

New Journal of Chemistry...

Electronic Supplementary Information

Synthesis and Optoelectronic Properties of Phenylenevinylenequinoline Macromolecules

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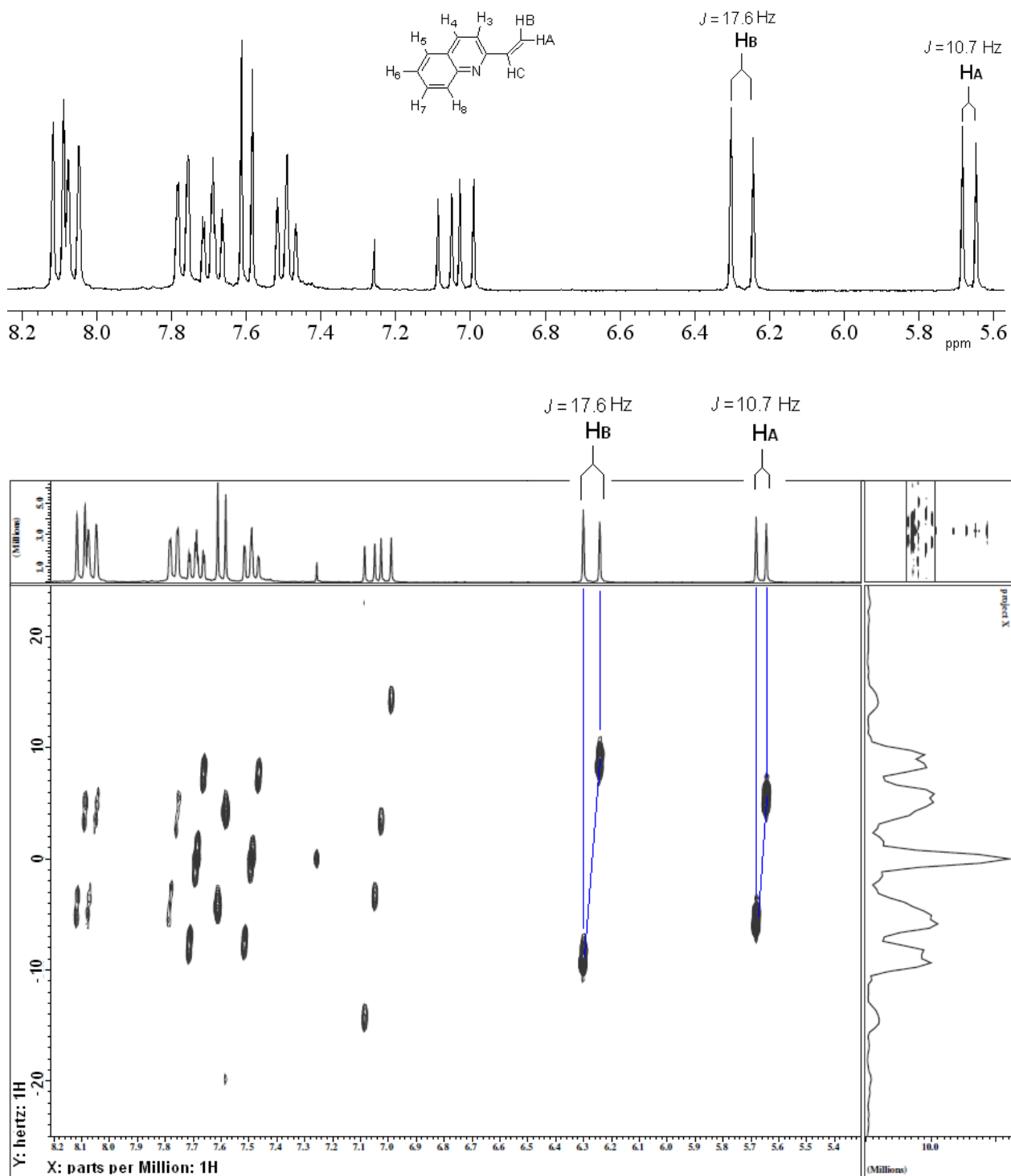
^bMaterials and manufacturing Directorate, Air Force Research Laboratory, 3005 Hobson Way, Wright-Patterson Air Force base, OH, 45433, USA.

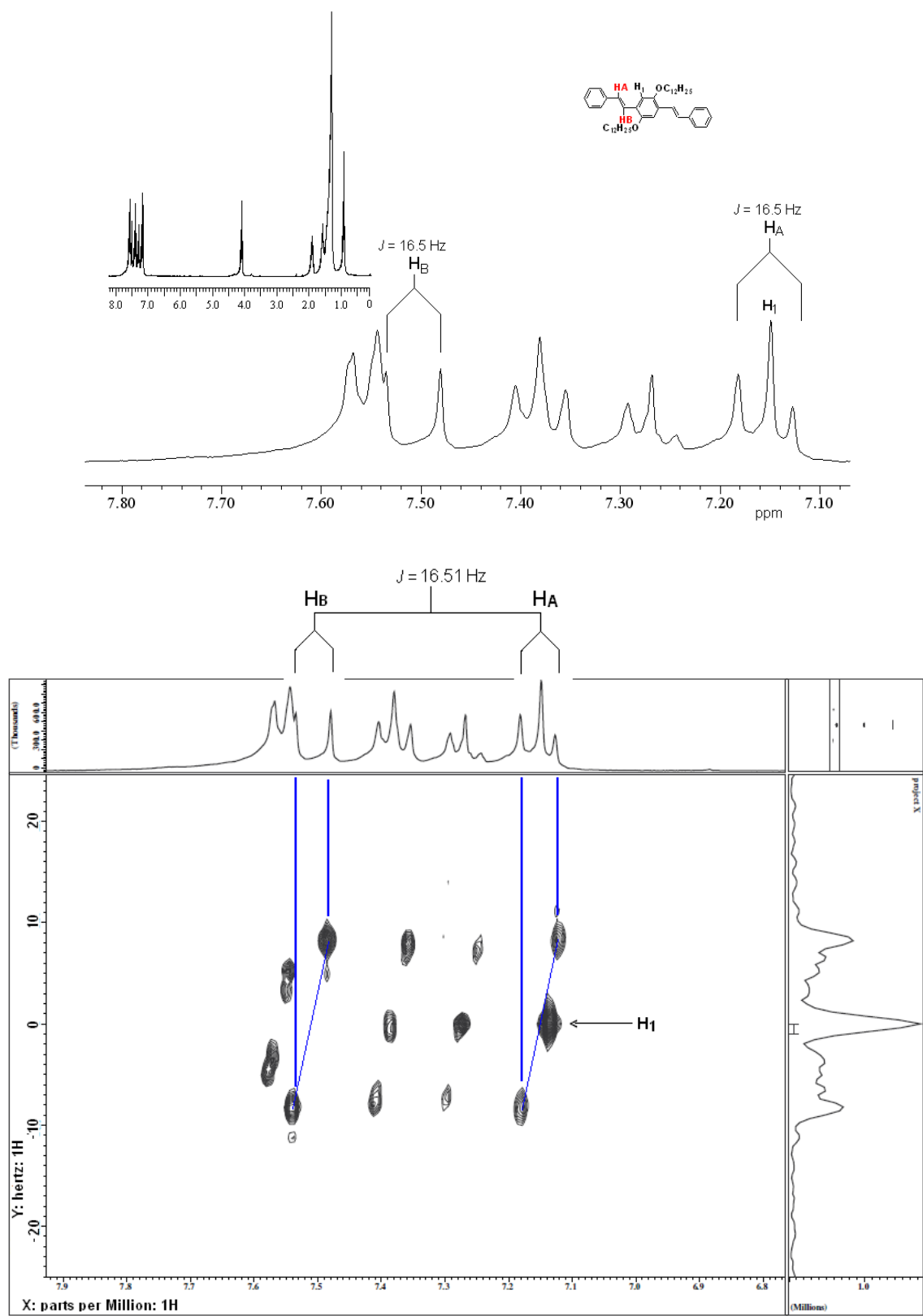
^cAzimuth Corporation, 4134 Linden Avenue, Suite 300, Dayton, OH 45431, USA

