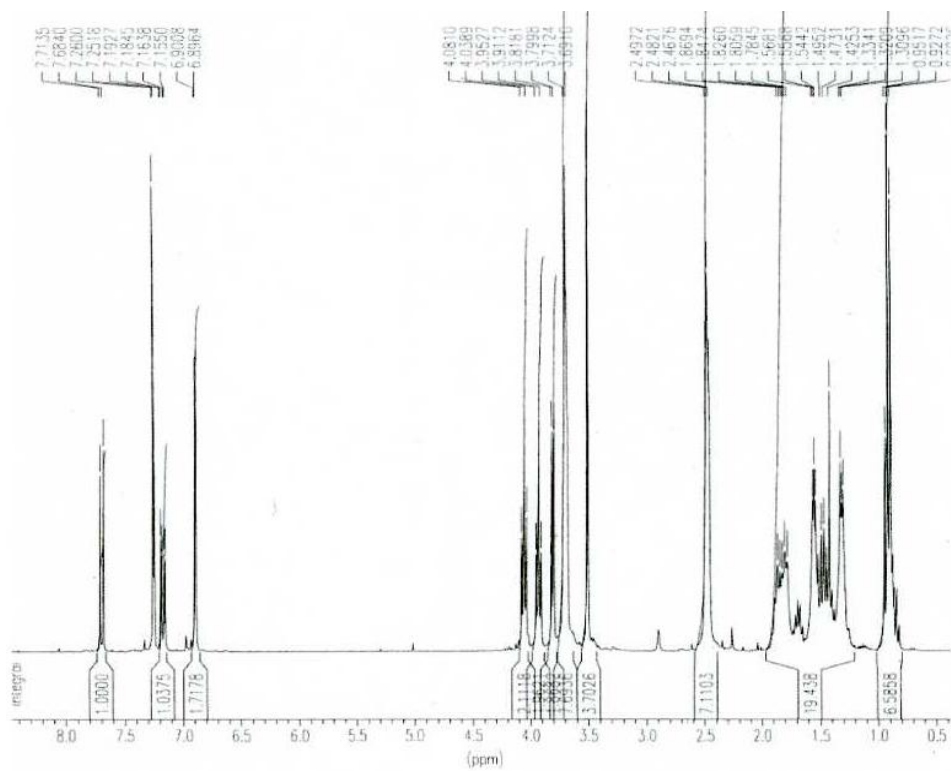
$^1\text{H-NMR}$  and  $^{13}\text{C-RMN}$  spectra of compound 11



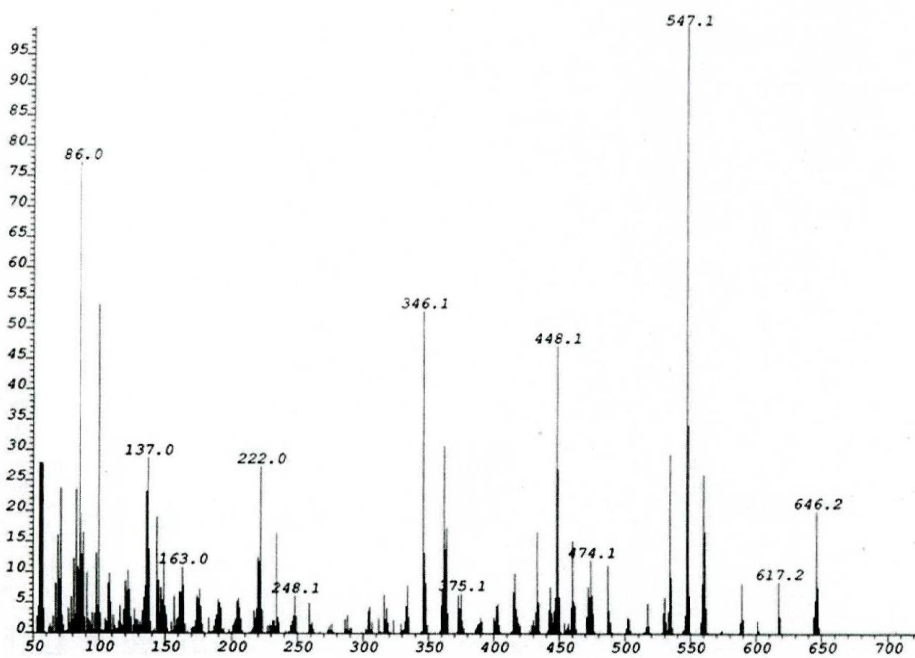
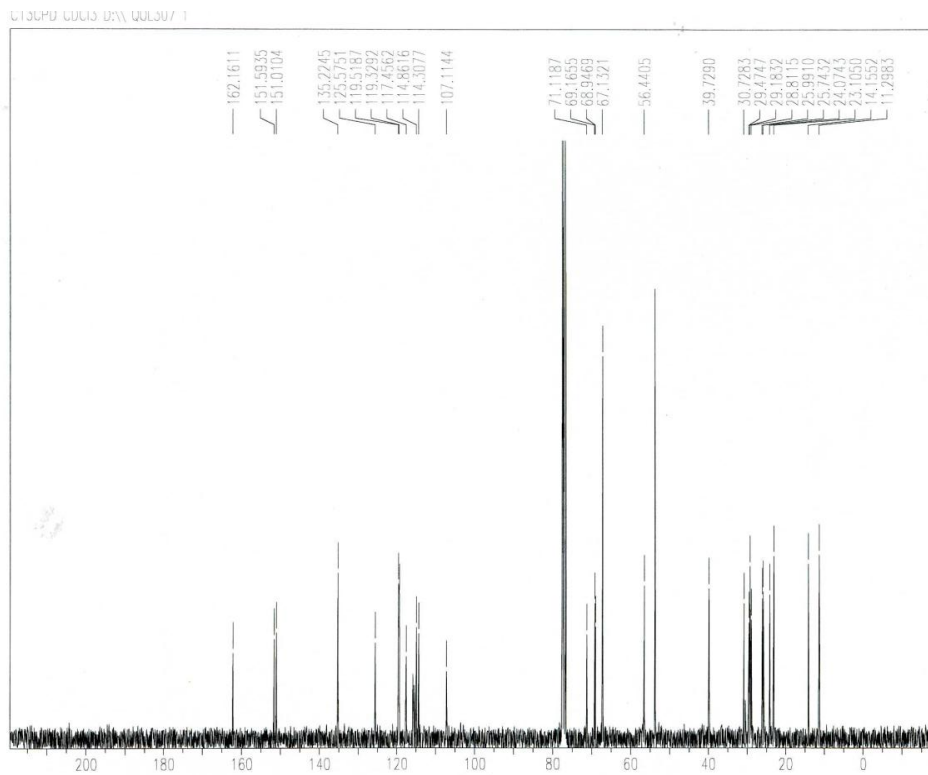
MS (EI) spectrum of compound 11



