

Supplementary Information

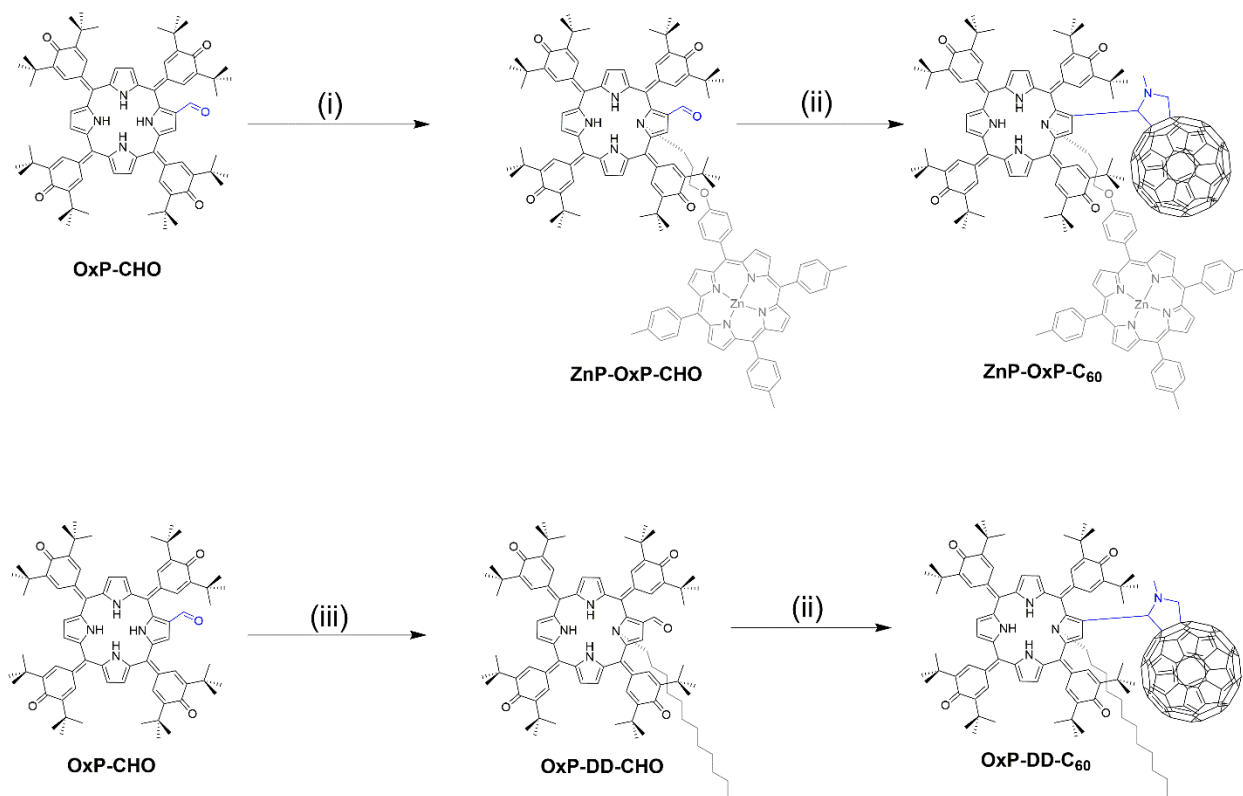
Electron and energy transfer in a porphyrin-oxoporphyrinogen- fullerene triad, ZnP-OxP-C₆₀

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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)/Na₂CO₃/acetone/reflux, (ii) C₆₀/N-methylglycine/toluene/reflux, (iii) n-1-bromodecane/ K₂CO₃/acetone/reflux.

