Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2017

Supporting Information

Laterally Stretched Polycyclic Aromatic Hydrocarbons: Synthesis of Dibenzophenanthroheptaphene and Tetrabenzotriphenyleno-pyranthrene Derivatives.

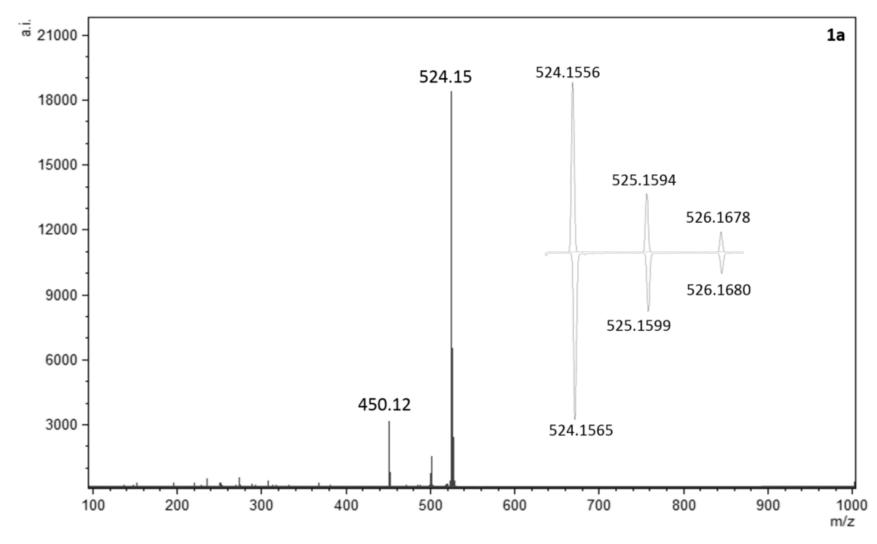
Bassam Alameddine,*† Rajamohanan Sobhana Anju,† Suchetha Shetty,† Noorullah Baig,† Fakhreia Al-Sagheer,‡ Saleh Al-Mousawi, ‡ Titus Andreas Jenny[§]

[†]Department of Mathematics and Natural Sciences, Gulf University for Science and Technology, Kuwait. [‡]Department of Chemistry, University of Kuwait, Kuwait.

[§]Department of Chemistry, University of Fribourg, Switzerland.

CONTENTS

- I. Experimental details (HR-MS of 1a-c, 2a-b, 4a-c, 9 and 10a,b and ¹H-NMR of 1c, 2b, 4a-c, 9, 10a-b, 13a,b.
- II. UV-Emission spectra of 9.
- III. II. Computational Details (3D optimized structures and their HOMO-LUMO configurations).



