Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Electron and energy transfer in a porphyrin-oxoporphyrinogen-fullerene triad, ZnP-OxP-C_{60}

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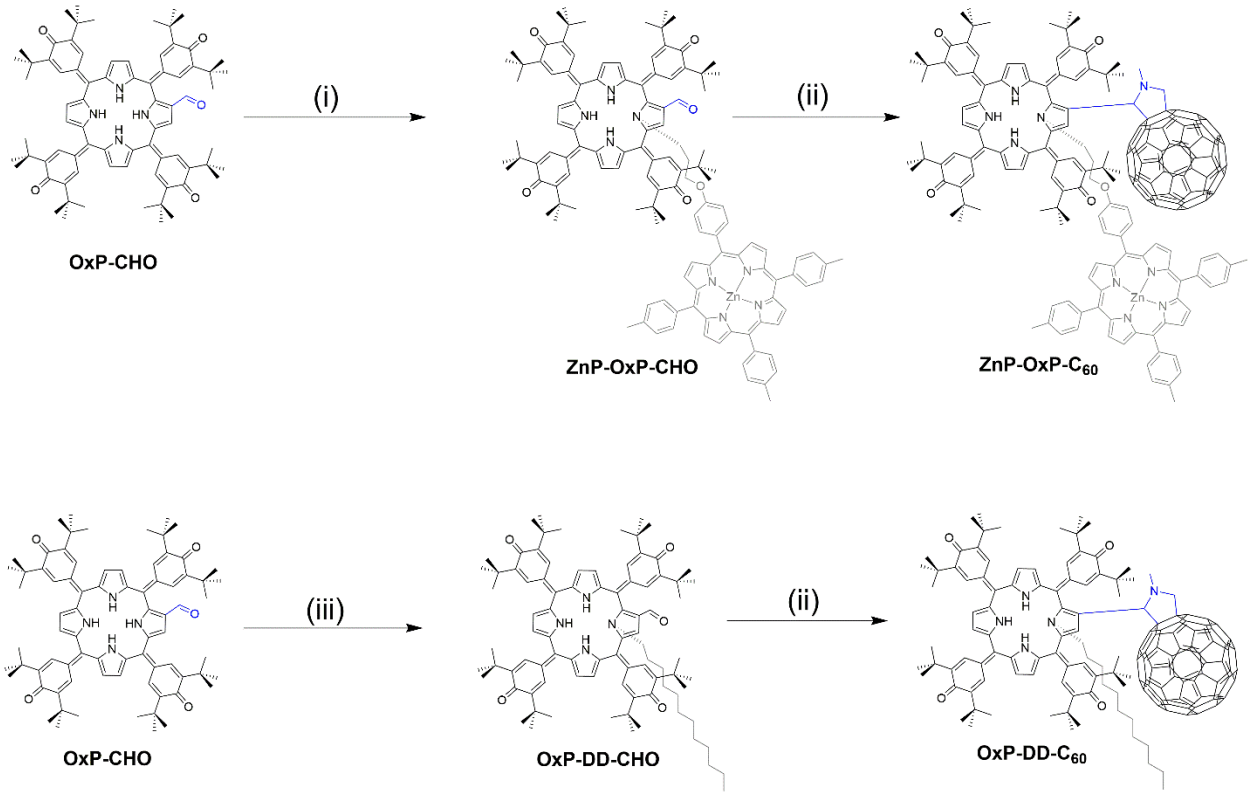
Synthesis Overview:



Scheme S1. Synthesis of the compounds. (i) [5-(4-(3-bromopropoxy)phenyl))-10,15,20-tri(4-methylphenyl)porphyrinato]zinc(II)/Na_2CO_3/acetone/reflux, (ii) C_{60}/N-methylglycine/toluene/reflux, (iii) n-1-bromodecane/ K_2CO_3/acetone/reflux.

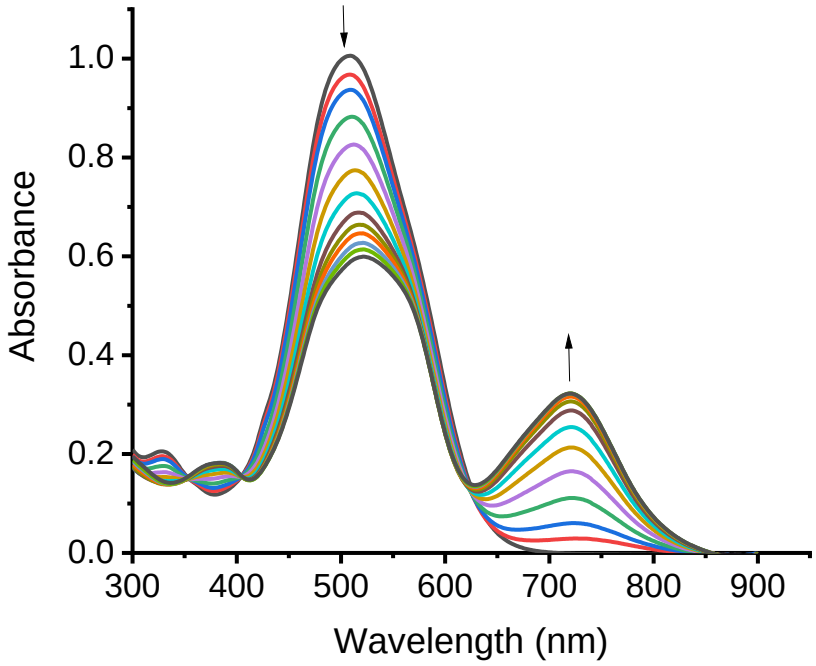
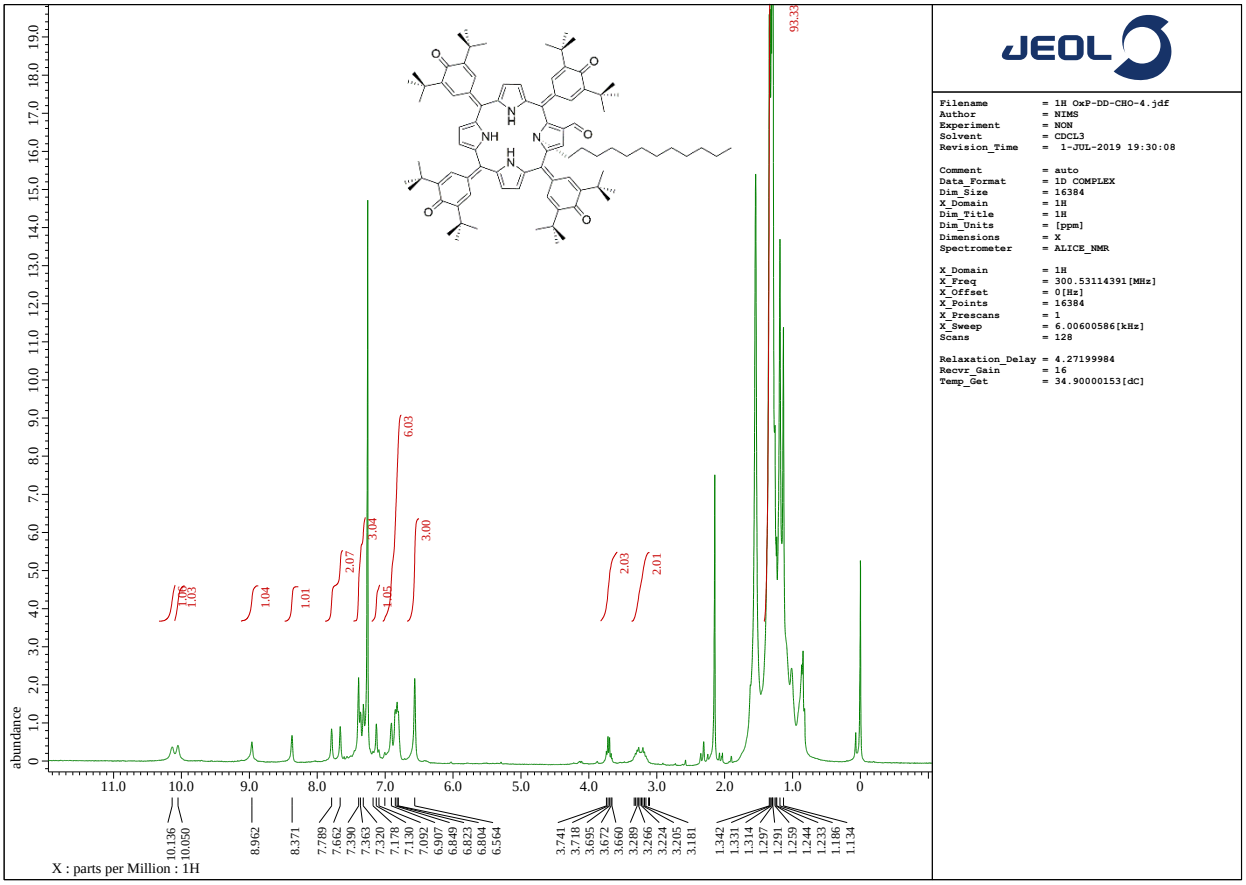


Figure S1. Spectral changes observed during increased addition of $NOBF_4$ (in methanol) to a solution of **OxP** in DCB.