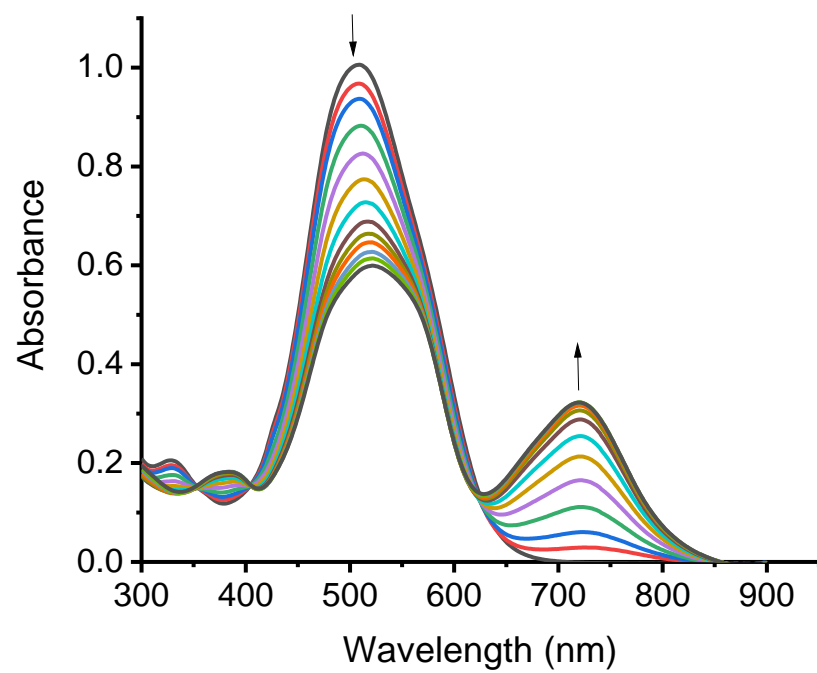
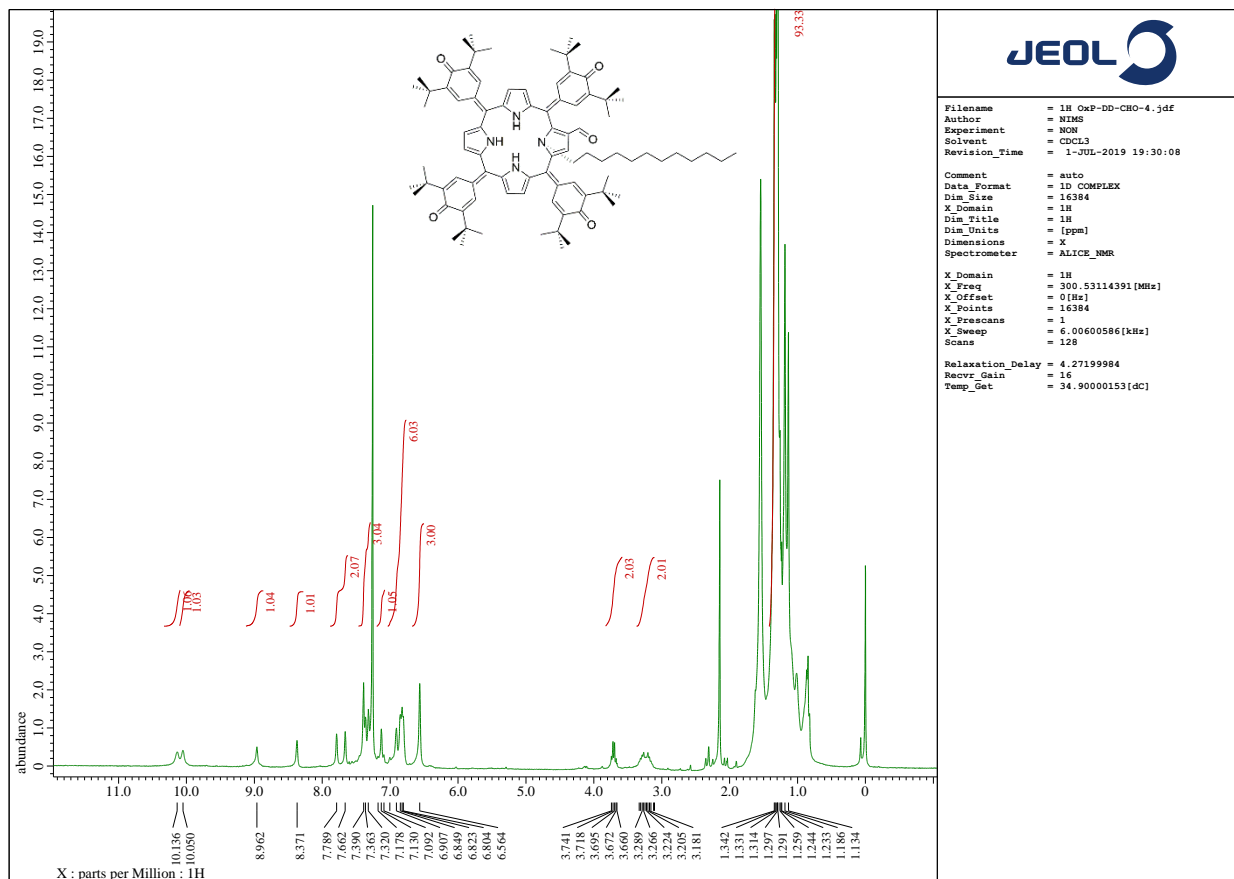