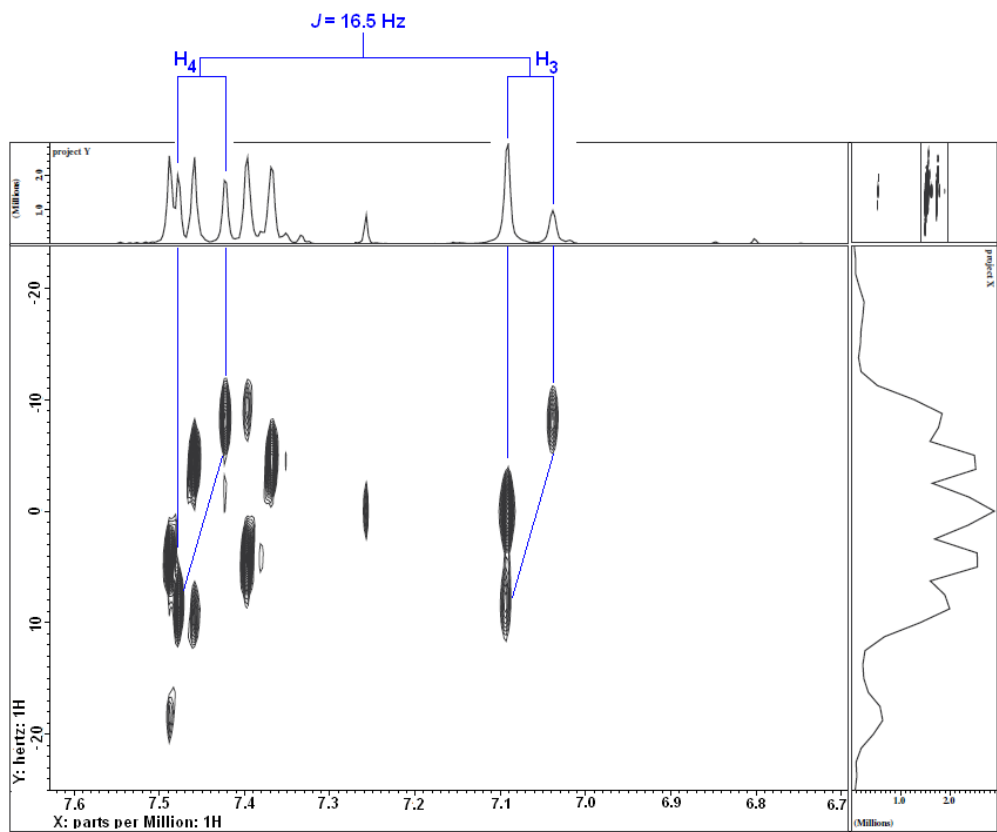
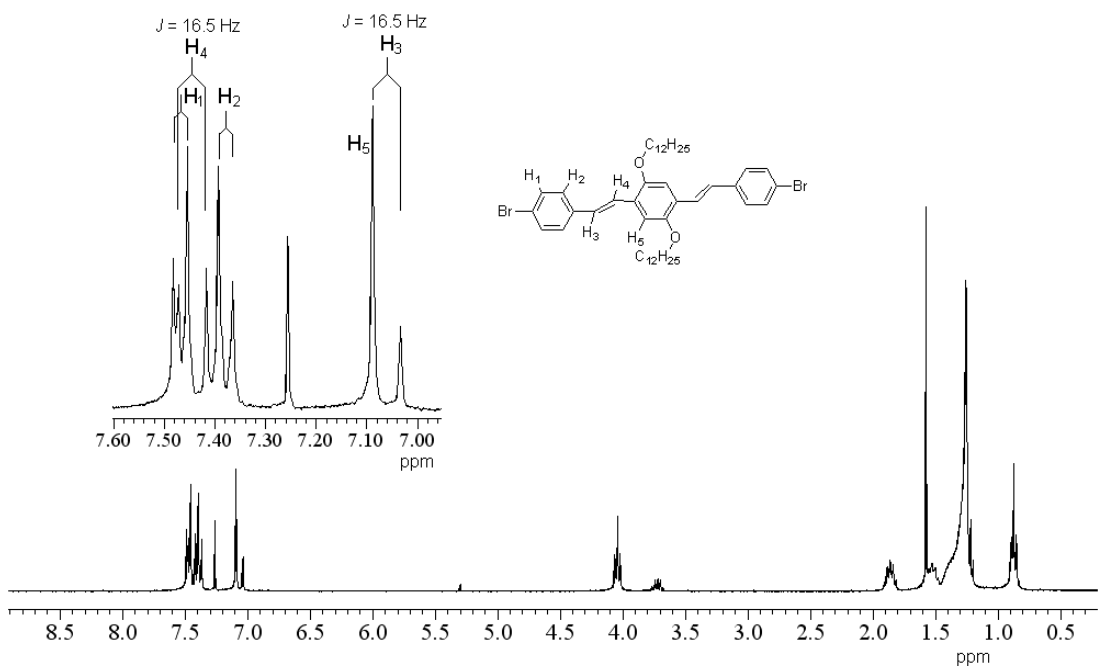
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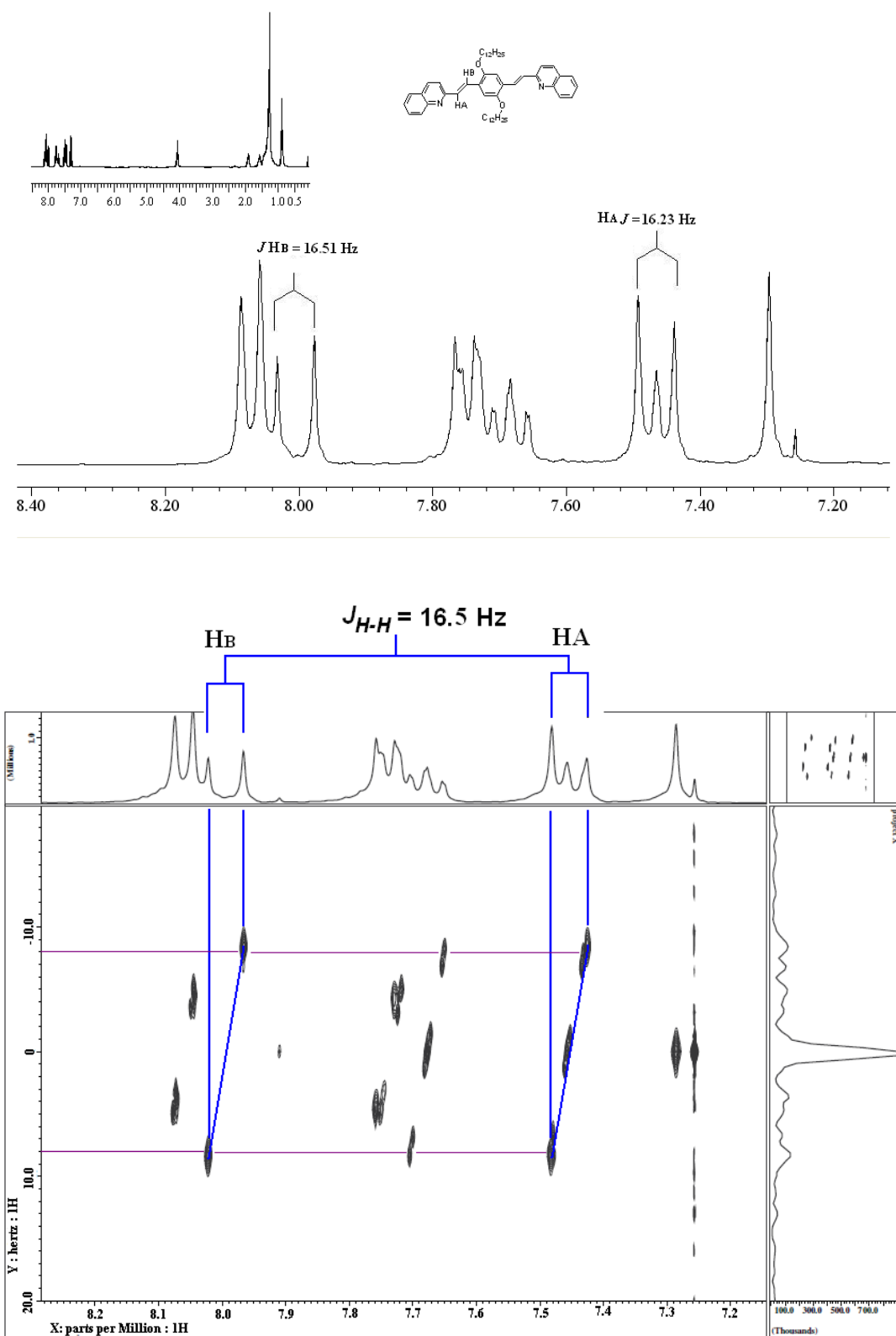
- I. ¹H, two dimensional *J*-Resolved, APT, DEPT-135, ¹³C NMR spectroscopy of intermediates and selected oligomers.**
- II. MALDI-TOF Spectrometry of selected oligomers.**
- III. Additional electronic spectra of 7QPV as example for the nQPV series**
- IV. Theoretical calculations**