^{1}H NMR spectrum of N_{21}-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**



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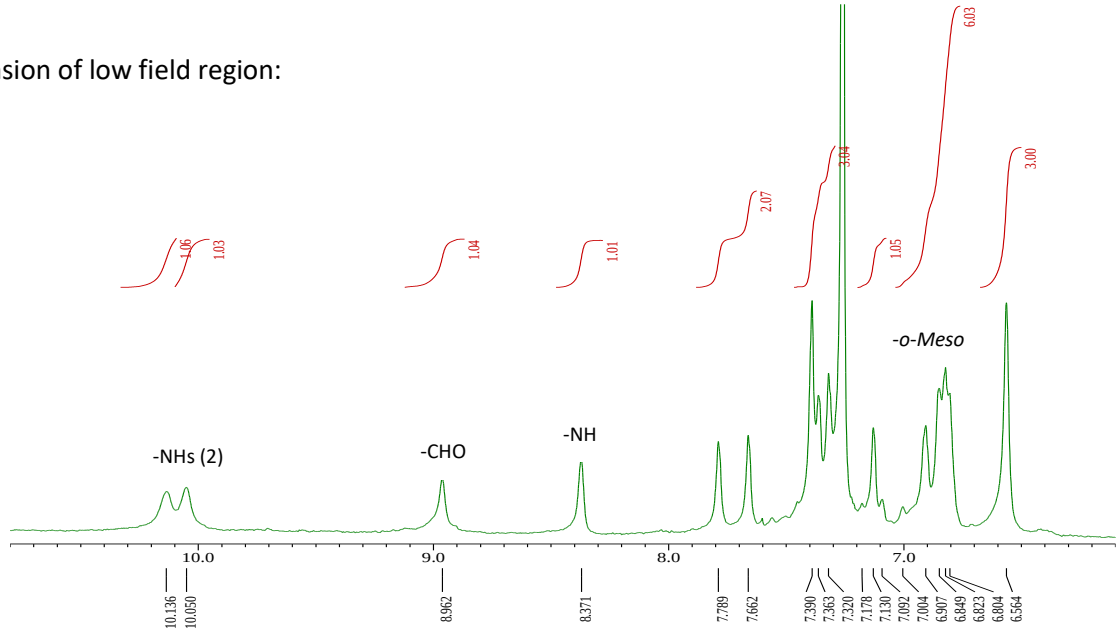
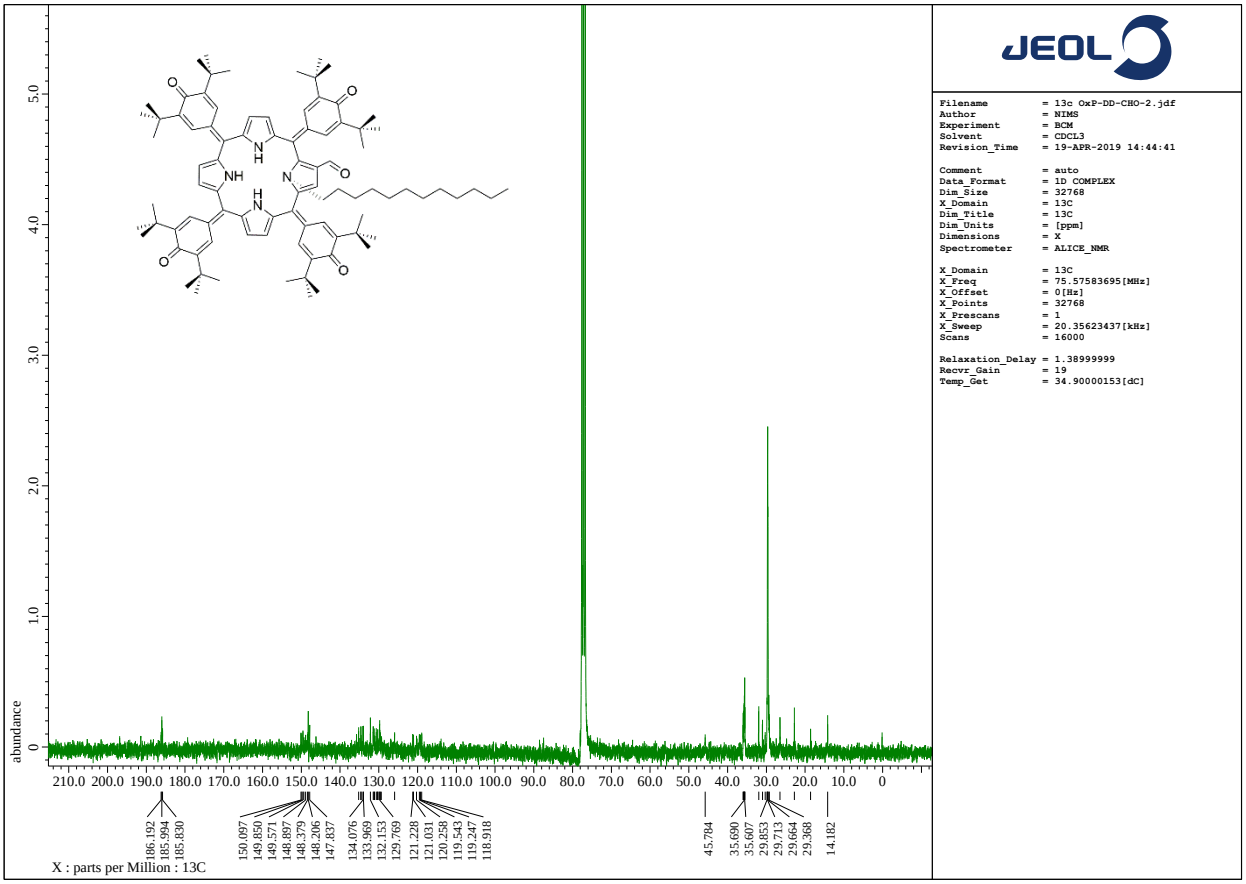
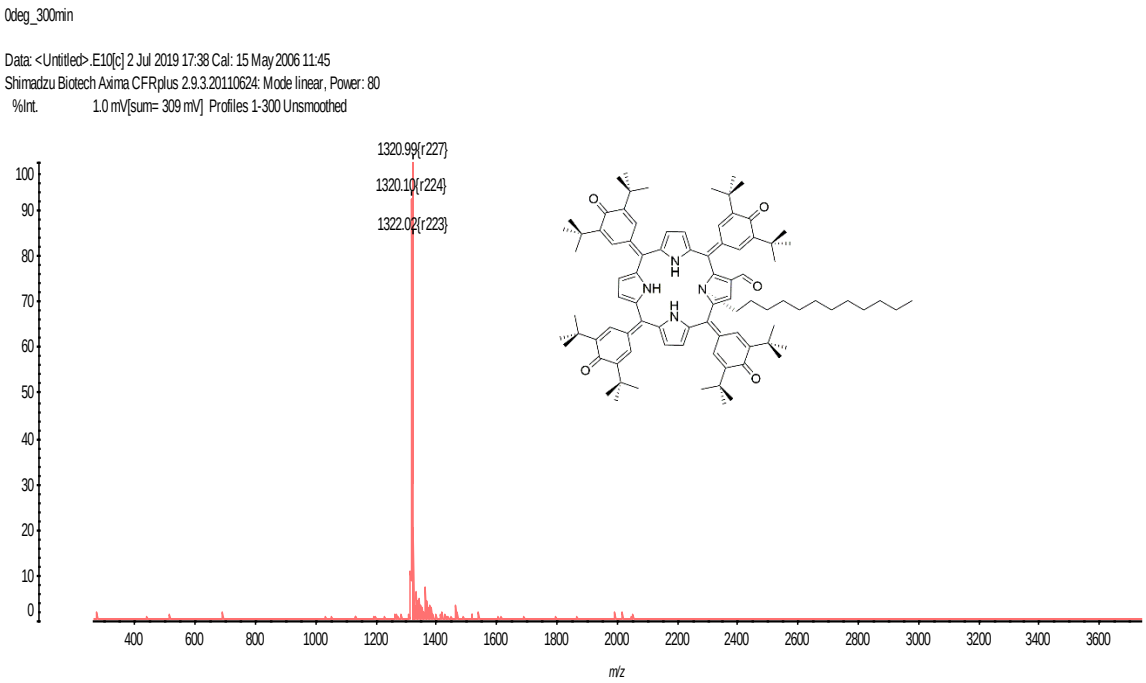