I. Experimental details MALDI 1a-c, 2a-b, 4a-c, 9 and 10a,b.

Figure S1. HR-MALDI spectrum of 1a

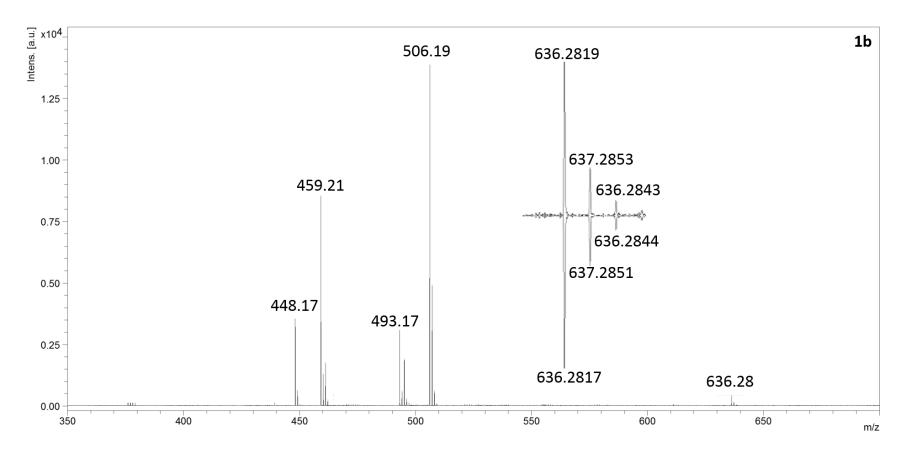


Figure S2. HR-MALDI spectrum of 1b

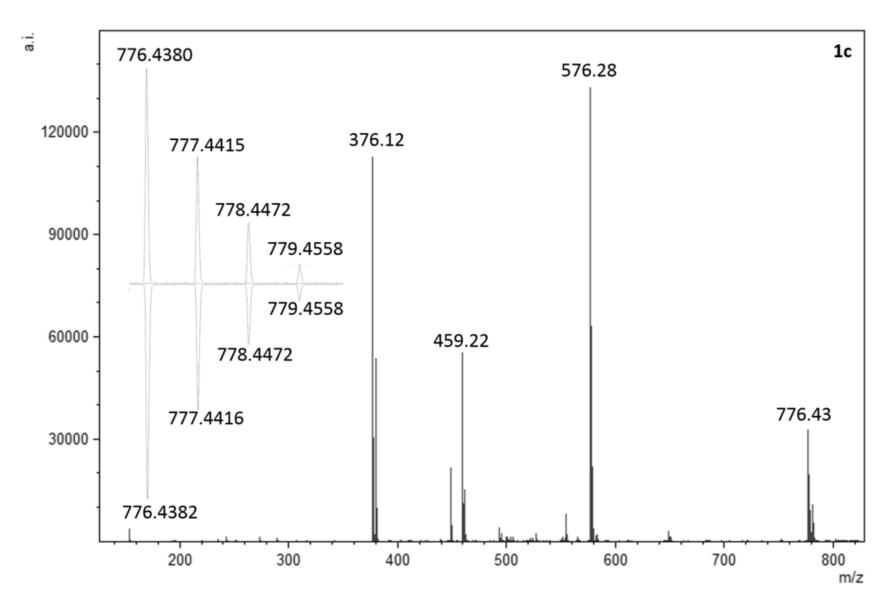


Figure S3. HR-MALDI spectrum of 1c