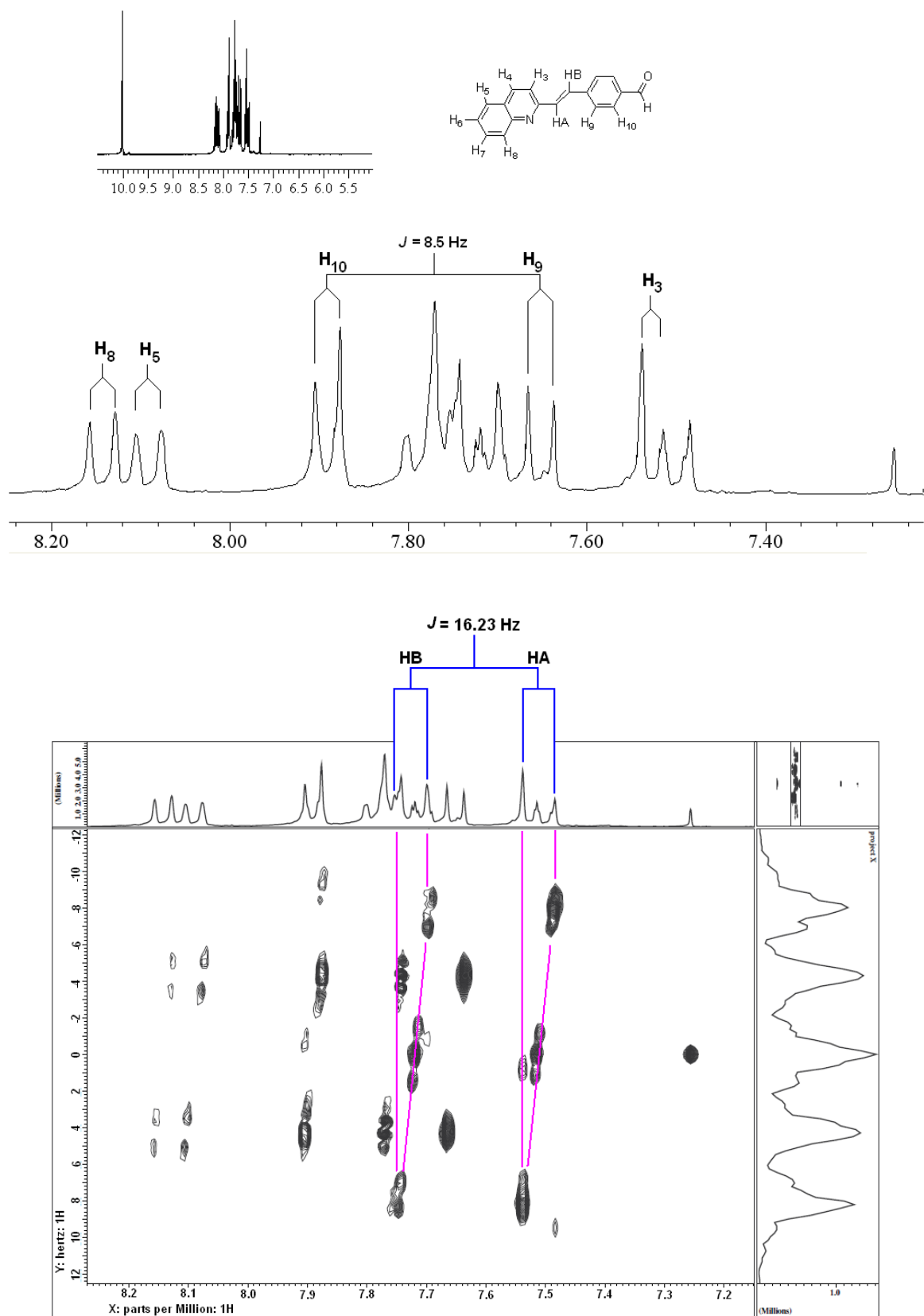
I. ^1H , two dimensional J -Resolved, APT, DEPT-135, ^{13}C NMR spectroscopy of intermediates and selected oligomers.