### <sup>1</sup>H-NMR spectrum of compound 9

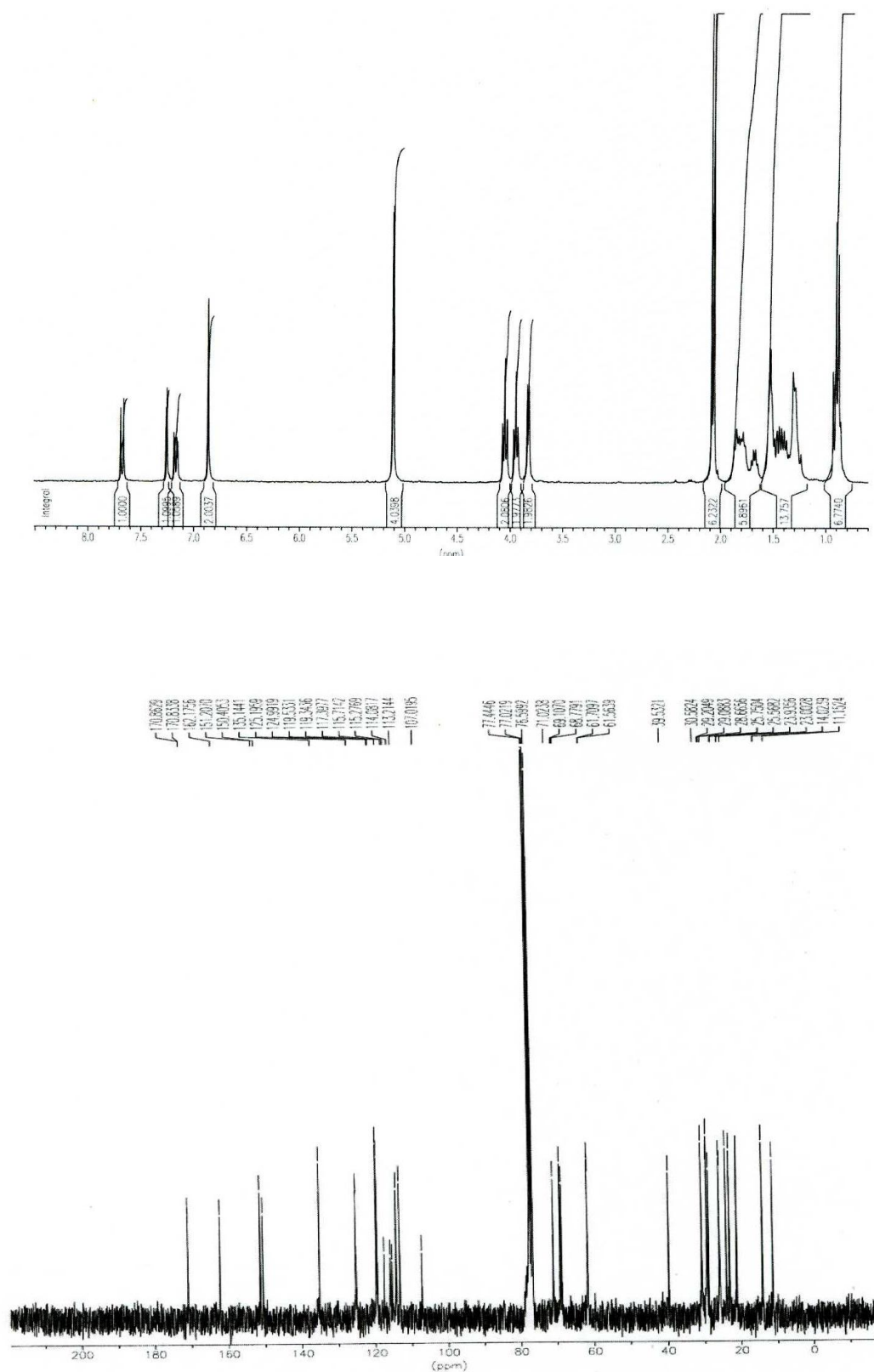


### <sup>13</sup>C-NMR and MS (EI) spectra of compound 9