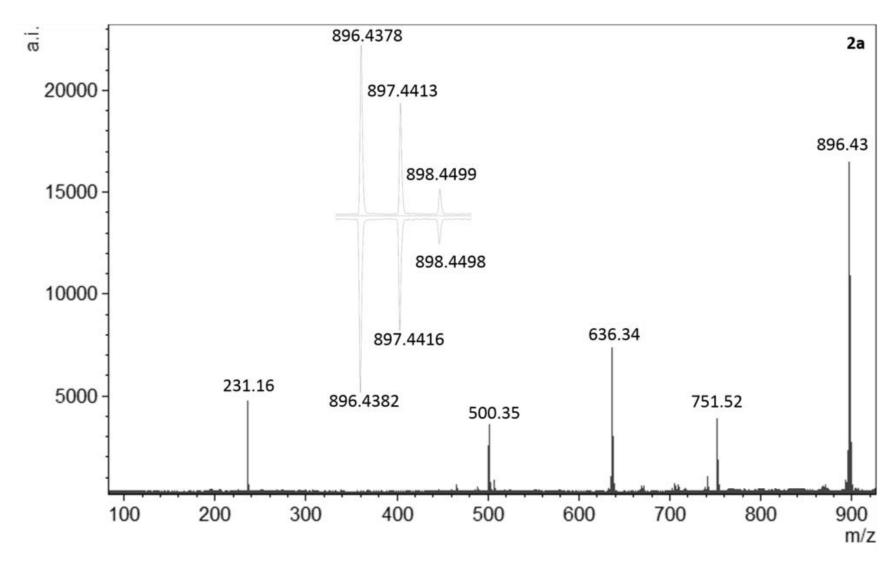


Figure S4. HR-MALDI spectrum of 2a

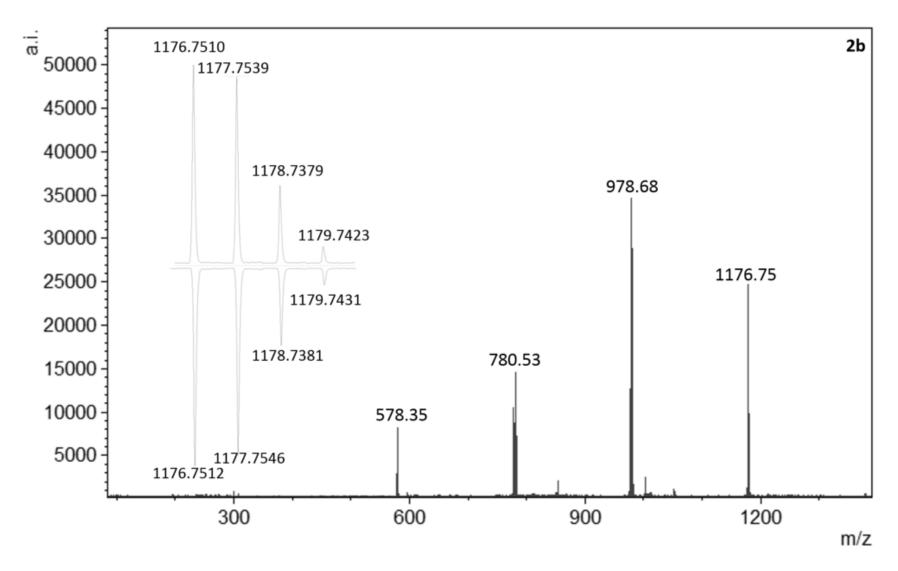


Figure S5. HR-MALDI spectrum of 2b

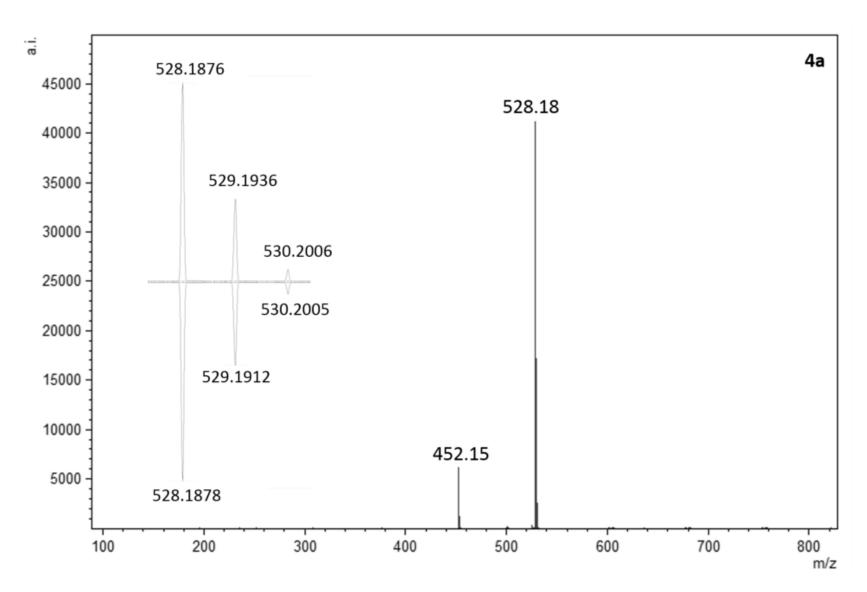


Figure S6. HR-MALDI spectrum of 4a

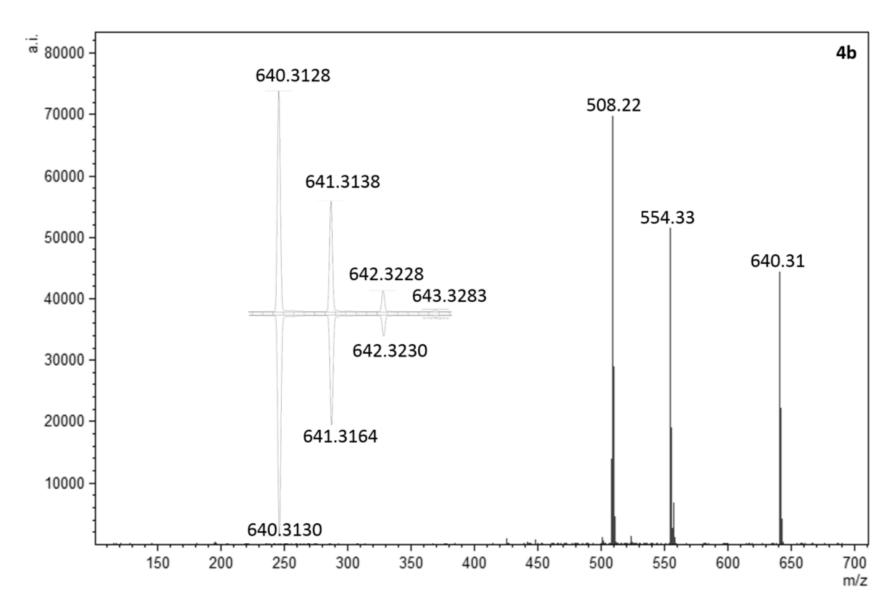