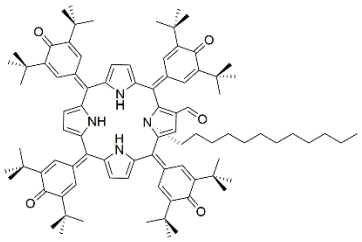
^{13}C NMR spectrum of N_{21}-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**

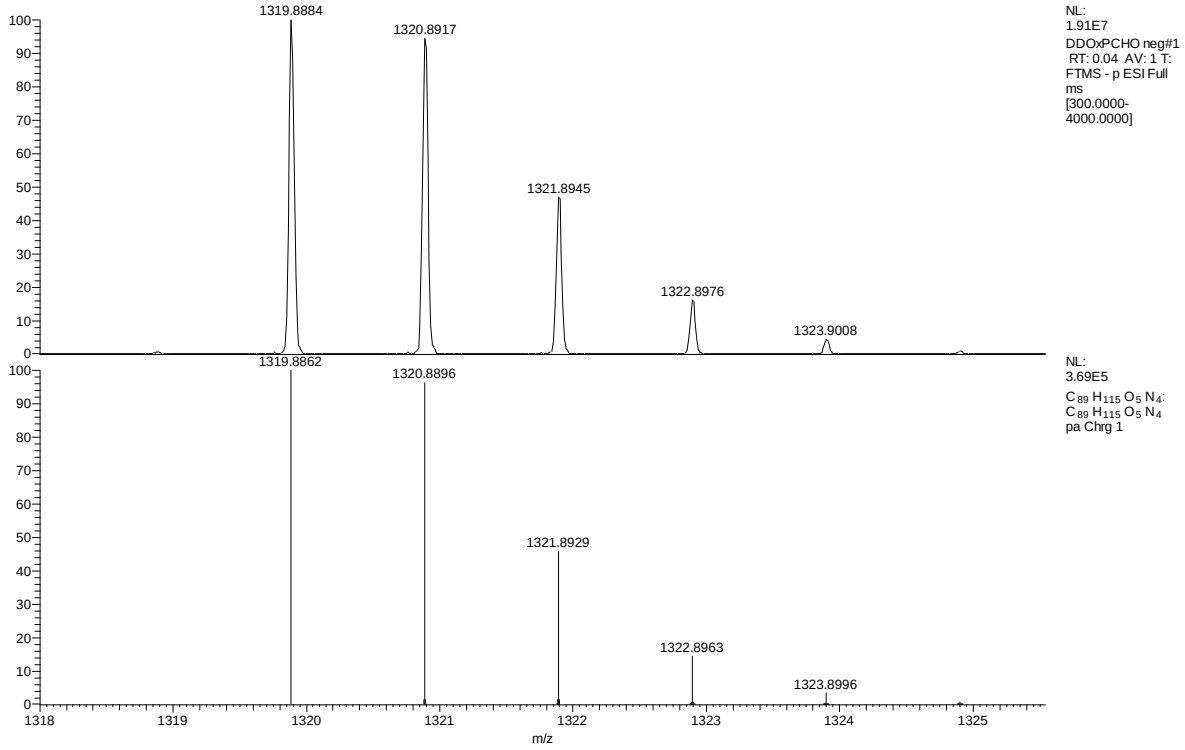


Mass spectrum of N_{21}-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**

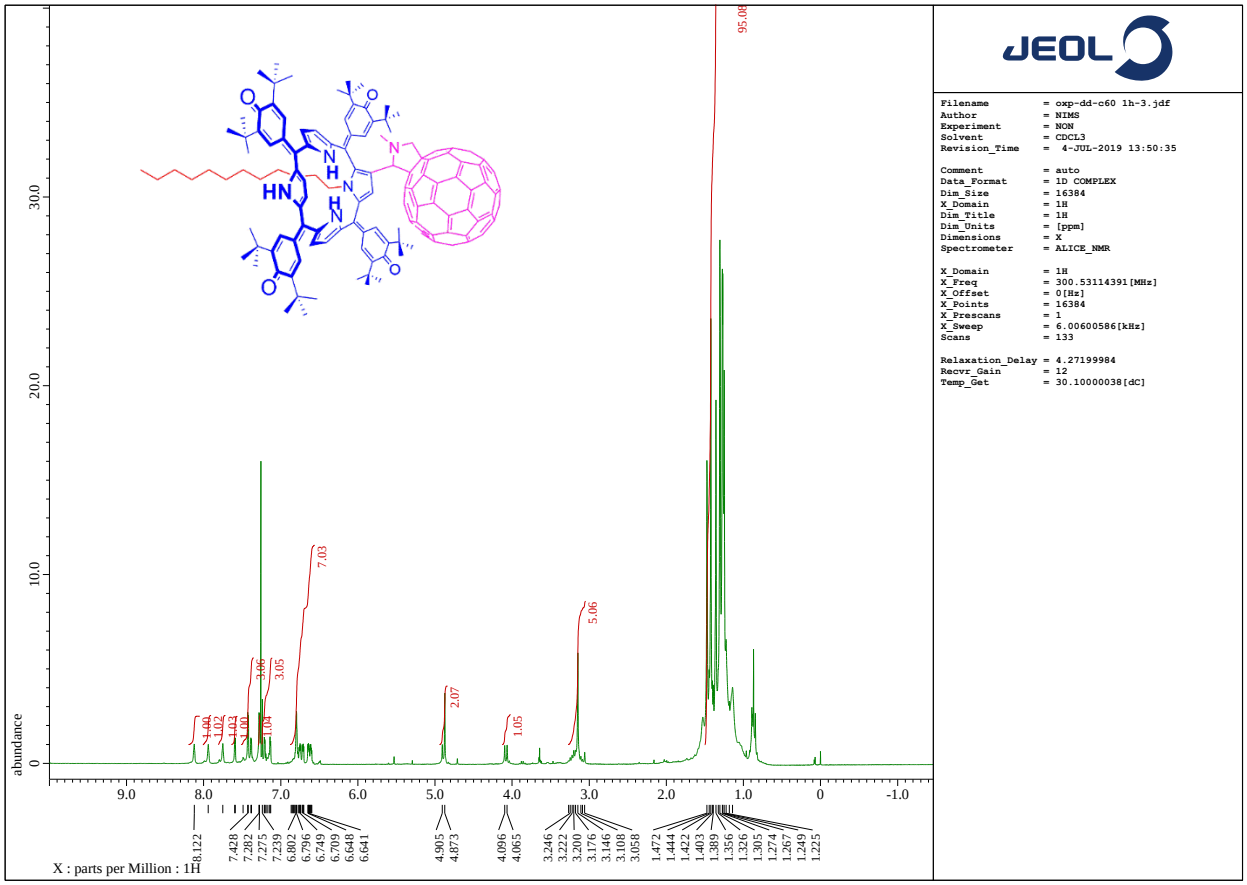


ESI-TOF-MS Spectrum of N_{21}-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**