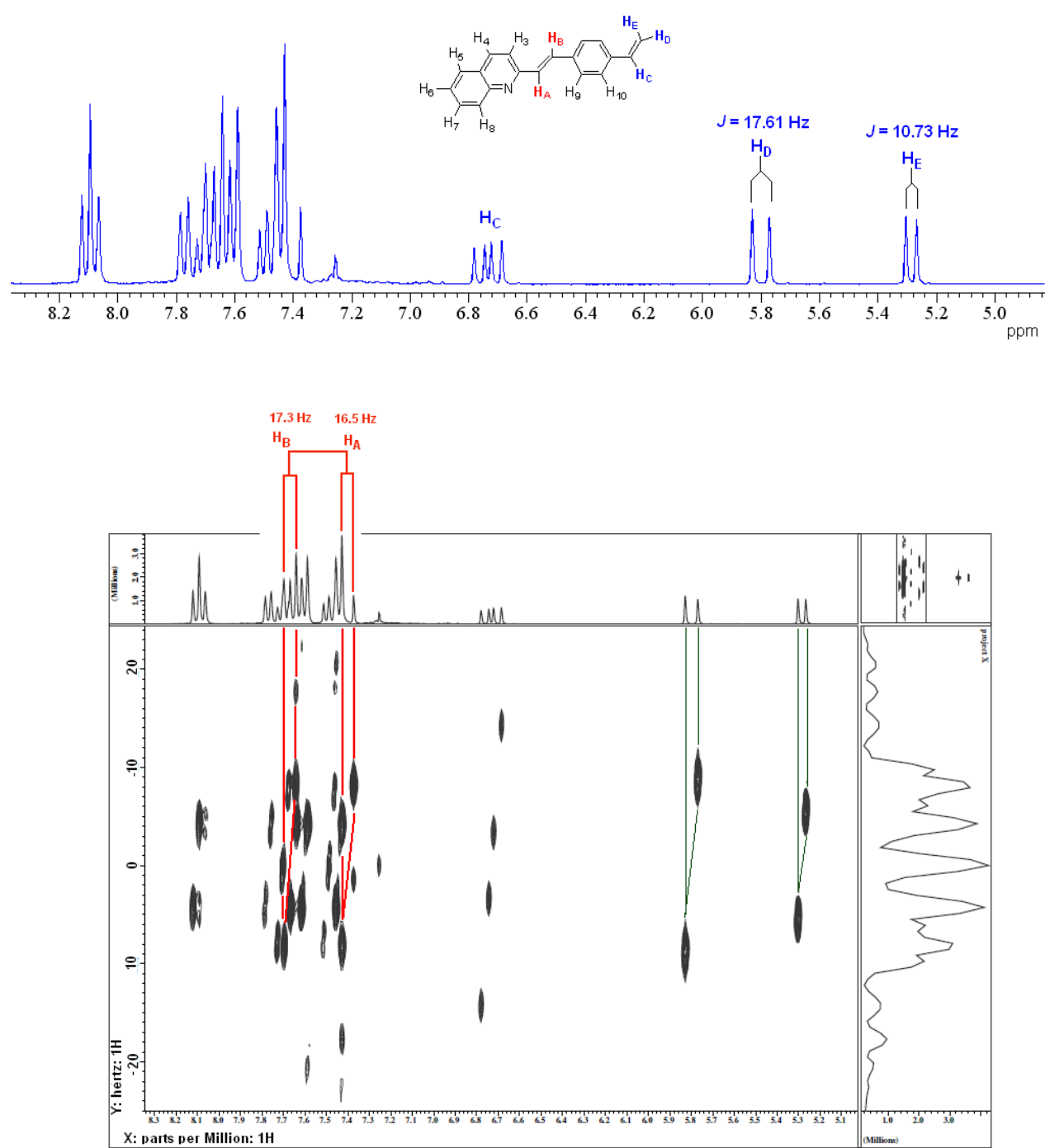


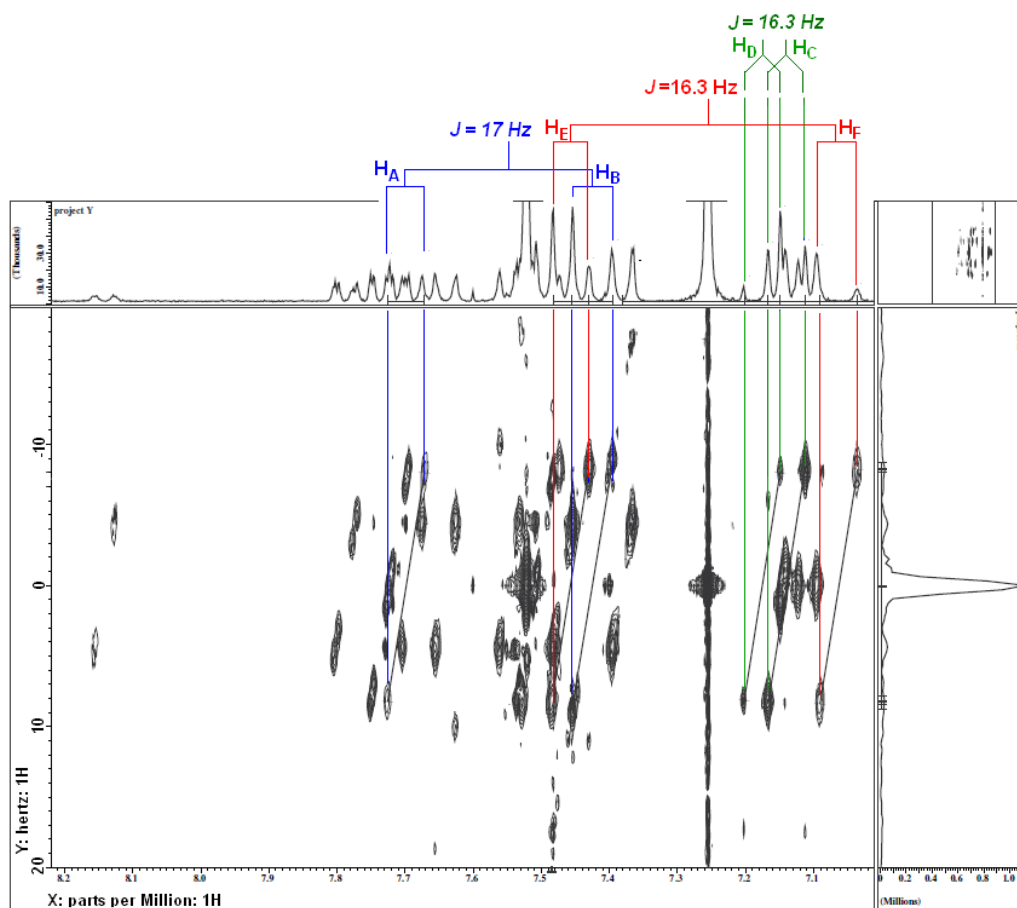
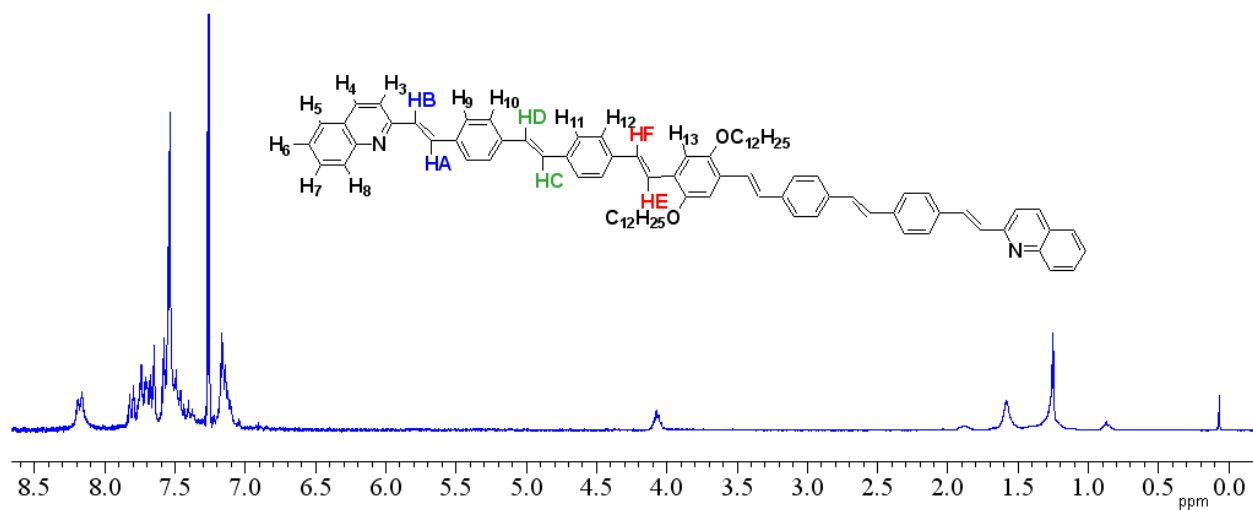