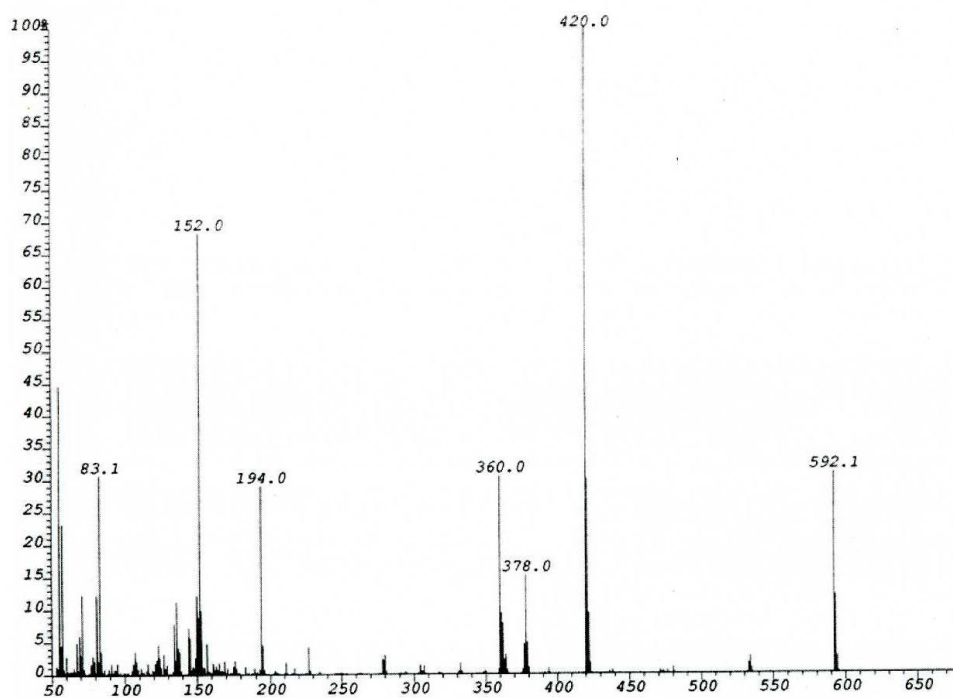




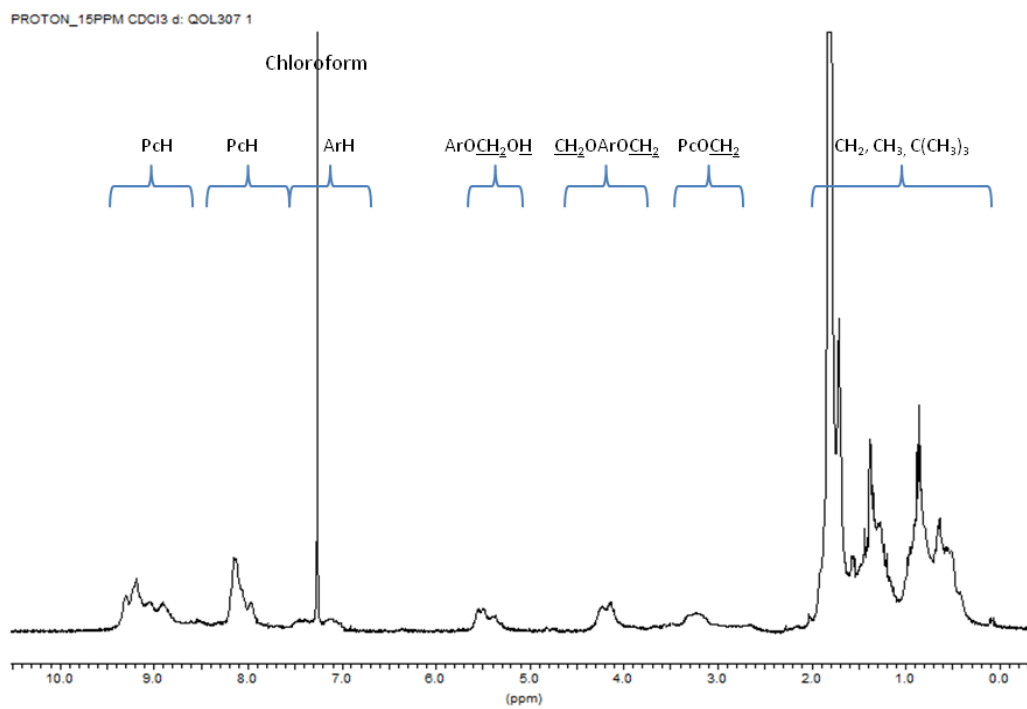
# $^1\text{H-NMR}$ and $^{13}\text{C-RMN}$ spectra of compound 8