^{1}H NMR spectrum of **OxP-DD-C$_{60}$** Dyad



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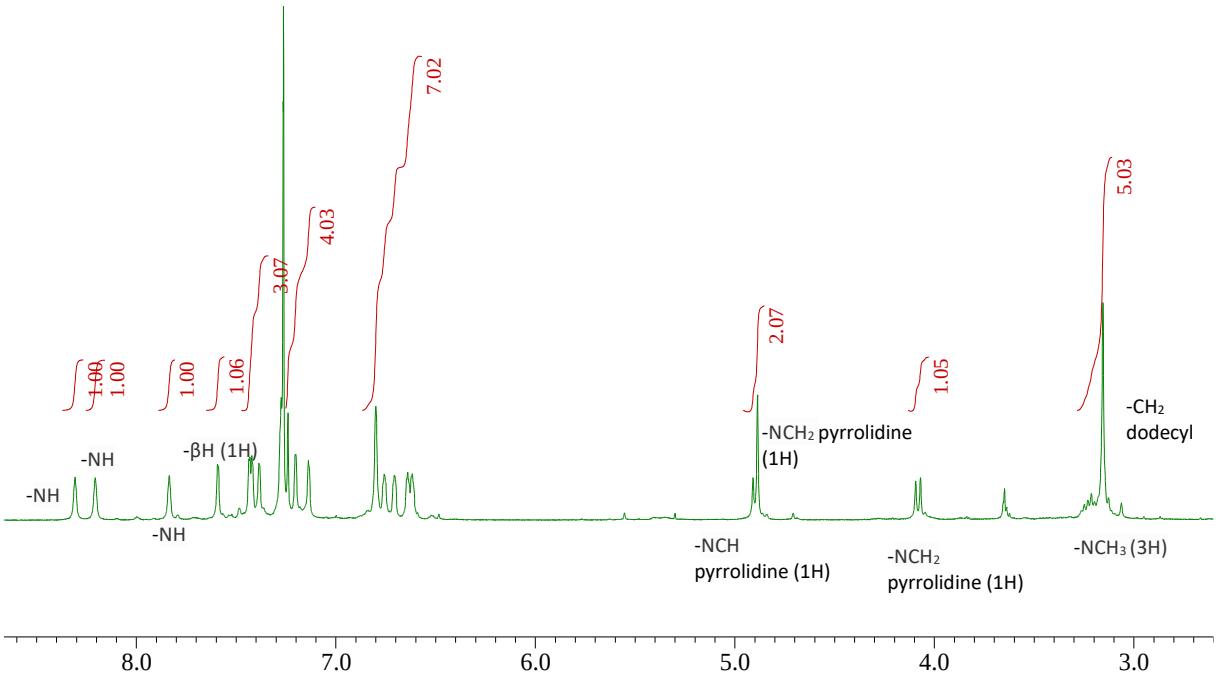
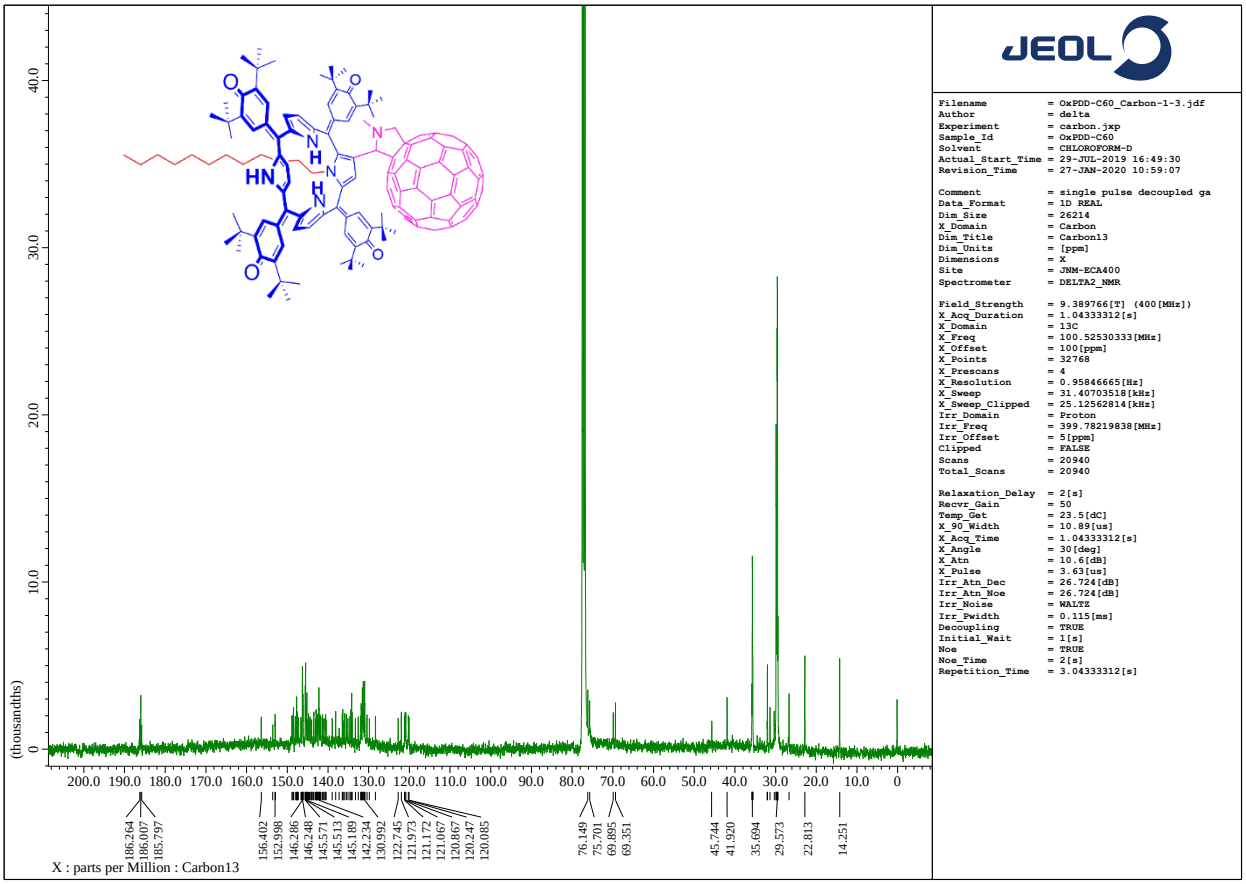
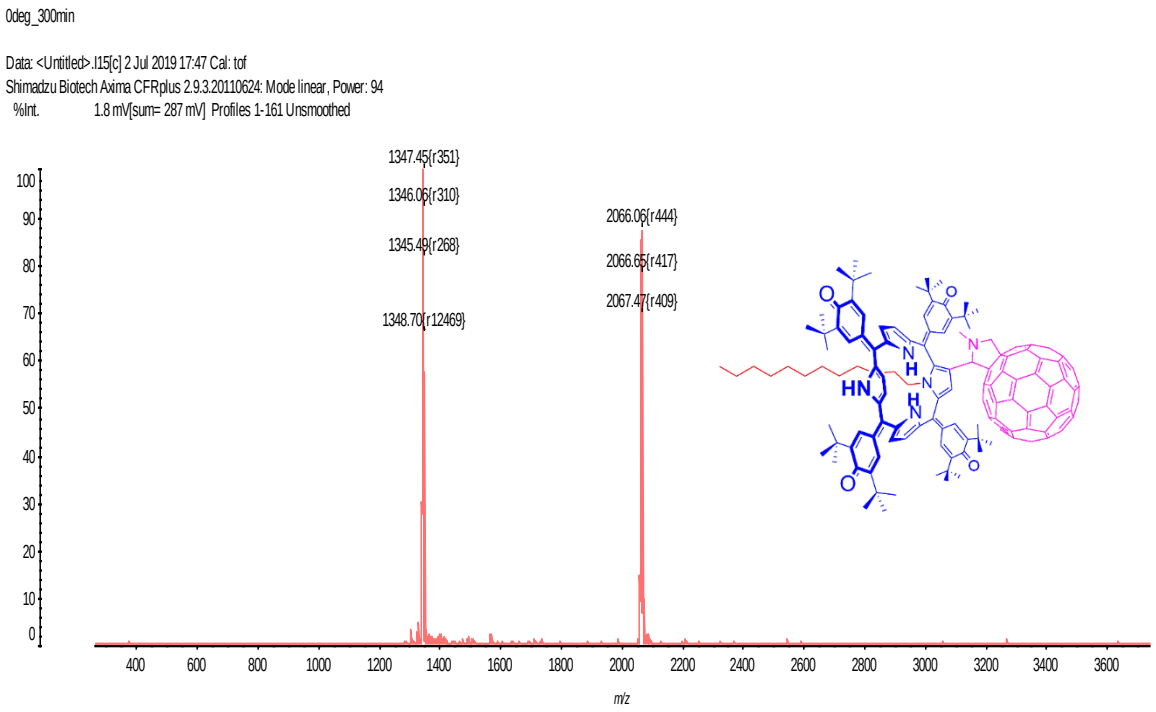


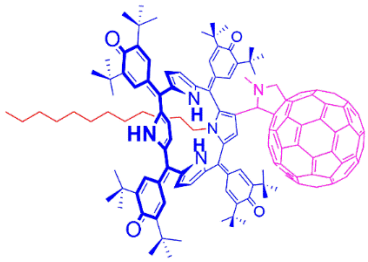
^{13}C NMR spectrum of **OxP-DD-C$_{60}$** Dyad