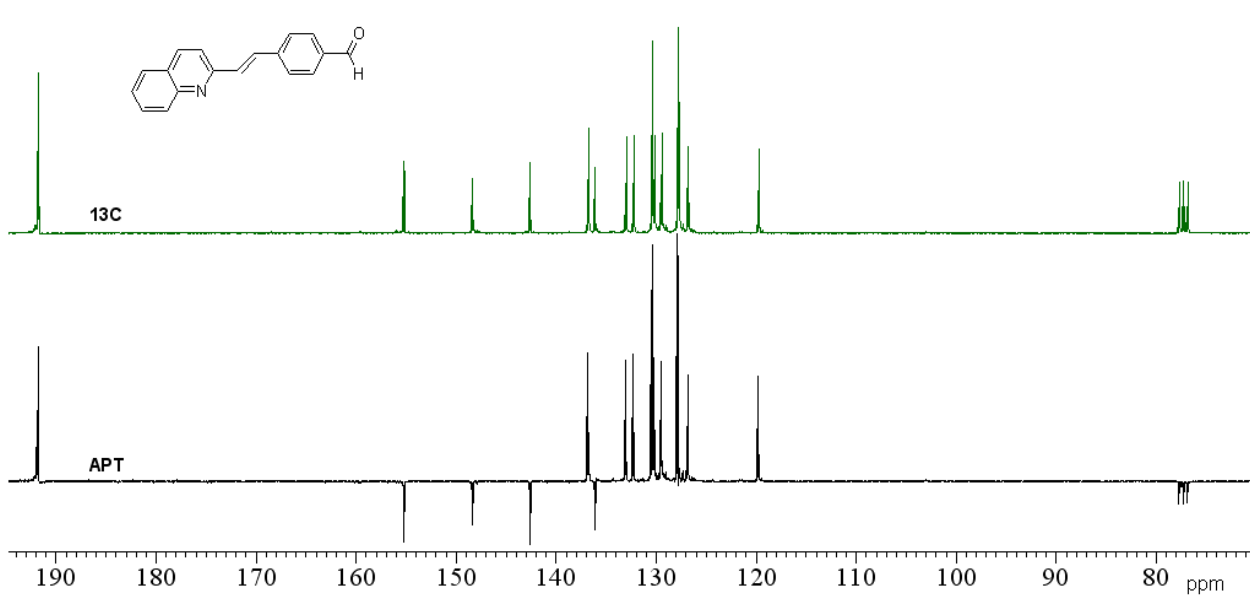
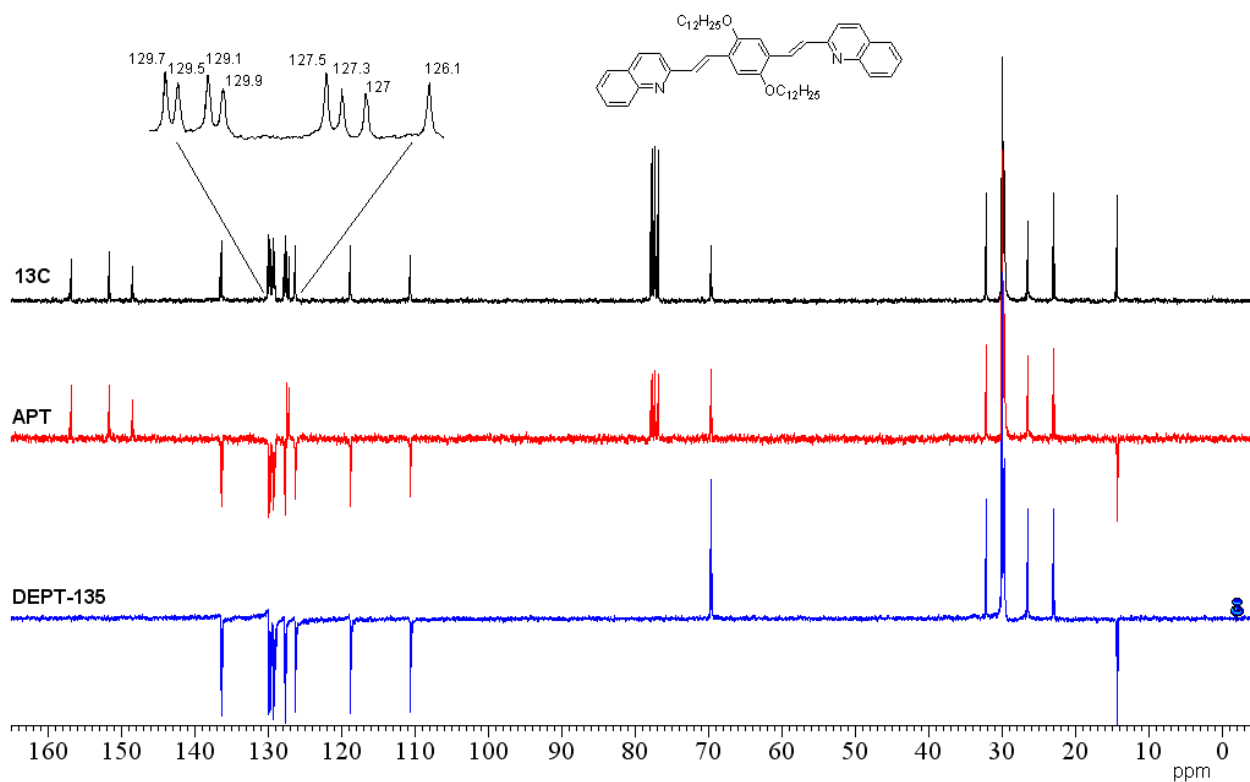


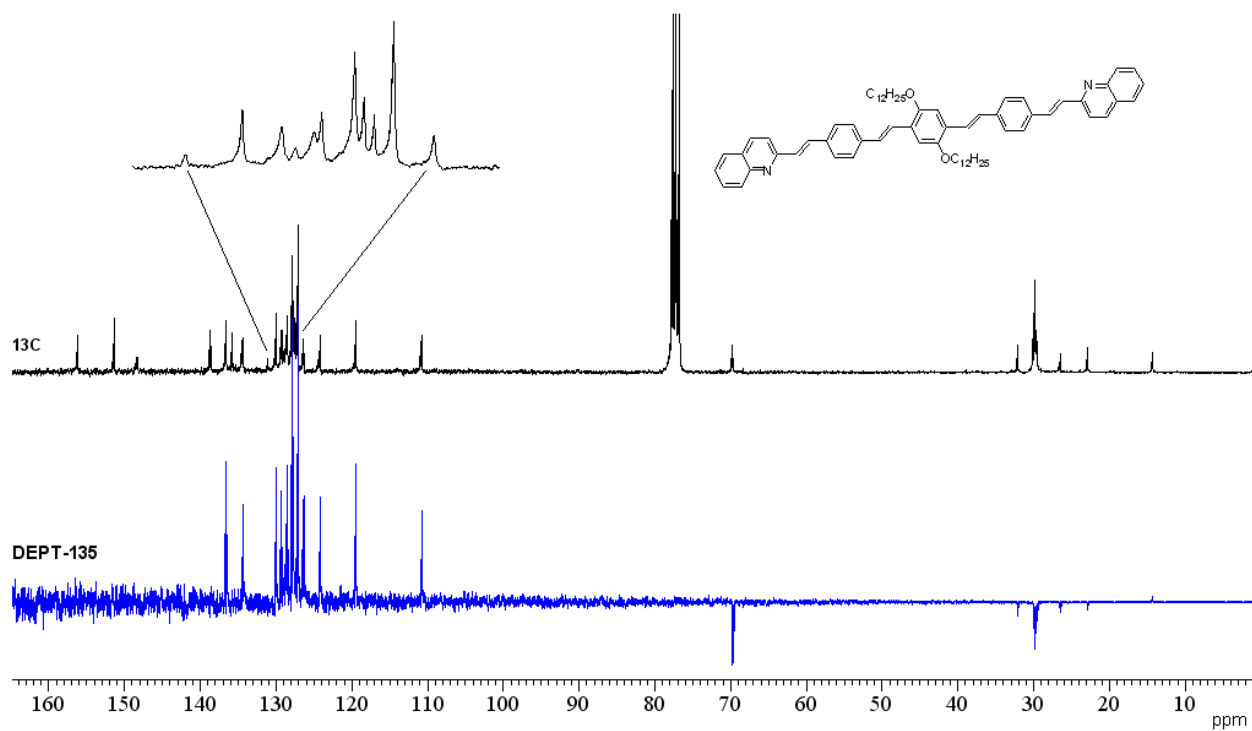
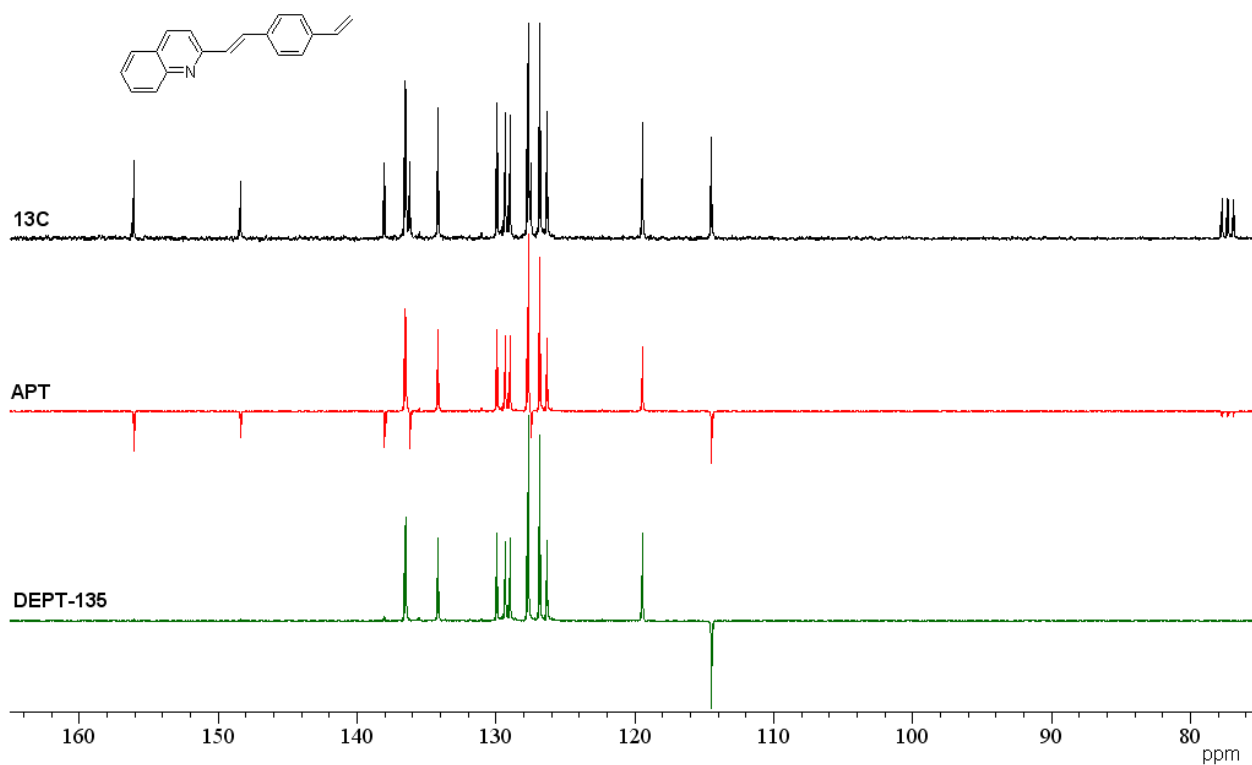