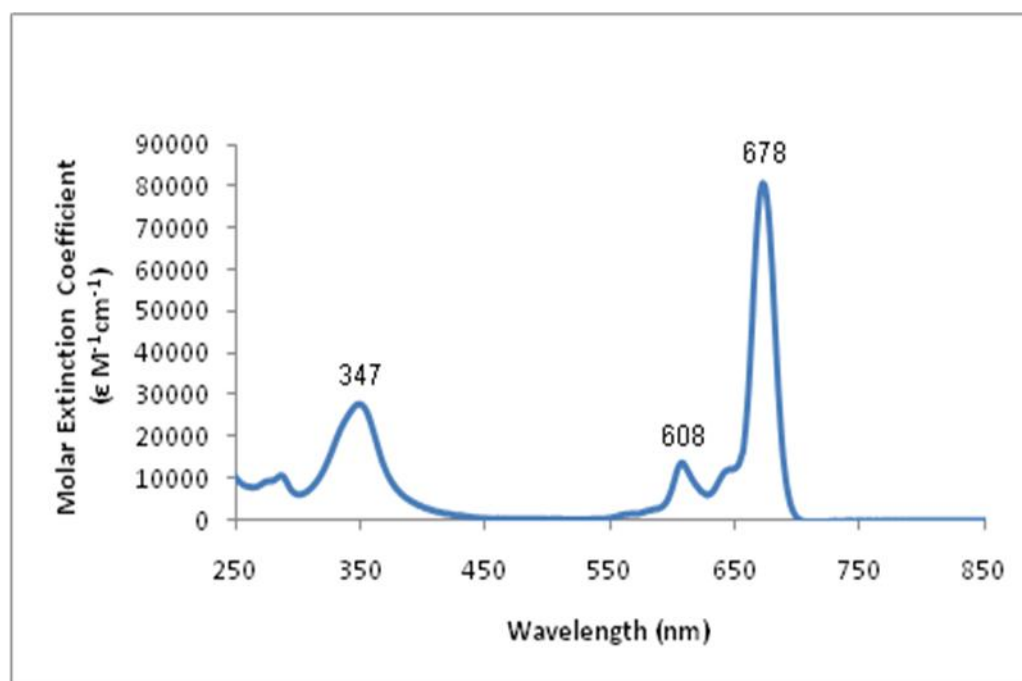
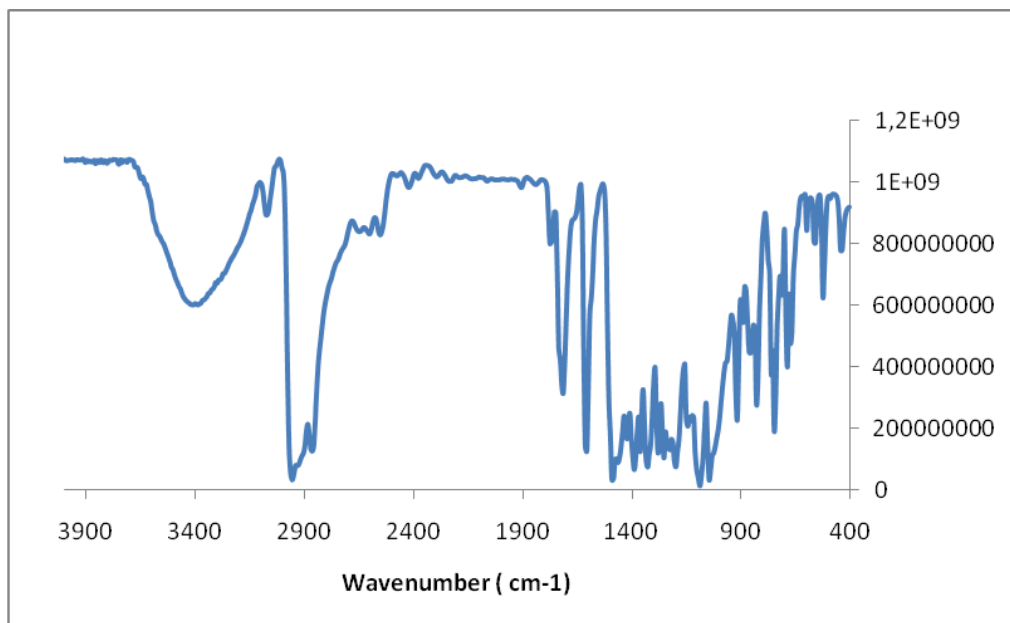
### MS (EI) spectrum of compound 8



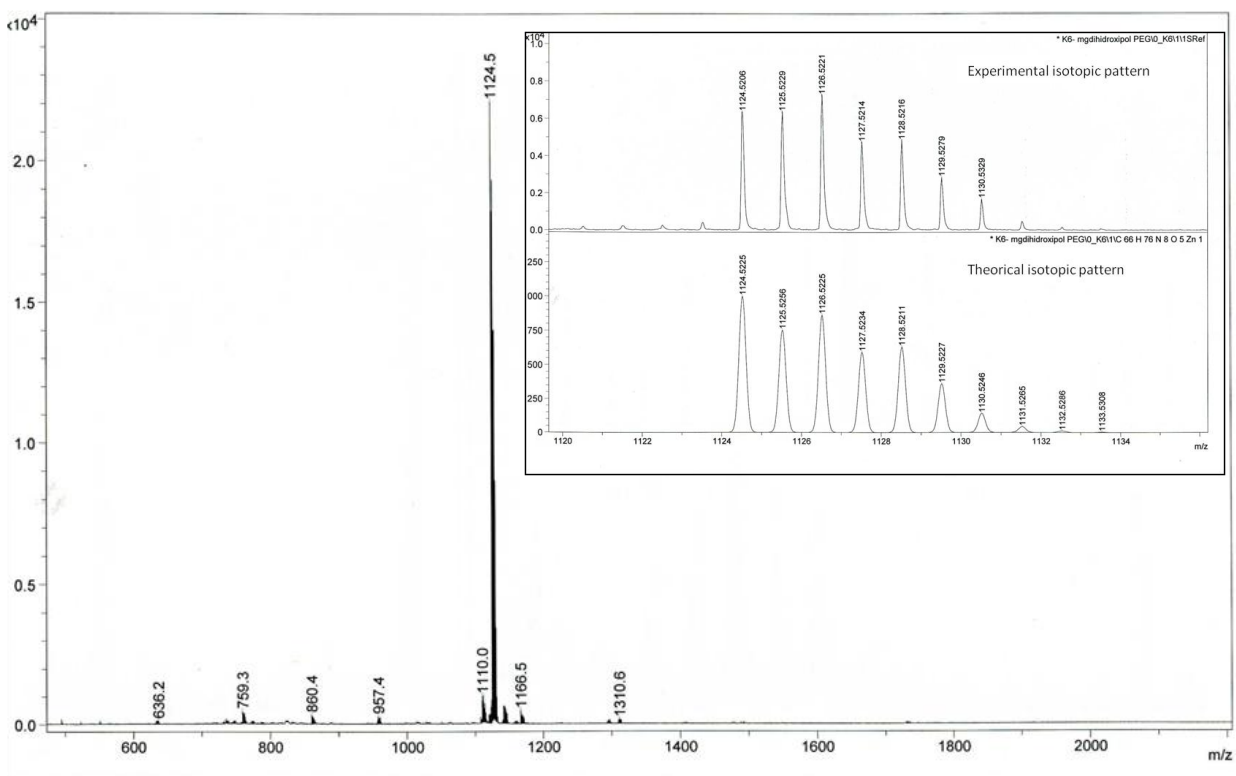
# <sup>1</sup>H-NMR spectrum of phthalocyanine 7