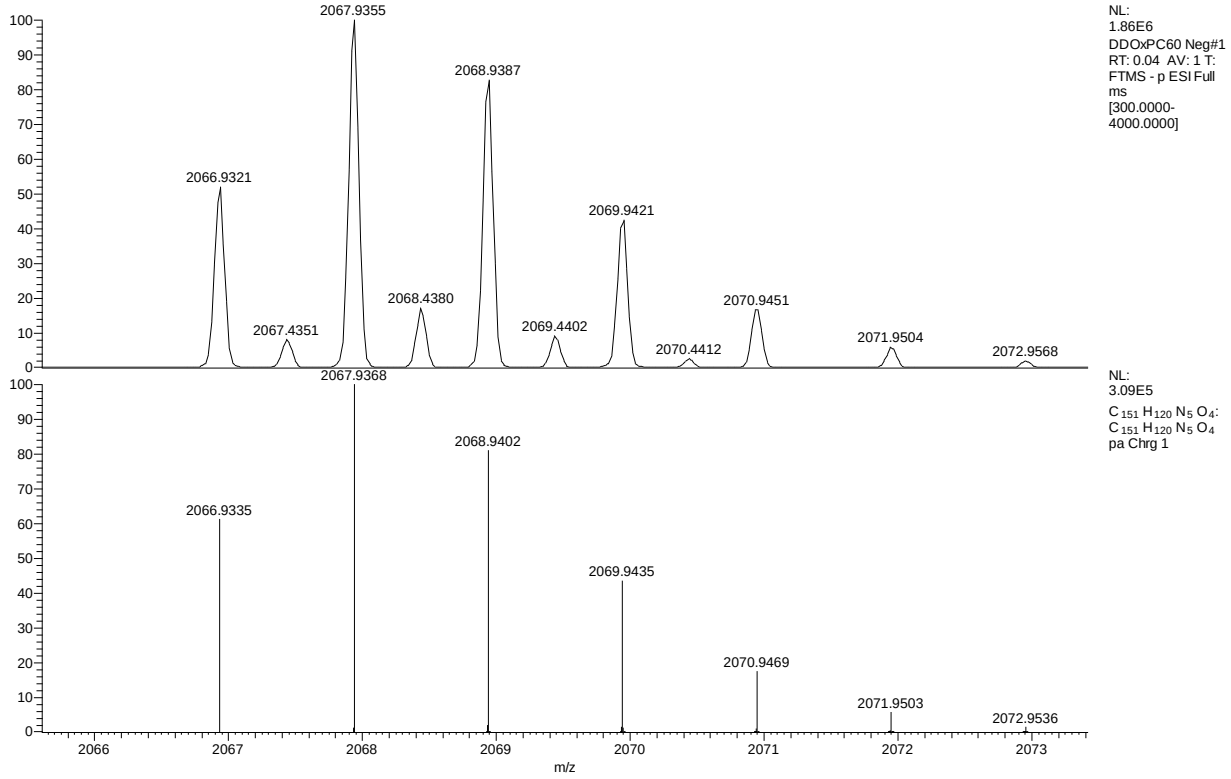


Mass spectrum of **OxP-DD-C_{60}** Dyad

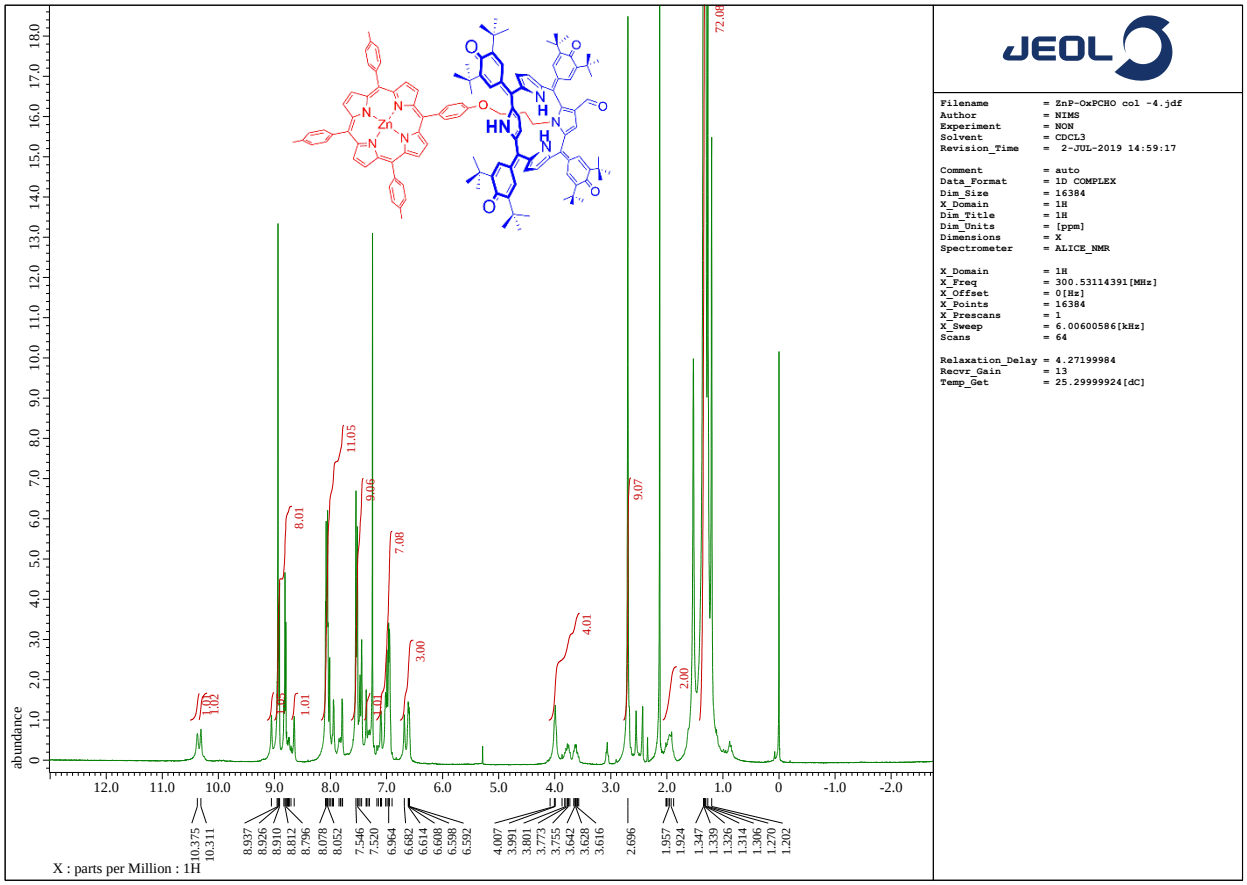


ESI-TOF-MS spectrum of **OxP-DD-C_{60}** Dyad





^{1}H NMR spectrum of **ZnP-OxP-CHO** Dyad



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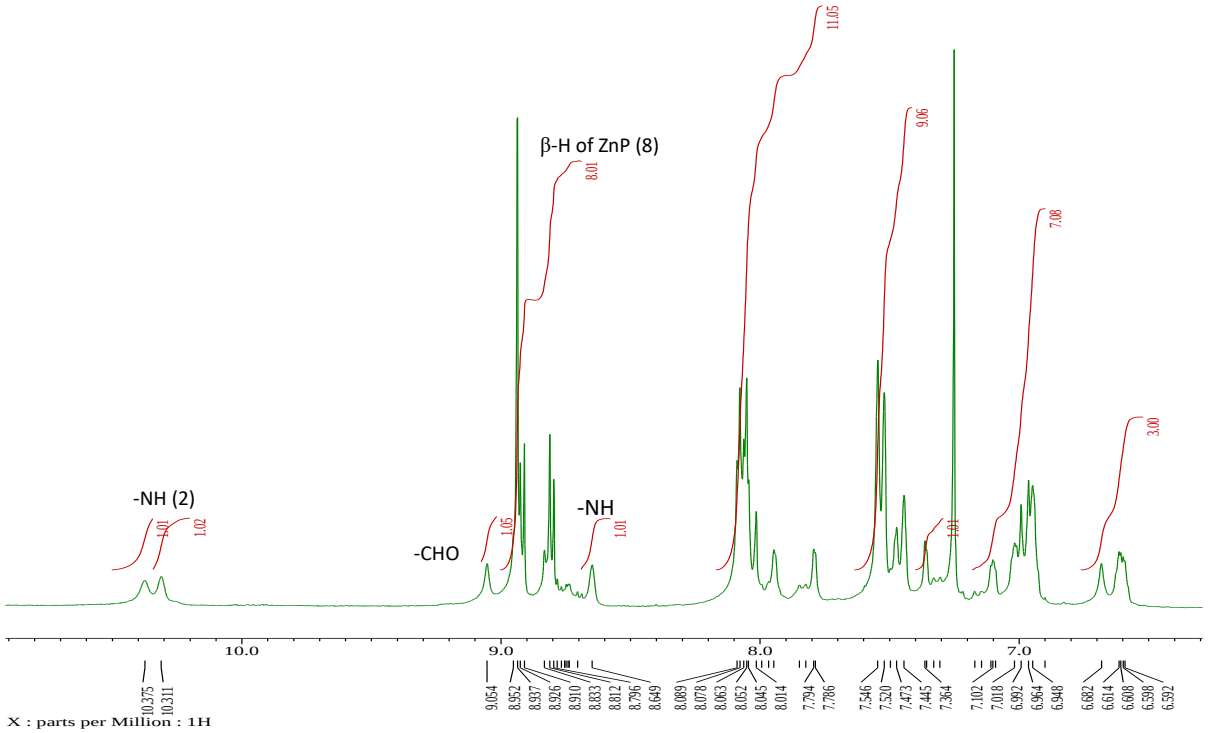