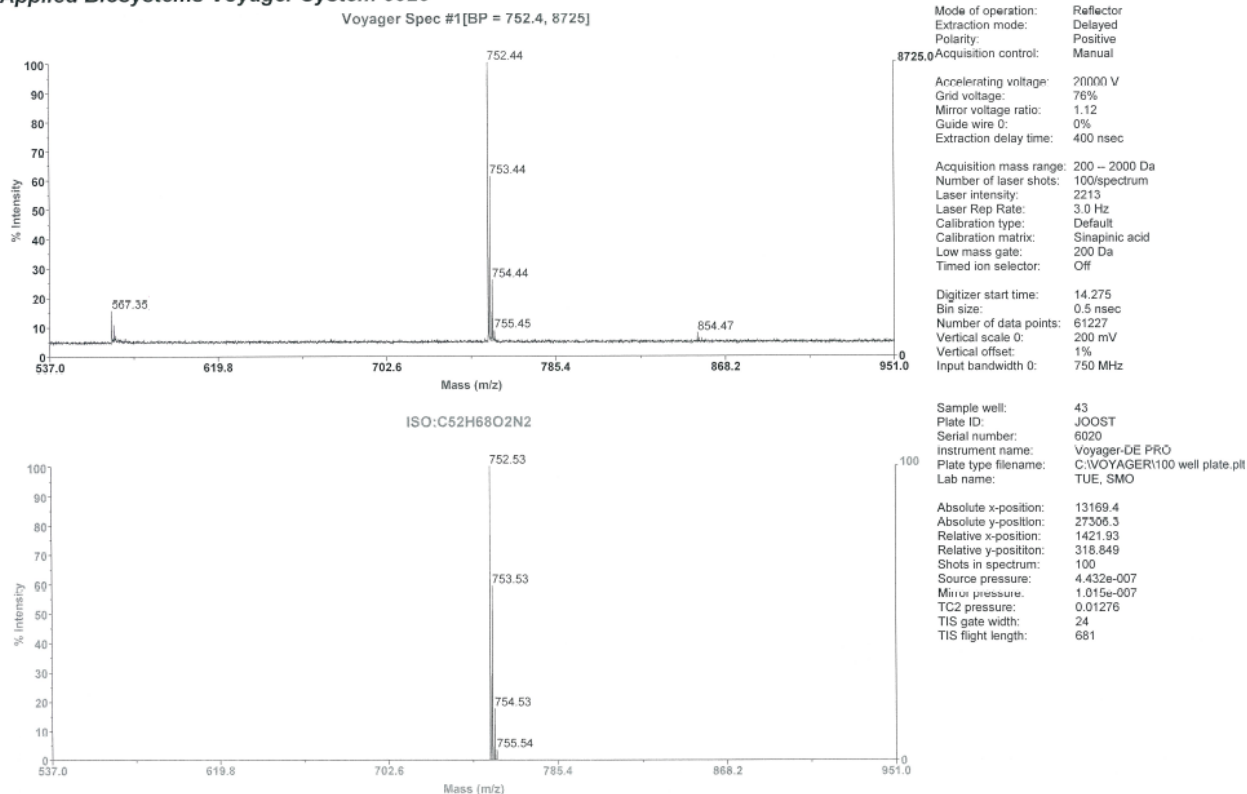






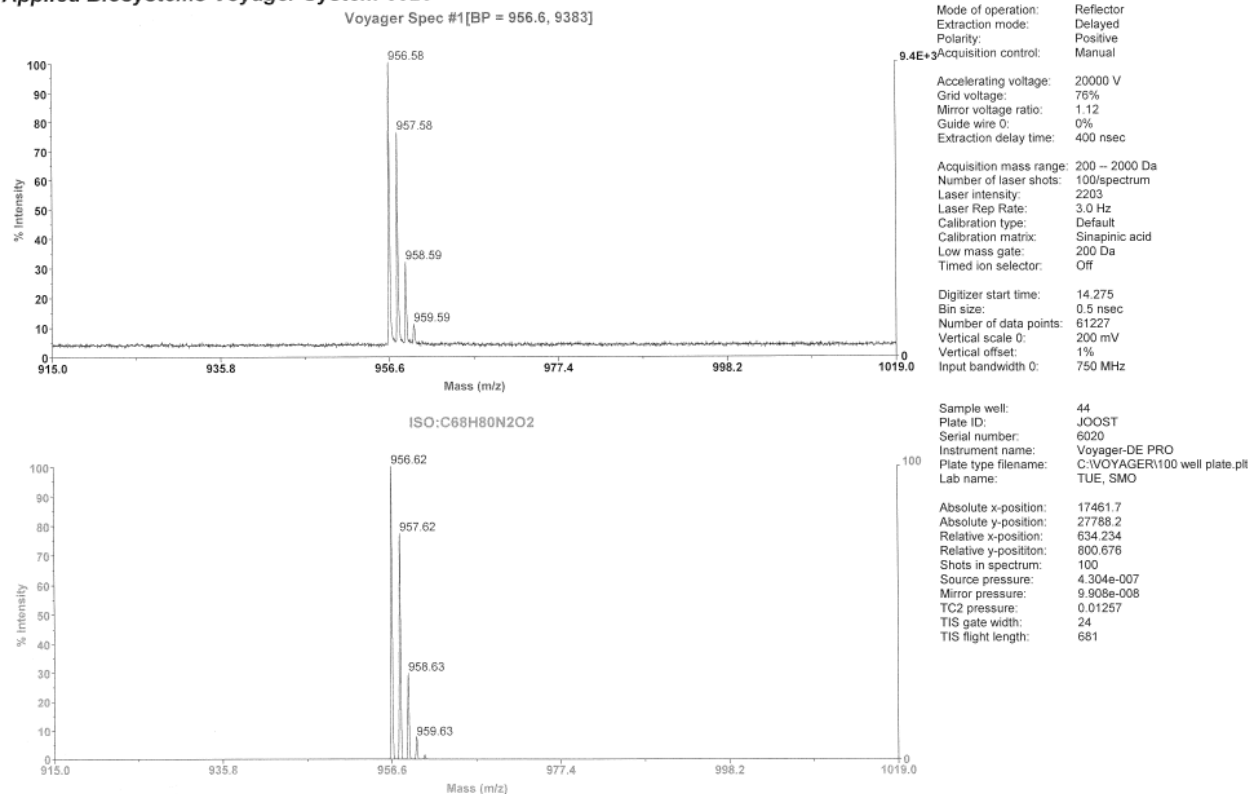
II. MALDI-TOF Spectrometry of selected oligomers.