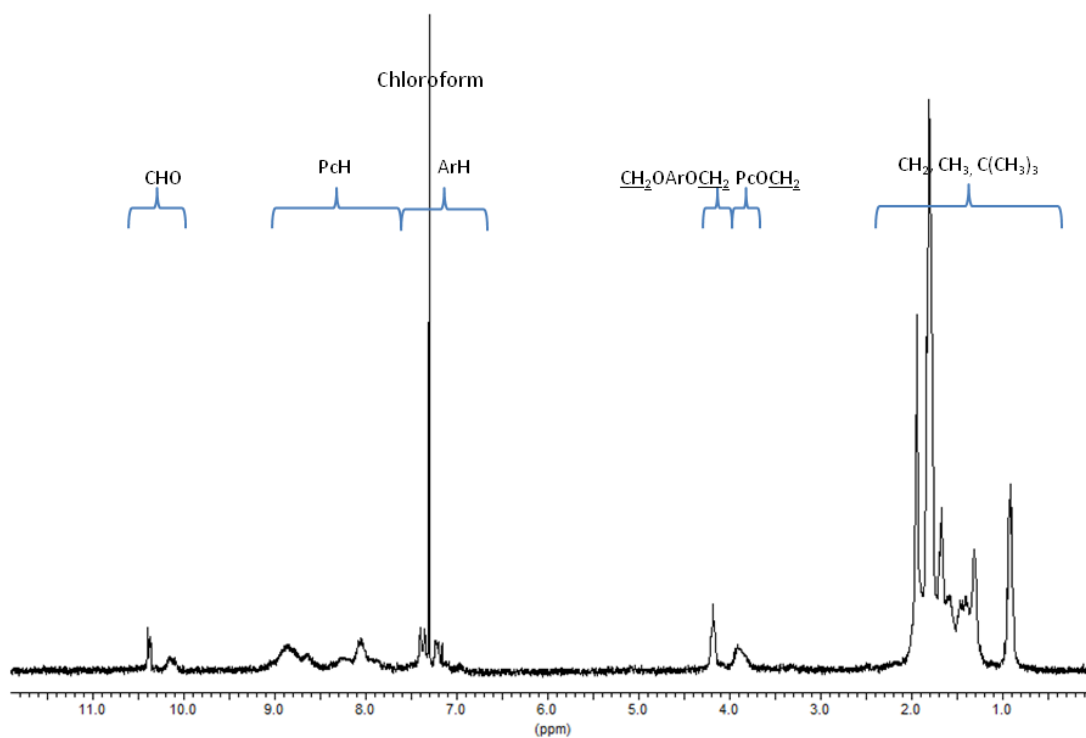
### FT-IR and UV-Vis. spectra of phthalocyanine 7