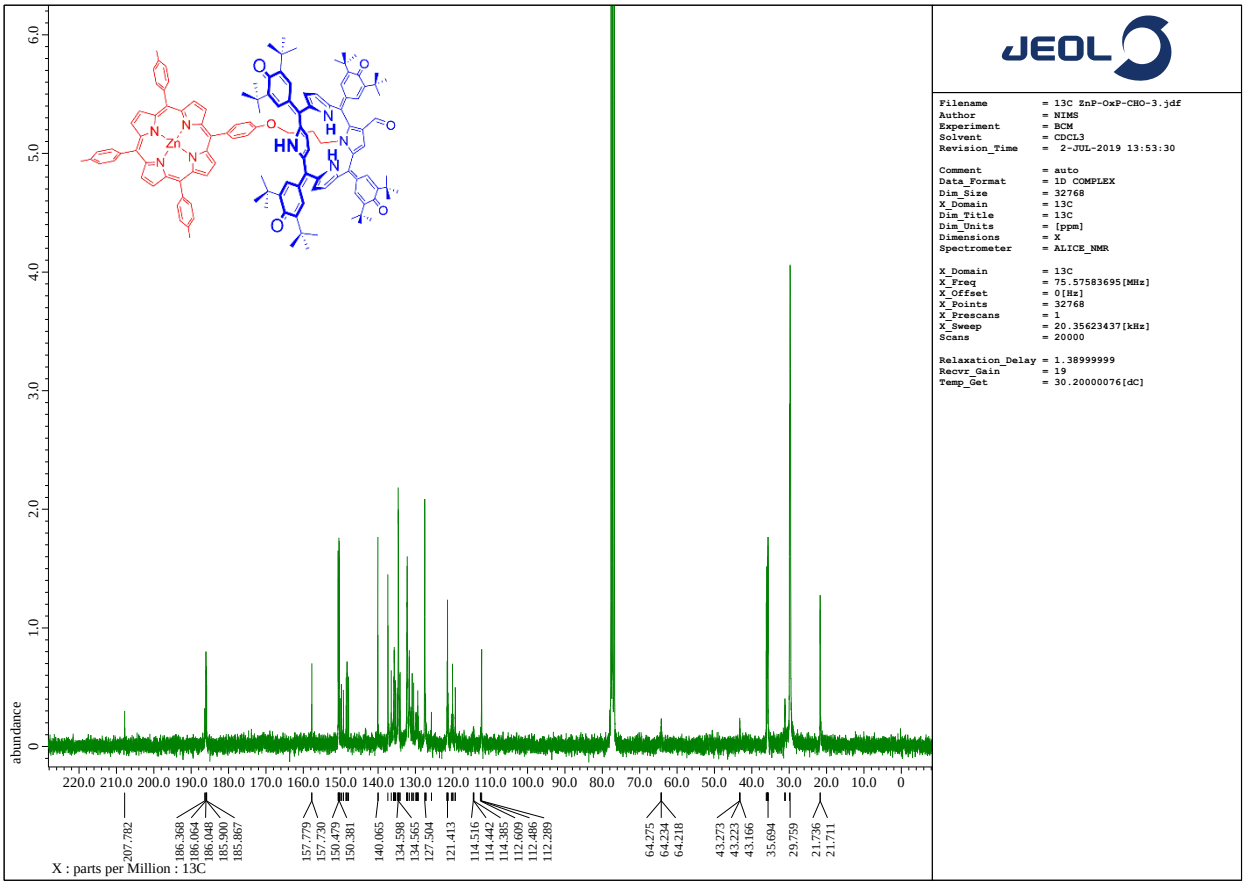


^{13}C NMR spectrum of **ZnP-OxP-CHO** Dyad



Mass spectrum of **ZnP-OxP-CHO** Dyad

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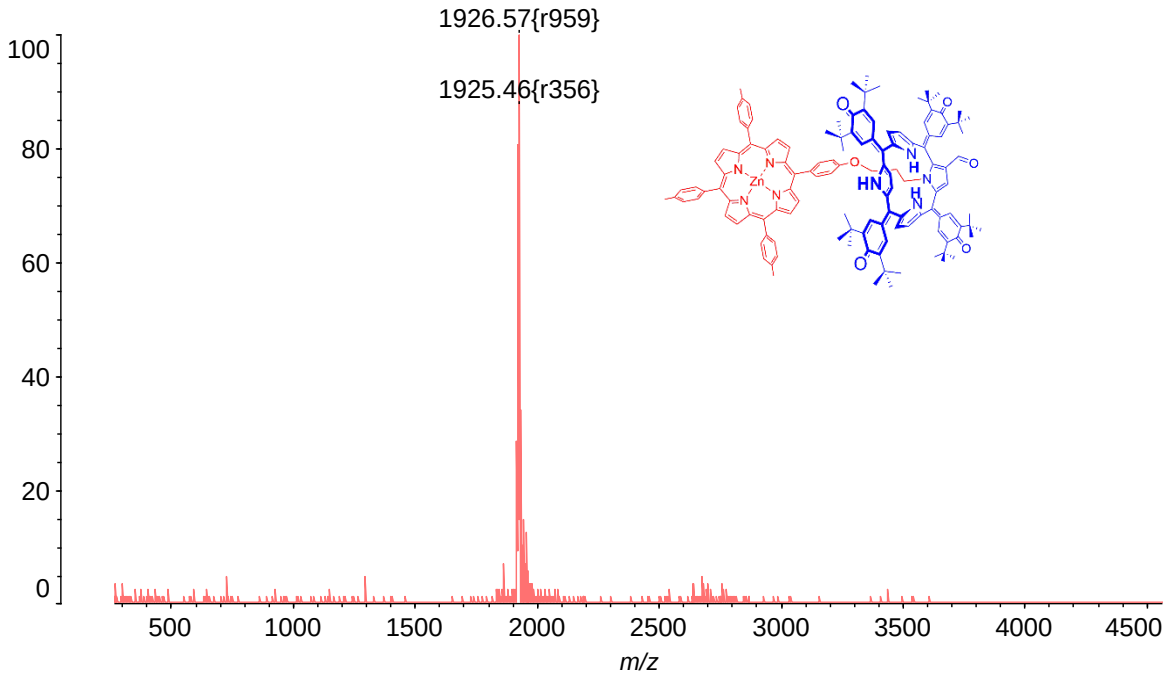
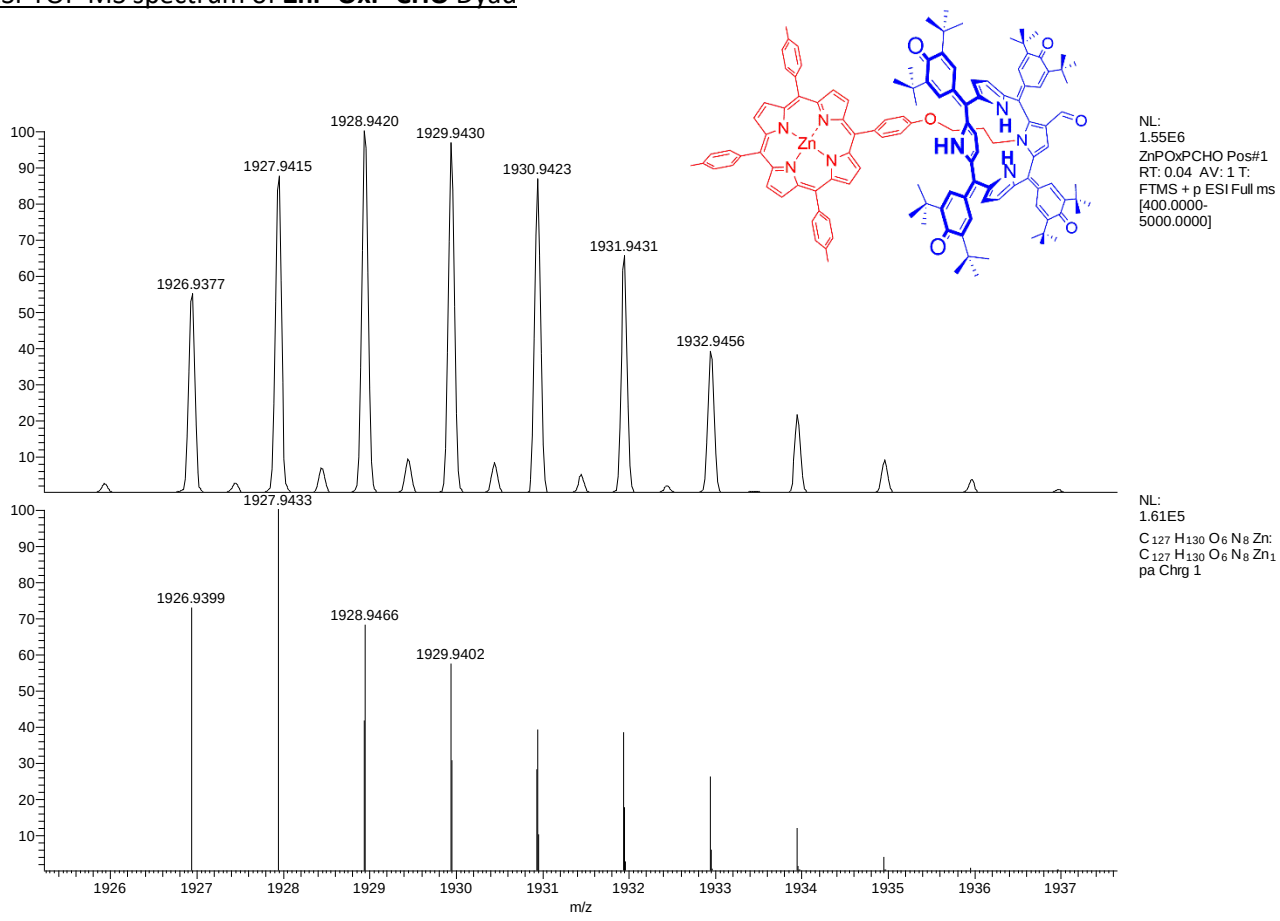
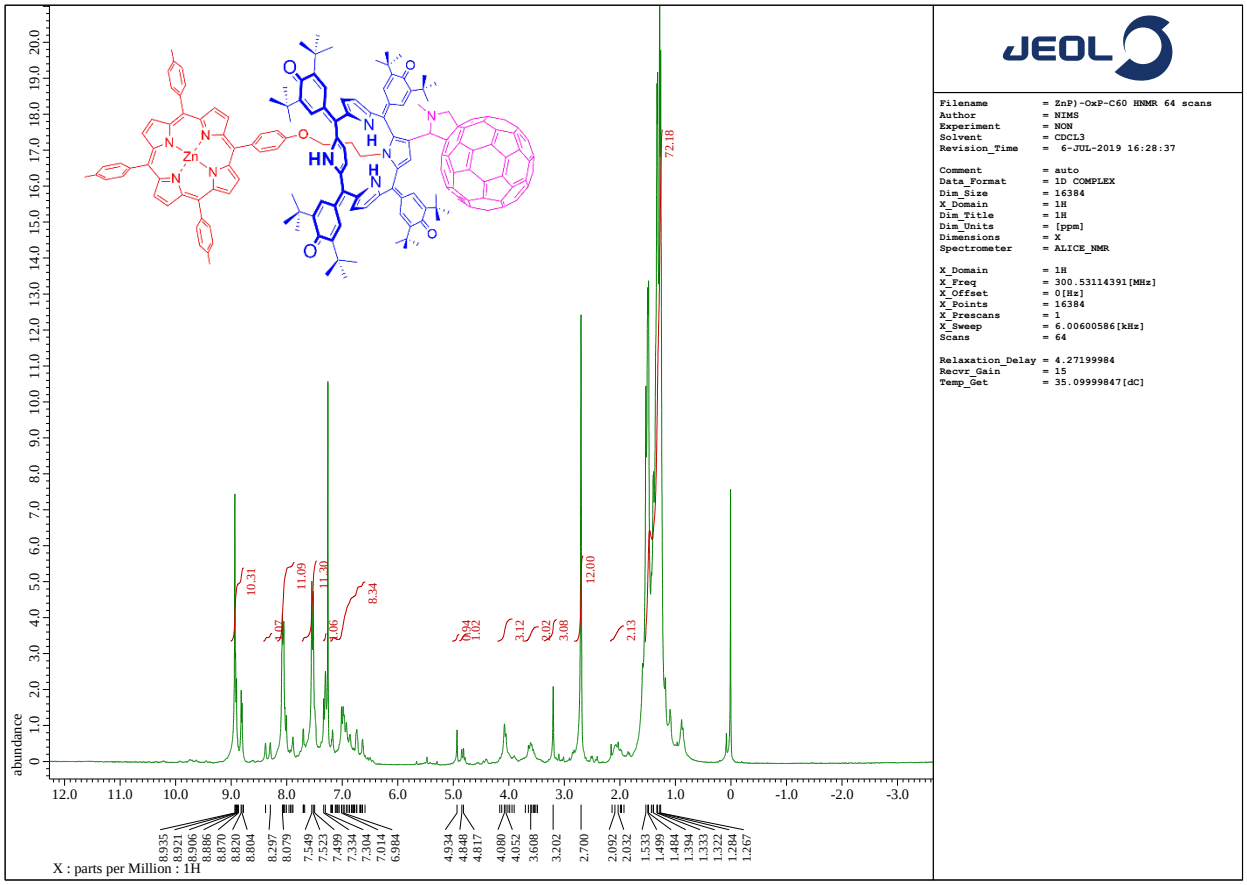