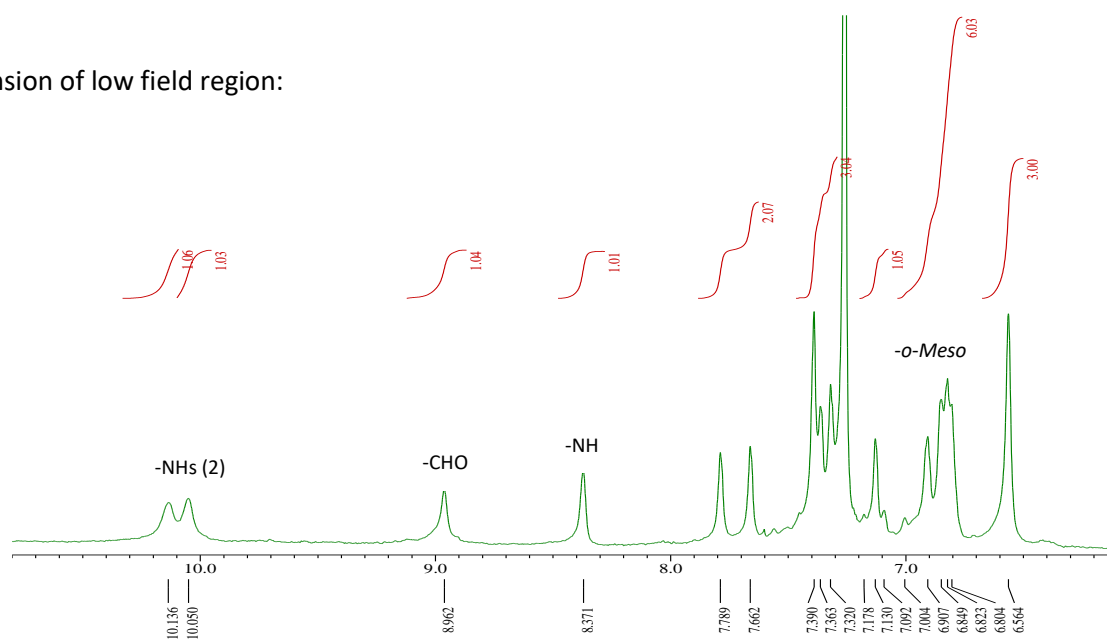