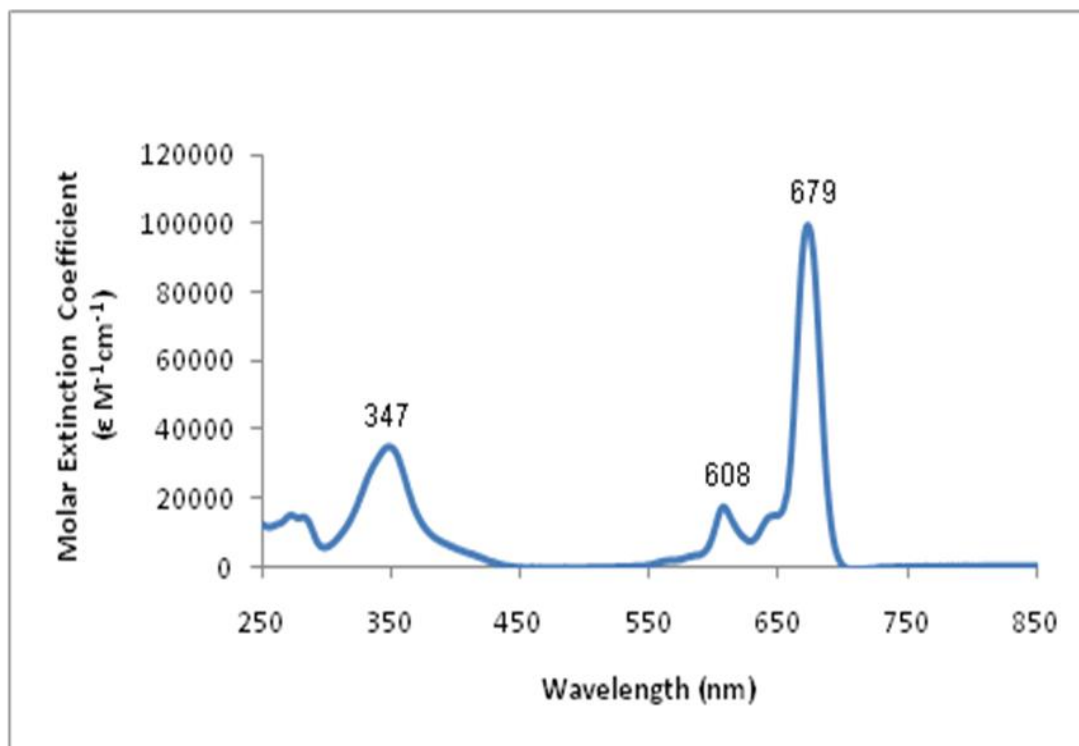
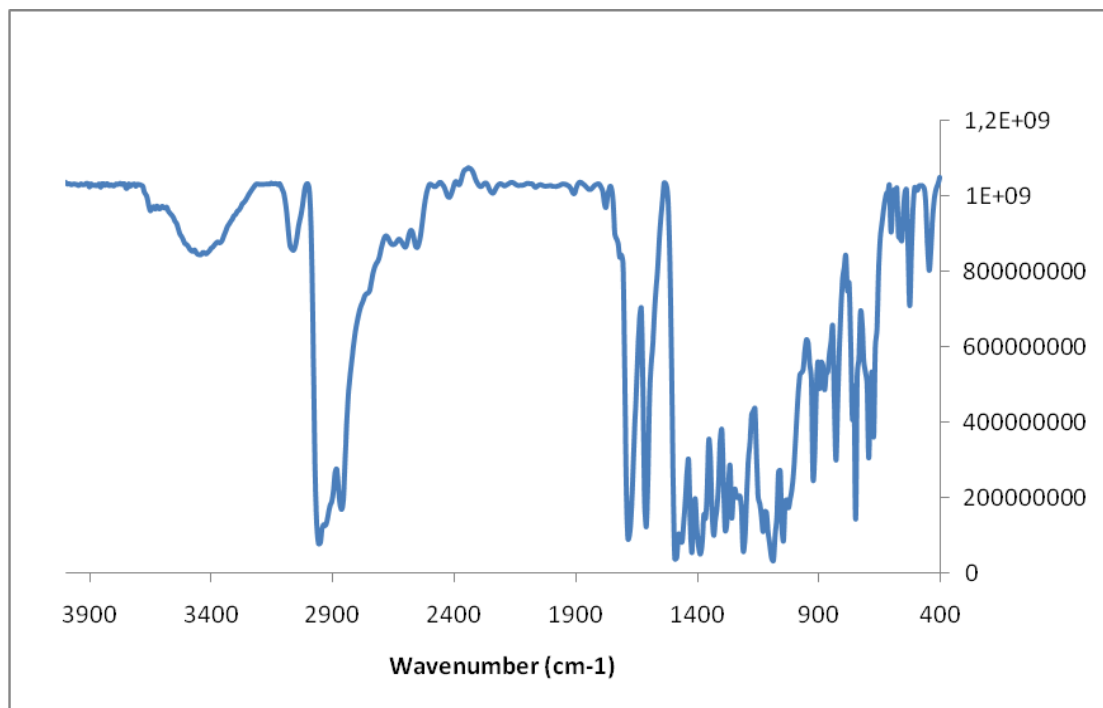
### MALDI-TOF spectrum and isotopic distribution pattern (inset) of phthalocyanine 7



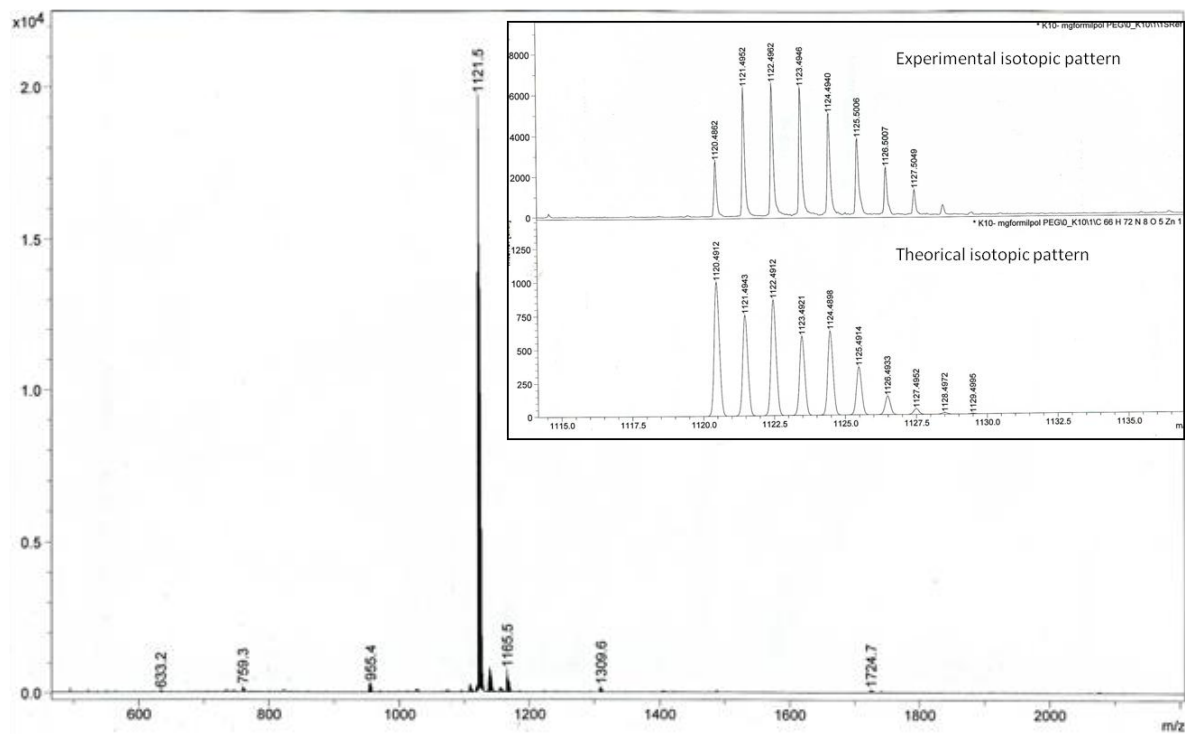
# <sup>1</sup>H-NMR spectrum of phthalocyanine 6