Applied Biosystems Voyager System 6020



MALDI-TOF MS spectrum of ***E*-3QPV** with DCTB matrix in the reflector positive ion mode together with a simulated spectrum of the product radical cation.

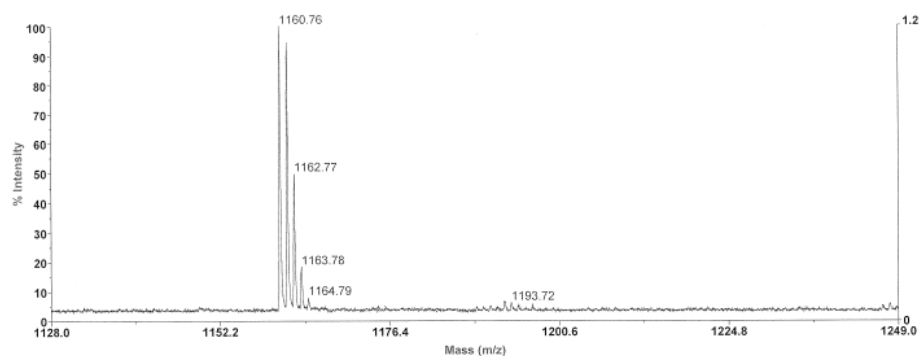
Applied Biosystems Voyager System 6020



MALDI-TOF MS spectrum of ***E,E*-5QPV** with DCTB matrix in the reflector positive ion mode together with a simulated spectrum of the product radical cation.

Applied Biosystems Voyager System 6020

Voyager Spec #1[BP = 808.4, 12672]

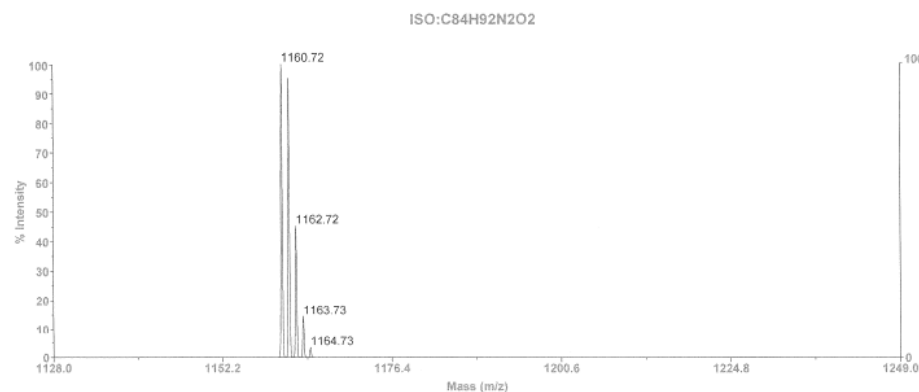


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Extraction mode: Delayed
Polarity: Positive
Acquisition control: Manual
Accelerating voltage: 20000 V
Grid voltage: 76%
Mirror voltage ratio: 1.12
Guide wire 0: 0%
Extraction delay time: 400 nsec
Acquisition mass range: 200 – 2500 Da
Number of laser shots: 100/spectrum
Laser intensity: 2253
Laser Rep Rate: 3.0 Hz
Calibration type: Default
Calibration matrix: Sinapinic acid
Low mass gate: 200 Da
Timed ion selector: Off

Digitizer start time: 14.275
Bin size: 0.5 nsec
Number of data points: 71796
Vertical scale 0: 200 mV
Vertical offset: 1%
Input bandwidth 0: 750 MHz

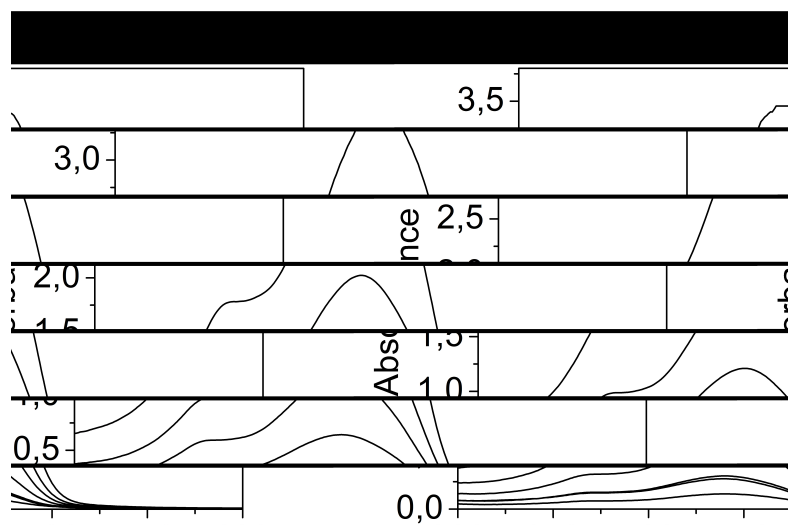
Sample well: 45
Plate ID: JOOST
Serial number: 6020
Instrument name: Voyager-DE PRO
Plate type filename: C:\VOYAGER\100 well plate.plt
Lab name: TUE, SMO

Absolute x-position: 22280
Absolute y-position: 27581.2
Relative x-position: 372.471
Relative y-position: 593.662
Shots in spectrum: 100
Source pressure: 3.79e-007
Mirror pressure: 9.072e-008
TC2 pressure: 0.01204
TIS gate width: 24
TIS flight length: 681