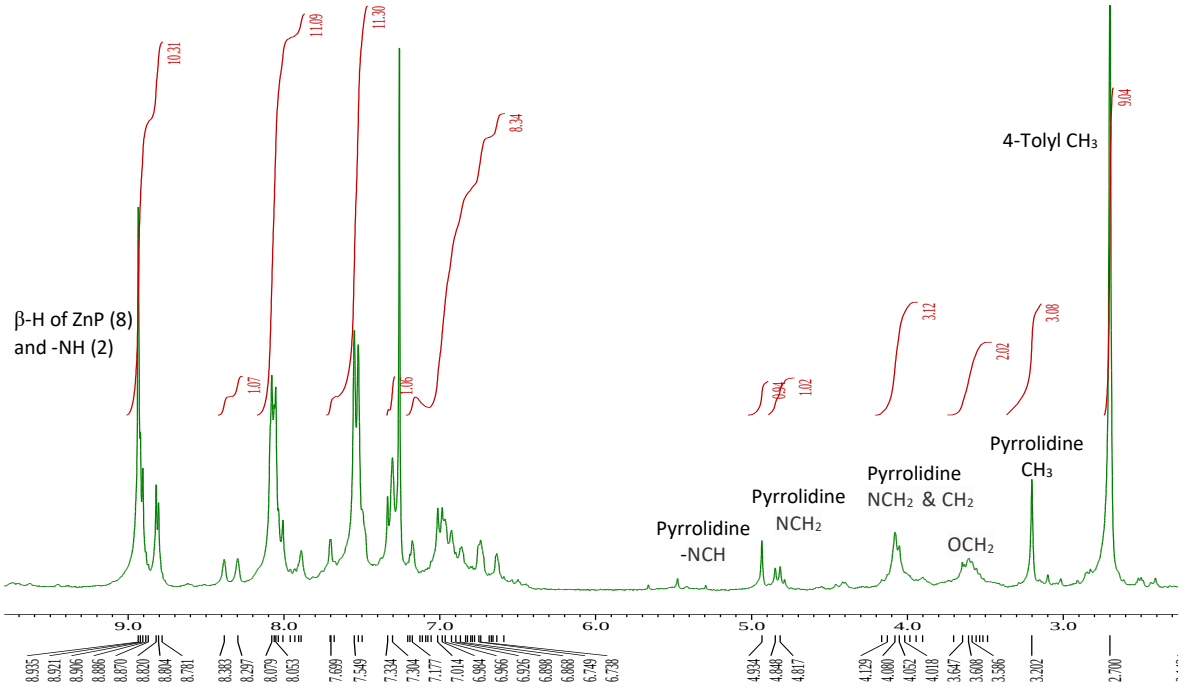
ESI-TOF-MS spectrum of **ZnP-OxP-CHO** Dyad