Figure S7. HR-MALDI spectrum of 4b

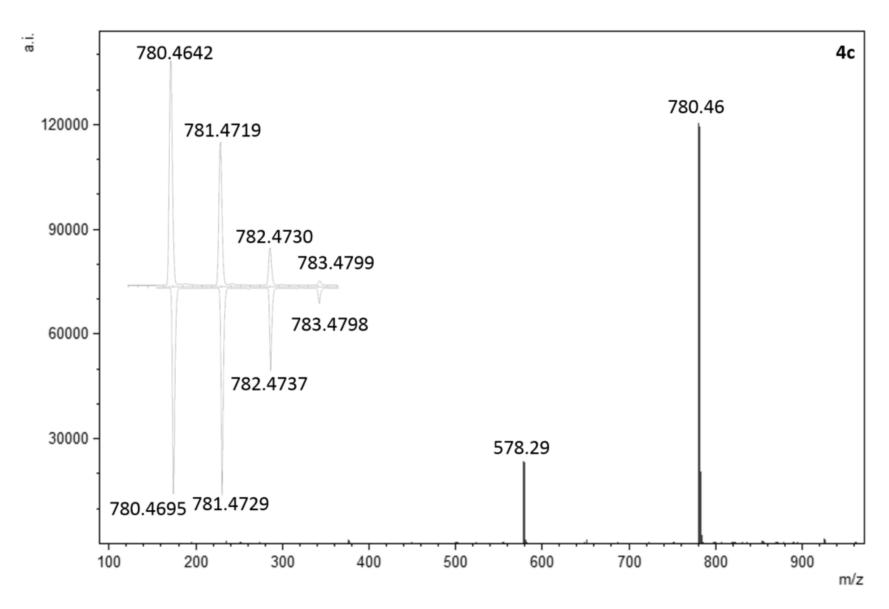


Figure S8. HR-MALDI spectrum of 4c

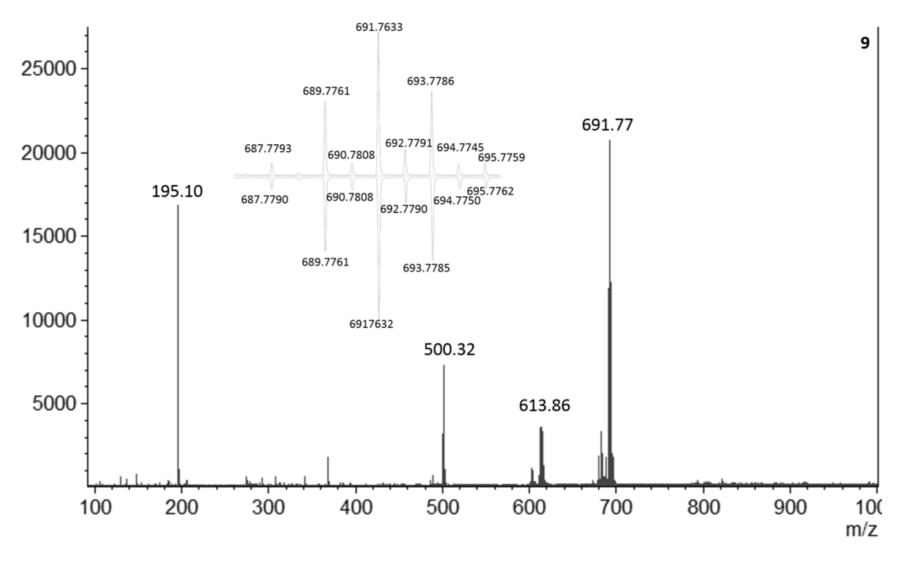


Figure S9. HR-MALDI spectrum of 9

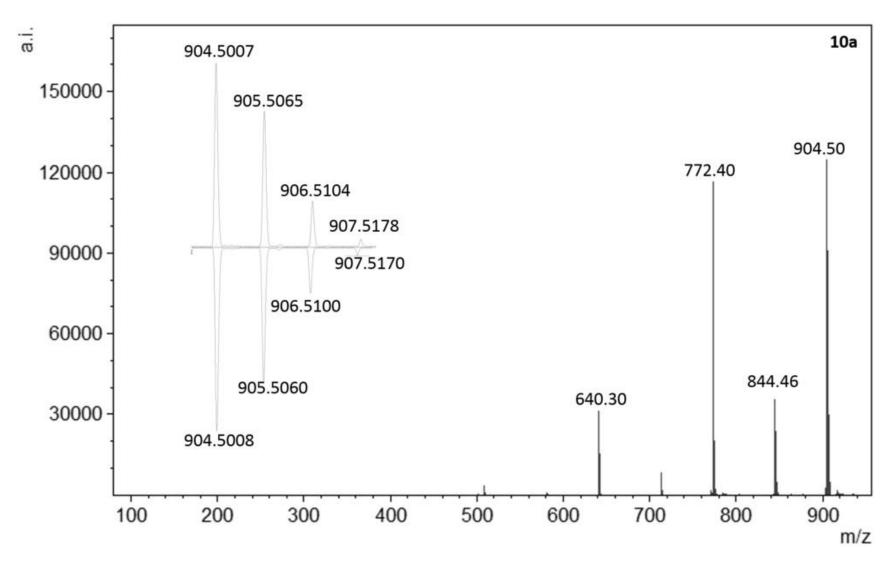
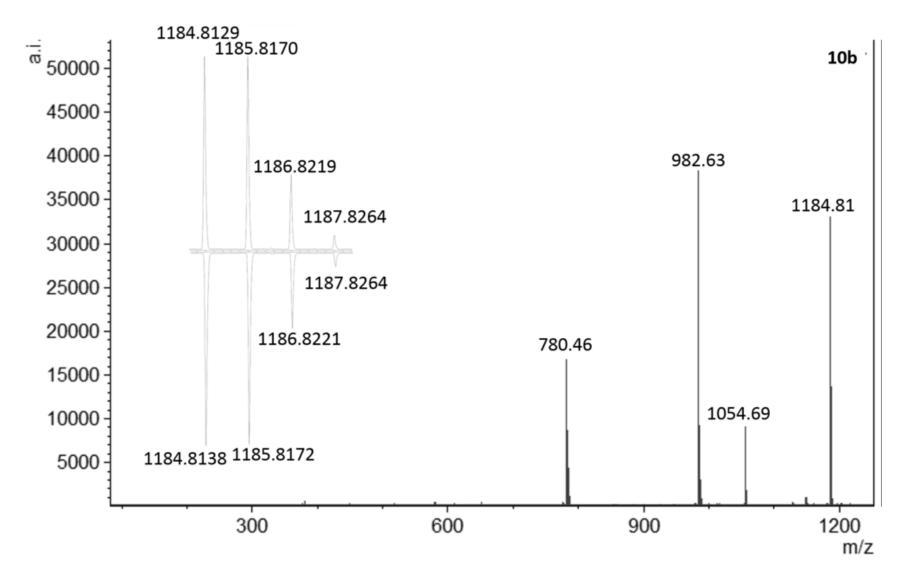