### FT-IR and UV-Vis. spectra of phthalocyanine 6

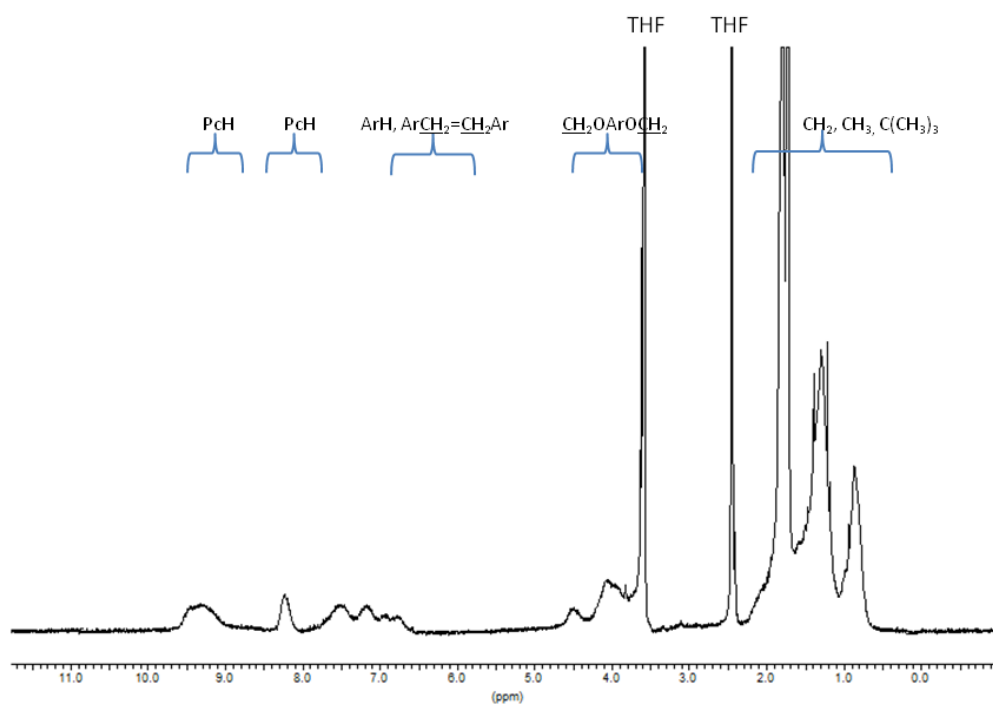


### MALDI-TOF spectrum and isotopic distribution pattern (inset) of phthalocyanine 6

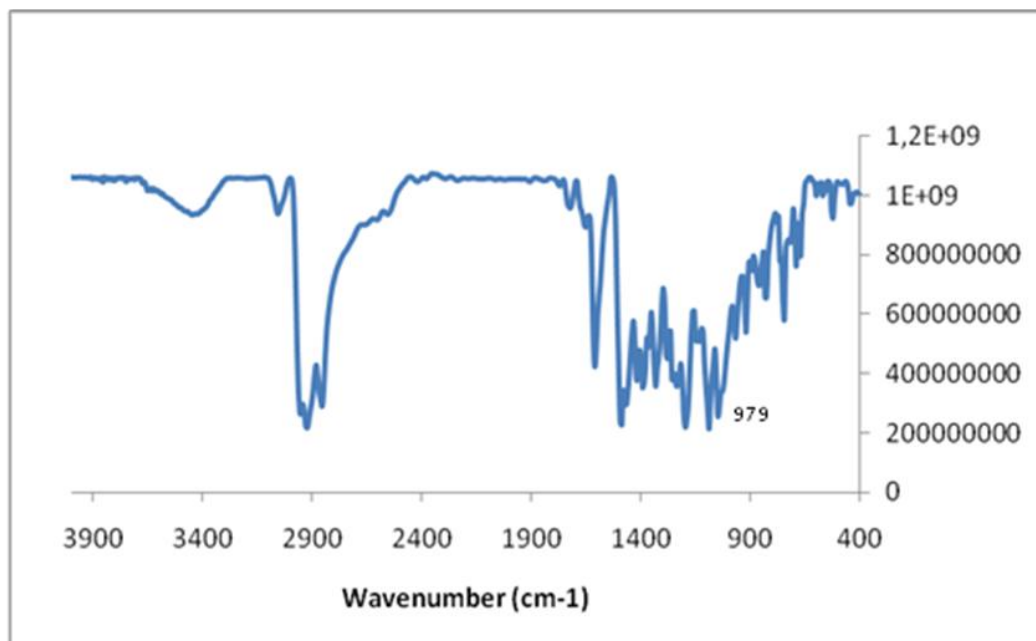


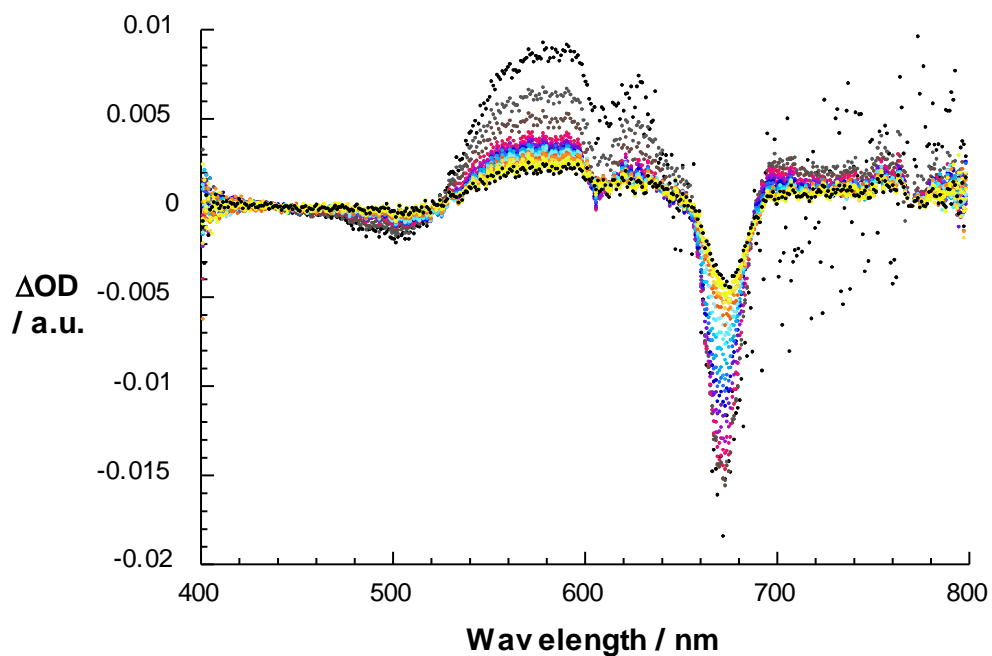


### <sup>1</sup>H-NMR spectrum of polymer 2

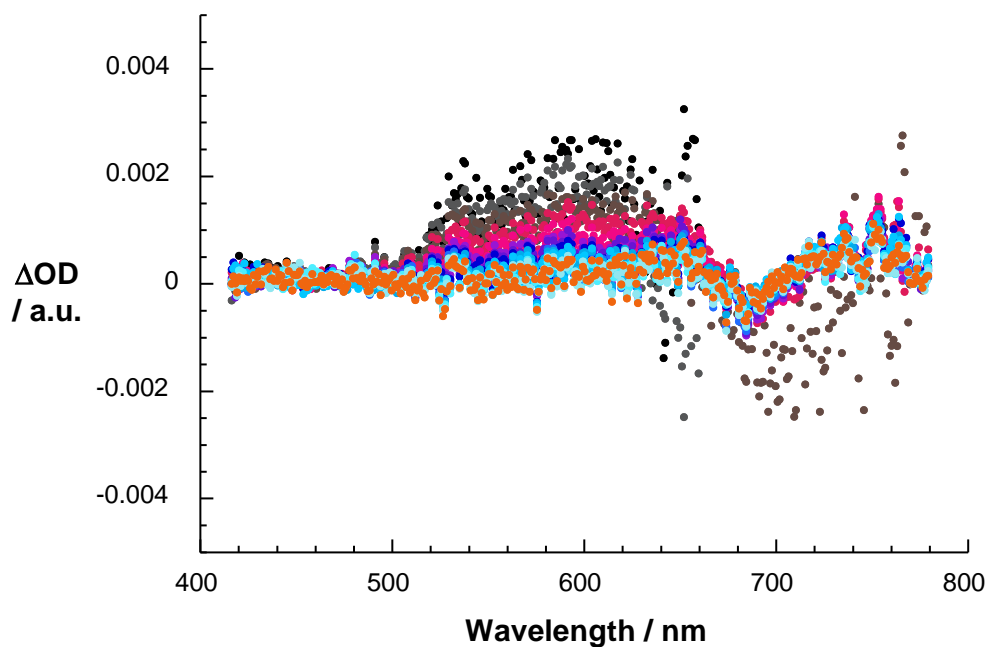


### FT-IR spectra of polymer 2





**Figure S1** Differential absorption spectra (visible range) obtained upon femtosecond laser flash photolysis (387 nm) of **2** in THF at room temperature with several time delays between 0 and 1000 ps, representing the ground state bleaching of PPV and ZnPc absorption bands and the formation / decay of the ZnPc singlet excited state – time evolution is from black and red to blue and yellow.



**Figure S2** Differential absorption spectra (visible) obtained upon femtosecond laser flash photolysis (387 nm) of SWNT/2 in THF at room temperature with several time delays between 0 and 10 ps representing the ground state bleaching of SWNT-bound ZnPc absorption bands and the ultrafast decay of the ZnPc singlet excited state leading to charge separation – time evolution is from black and red to blue and yellow.