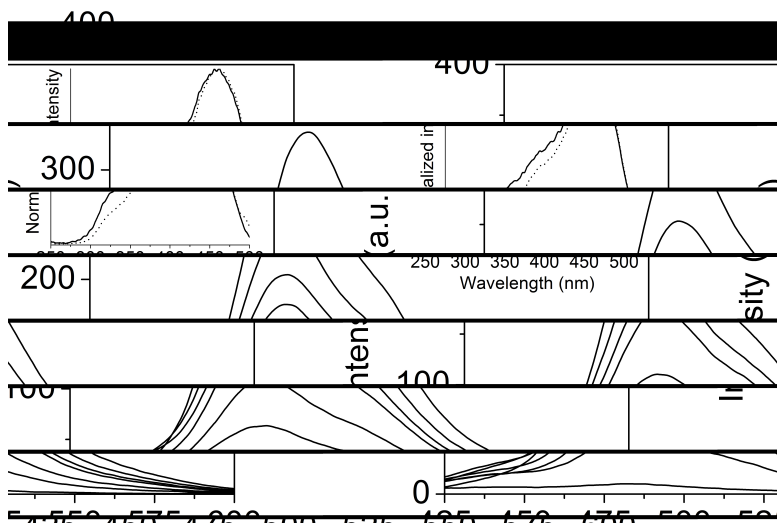
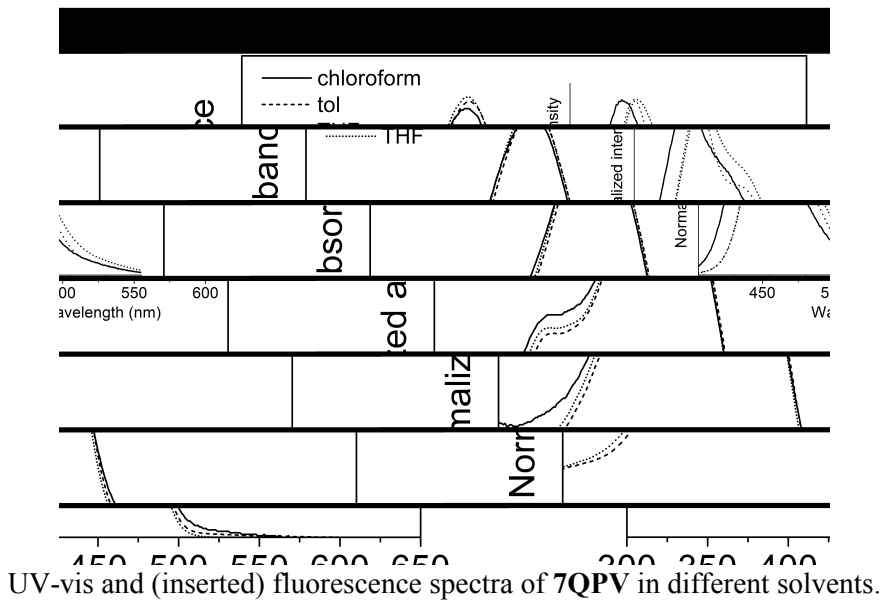


MALDI-TOF MS spectrum of *E,E,E*-7QPV with DCTB matrix in the reflector positive ion mode together with a simulated spectrum of the product radical cation.

III. Additional electronic spectra of 7QPV as example for the nQPV series

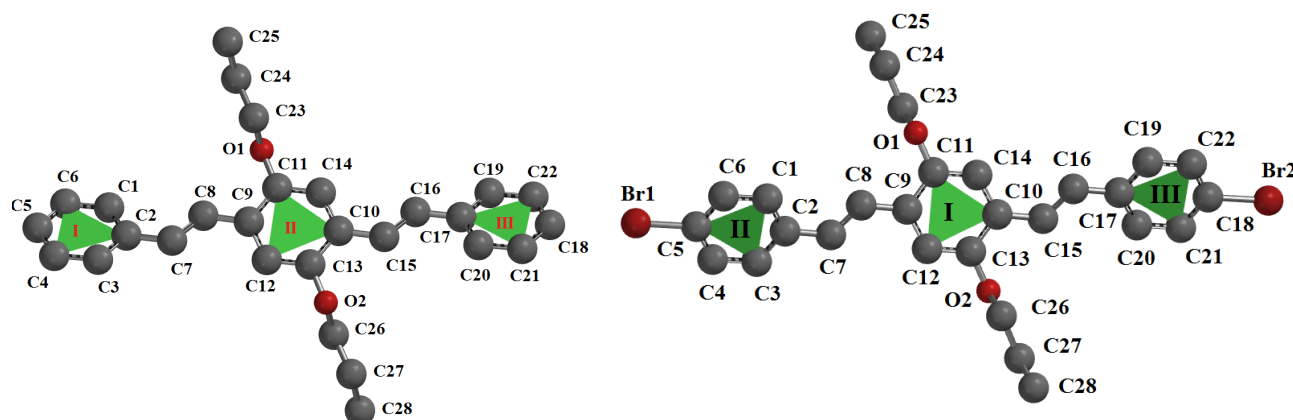


UV-Vis spectra of 7QPV in chloroform at different concentrations between $1.77 \cdot 10^{-5}$ to $7.12 \cdot 10^{-7}$ M.



Fluorescence spectra of **7QPV** at different excitation wavelength; from bottom to top: 300, 320, 340, 360, 380, 400, 420nm. Inserted: excitation spectra at 487nm (solid line) and 517nm as emission wavelength.

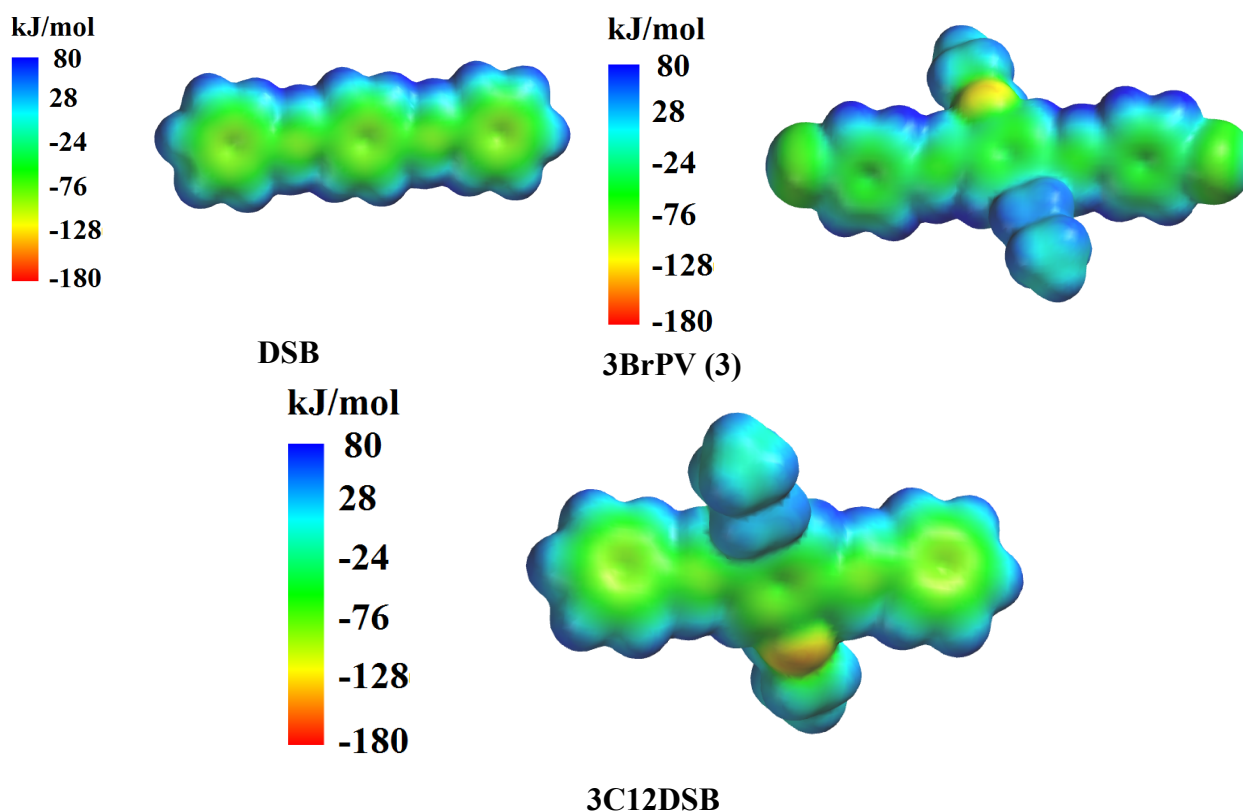
IV.- Theoretical calculations



3C12DSB

3BrPV (3)

Minimum energy (optimized) structure of **3C12DSB** and **3BrPV** by DFT/6-311+G(d,p).



Molecular electrostatic potential (MEP) in gas phase of **3DSB**, **3BrPV** and **3C12DSB** trimers