Figure S10 HR-MALDI spectrum of 10a





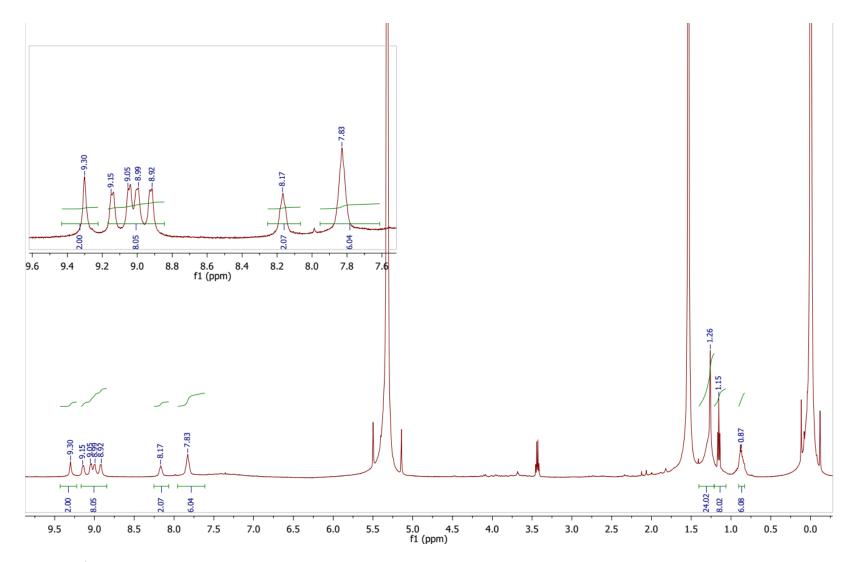


Figure S12. ¹H NMR spectrum of 1c

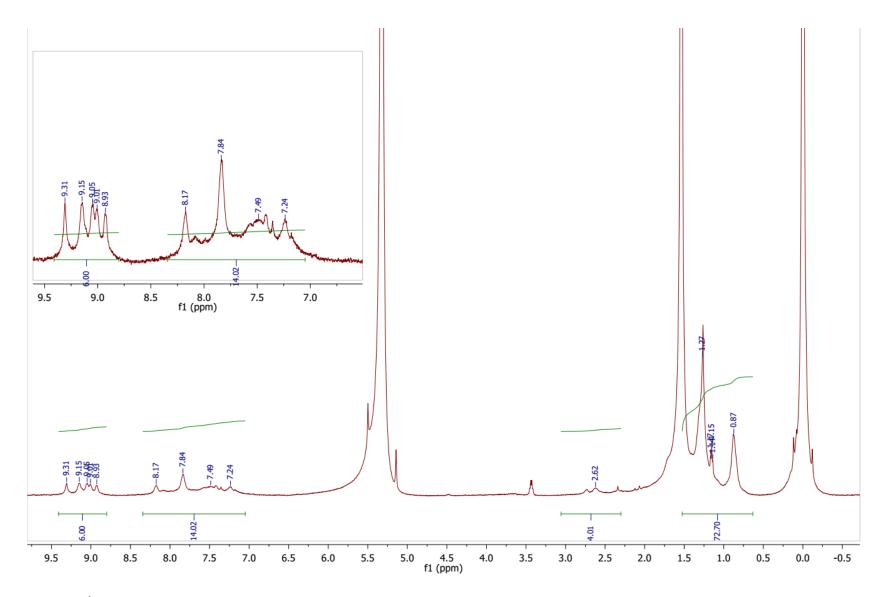


Figure S13. ¹H NMR spectrum of 2b

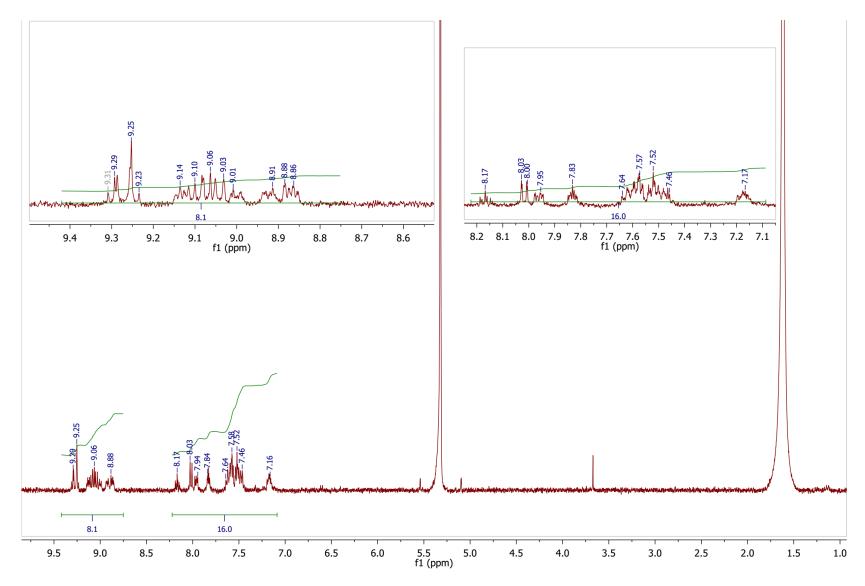


Figure S14. ¹H NMR spectrum of 4a

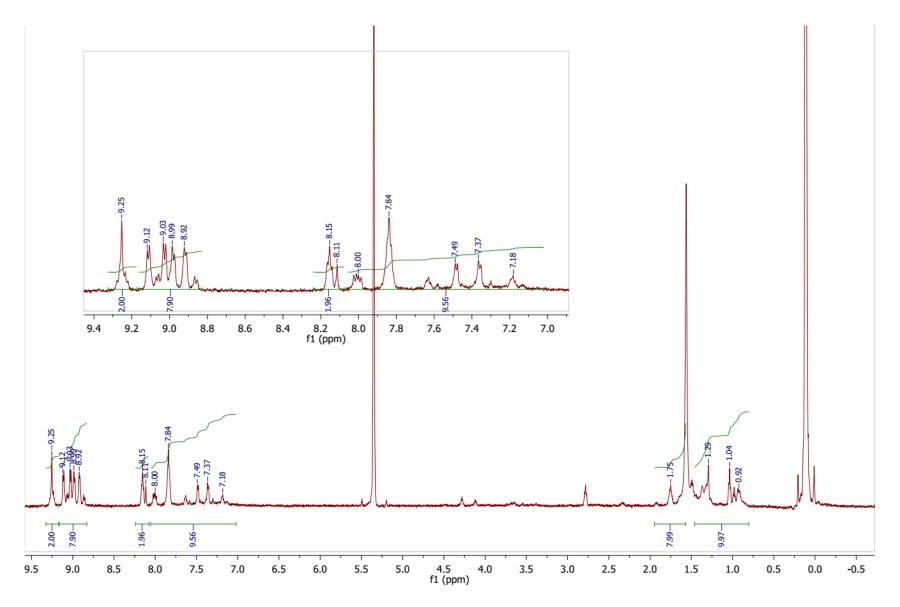


Figure S15. ¹H NMR spectrum of 4b