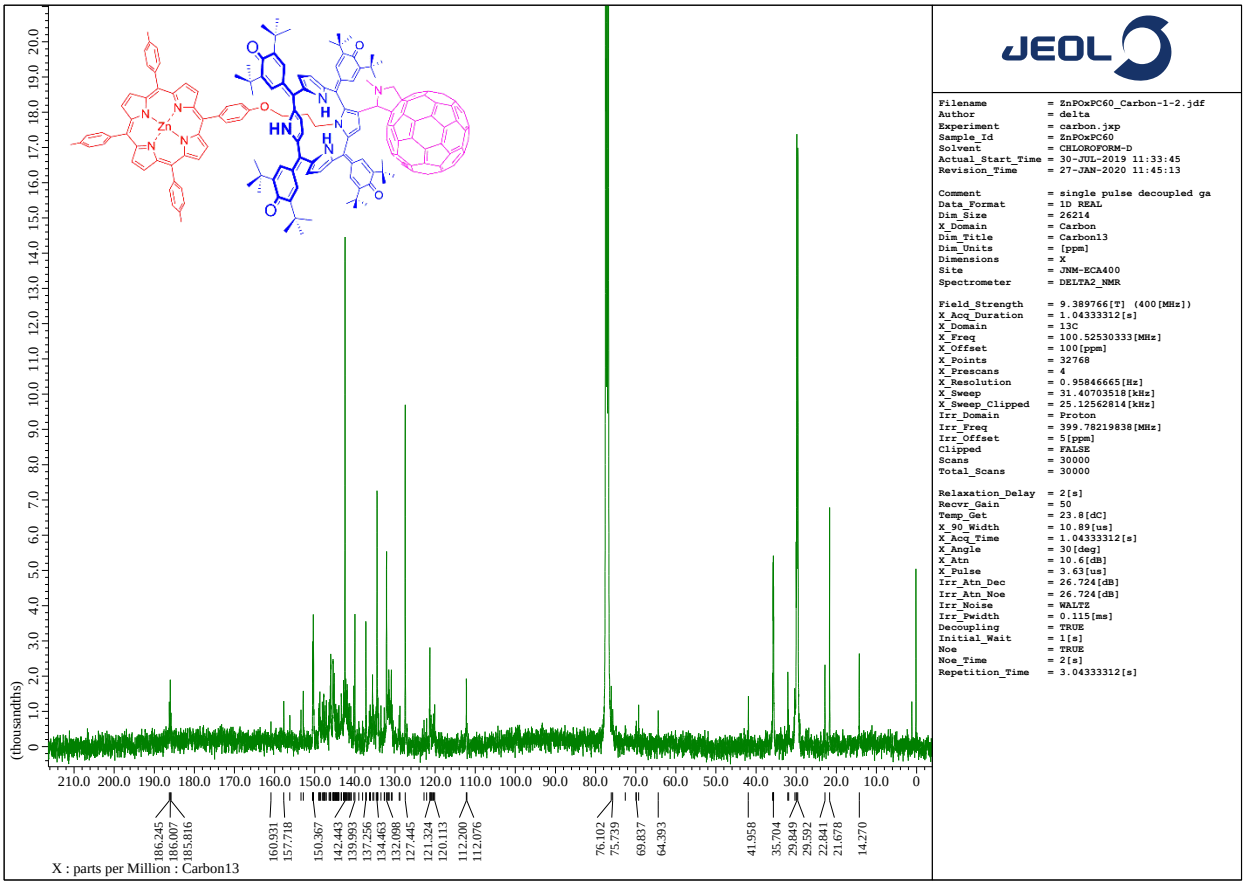
^{1}H NMR spectrum of **ZnP-OxP-C$_{60}$** Triad



Expansion of low field region:



^{13}C NMR spectrum of **ZnP-OxP-C$_{60}$** Triad



Mass spectrum of **ZnP-OxP-C_{60}** Triad

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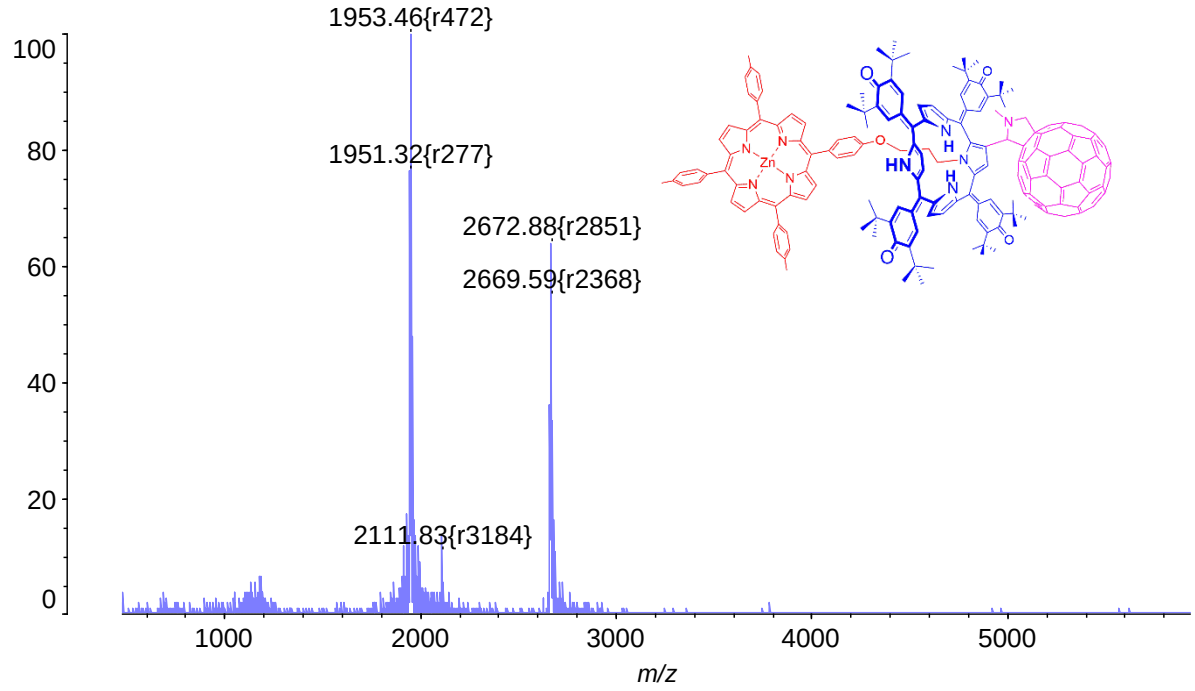
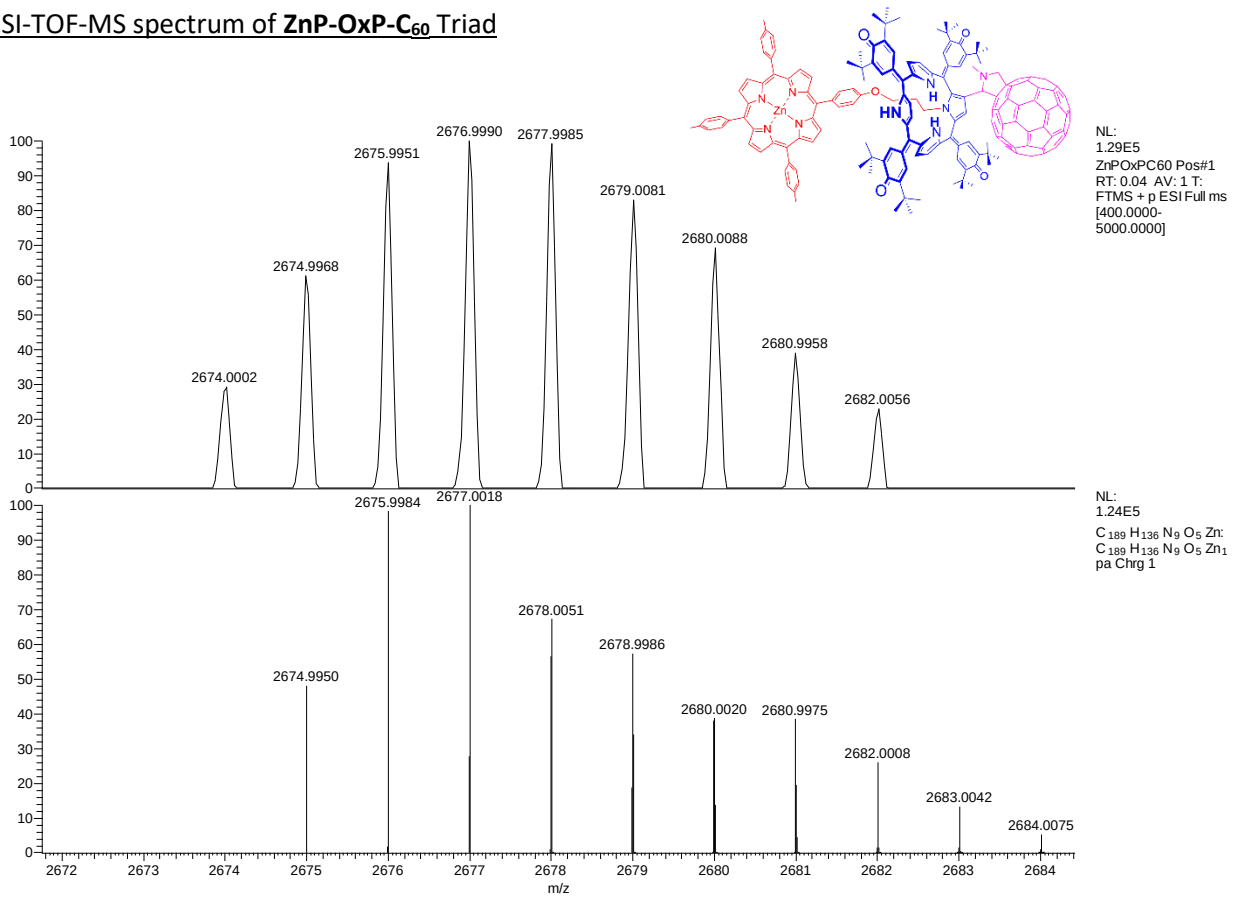


ESI-TOF-MS spectrum of **ZnP-OxP-C_{60}** Triad



Overlaid ^{13}C NMR spectra of **ZnP-OxP-C_{60}** Triad and **ZnP-OxP-CHO** Dyad (Shows reaction of 2-formyl group)