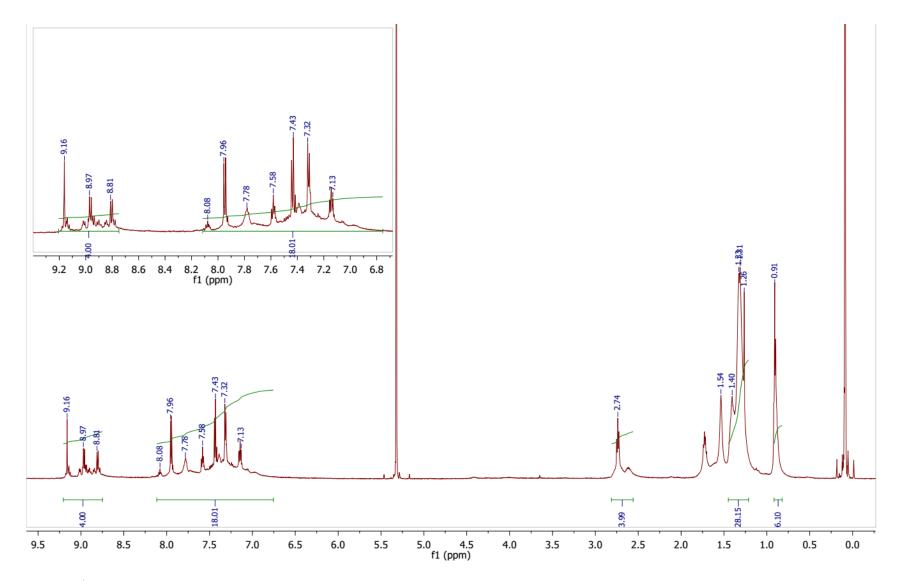


Figure S16. ¹H NMR spectrum of 4c

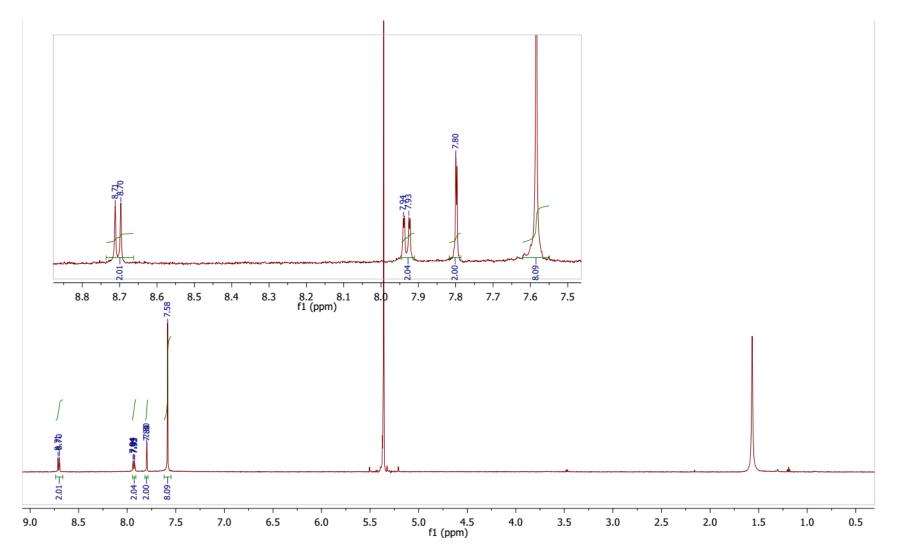


Figure S17. ¹H NMR spectrum of 9

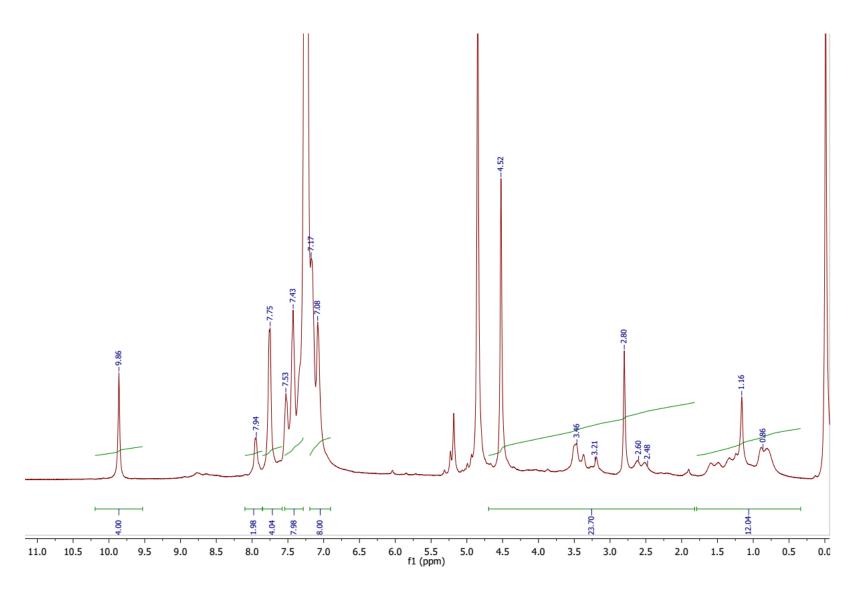


Figure S18. ¹H NMR spectrum of 10a

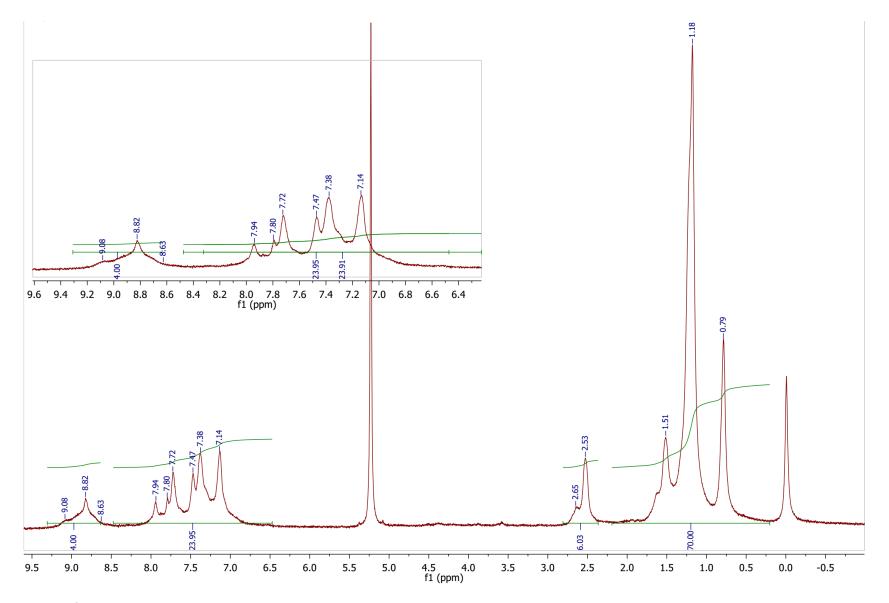


Figure S19. ¹H NMR spectrum of 10b

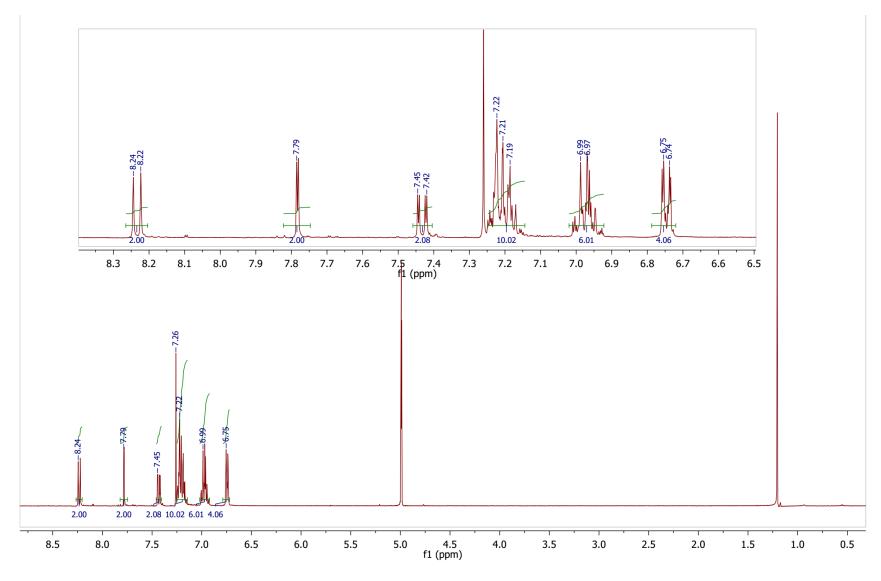


Figure S20. ¹H NMR spectrum of 13a

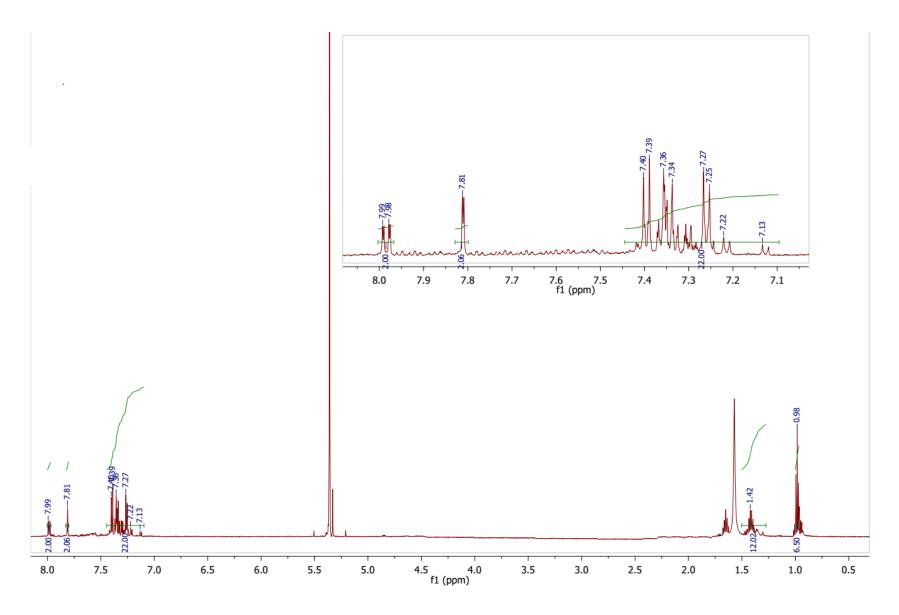


Figure S21. ¹H NMR spectrum of 13b

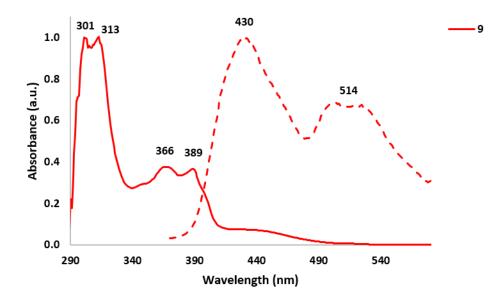


Figure S22. Normalized absorption and emission spectra for the pentaphene derivatives 9 in THF. The solid lines represent absorption spectra and the dotted lines correspond to emission spectra.

II. Computational details

basis set with R = H (1a and 2-H) or Me (1-Me and 2-Me) instead of the alkyl groups for simplicity. No **Optimized structure** номо LUMO 1a 1Me $\mathbf{2}_{\mathrm{H}}$ 2Me

Table S1. Optimized structures and HOMO-LUMO frontier orbitals of DBPH and TBTP at the level of the B3LYP/6-31 G*