Figure S1. Spectral changes observed during increased addition of NOBF_4 (in methanol) to a solution of **OxP** in DCB.

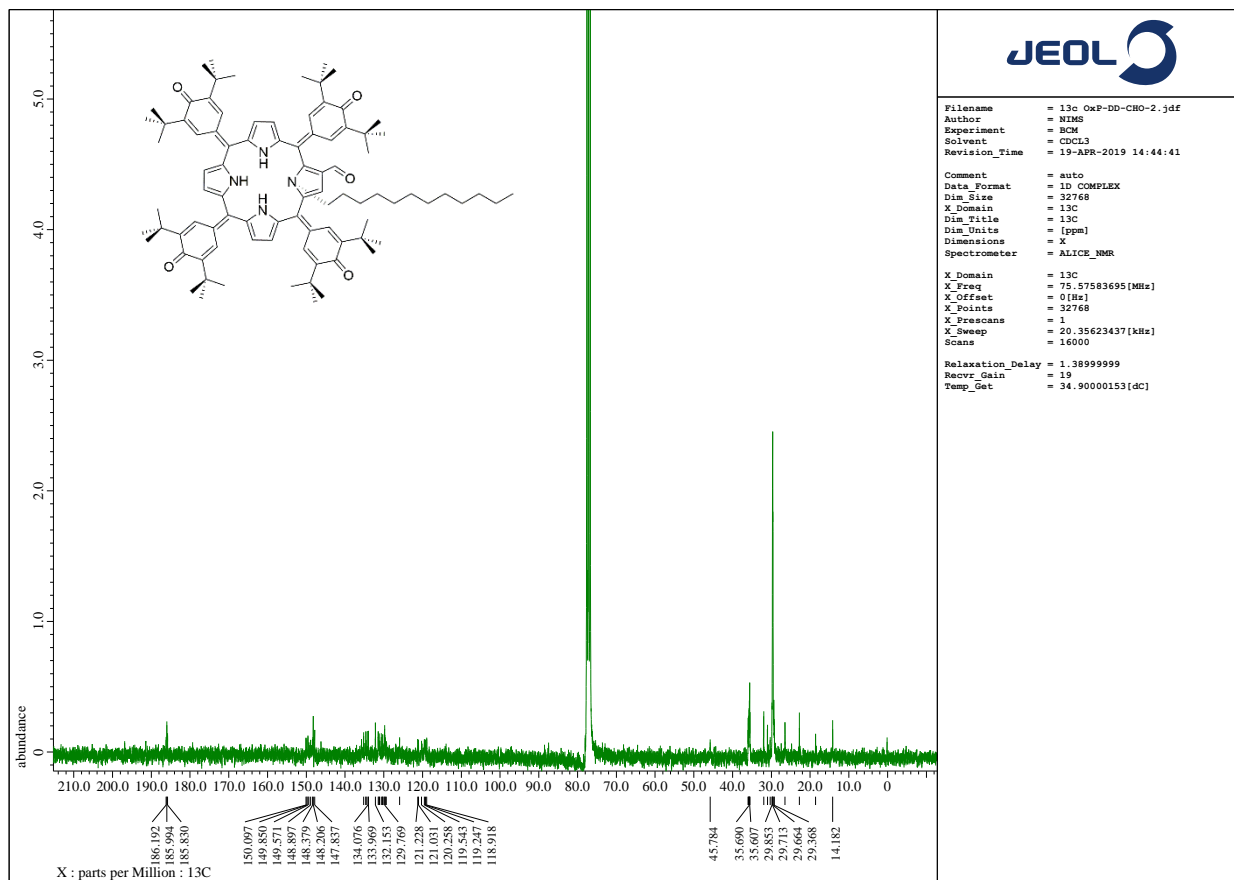
¹H NMR spectrum of N₂₁-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**



Expansion of low field region:



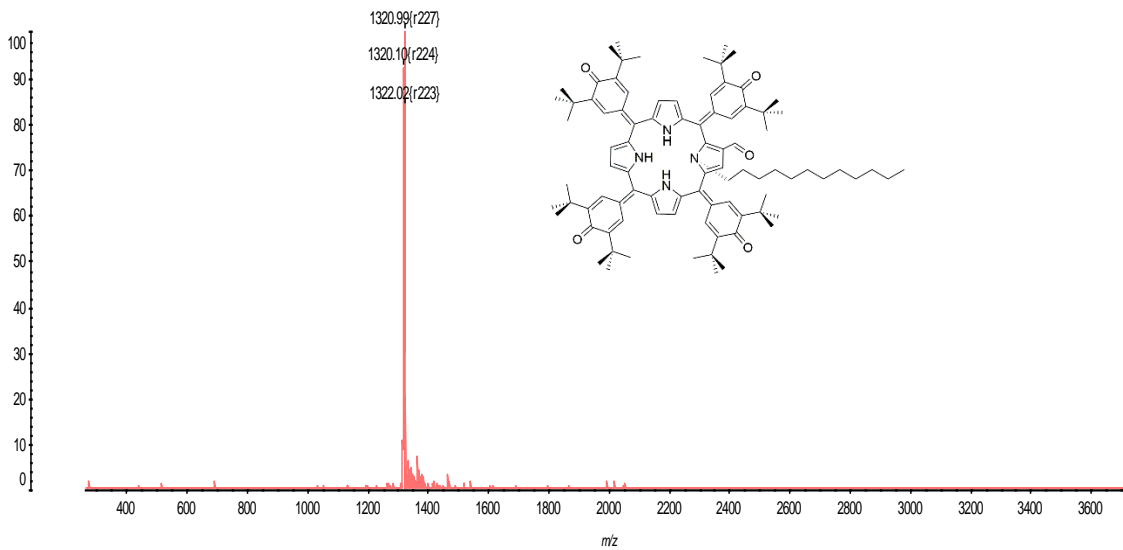
¹³C NMR spectrum of N₂₁-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen OxP-DD-CHO



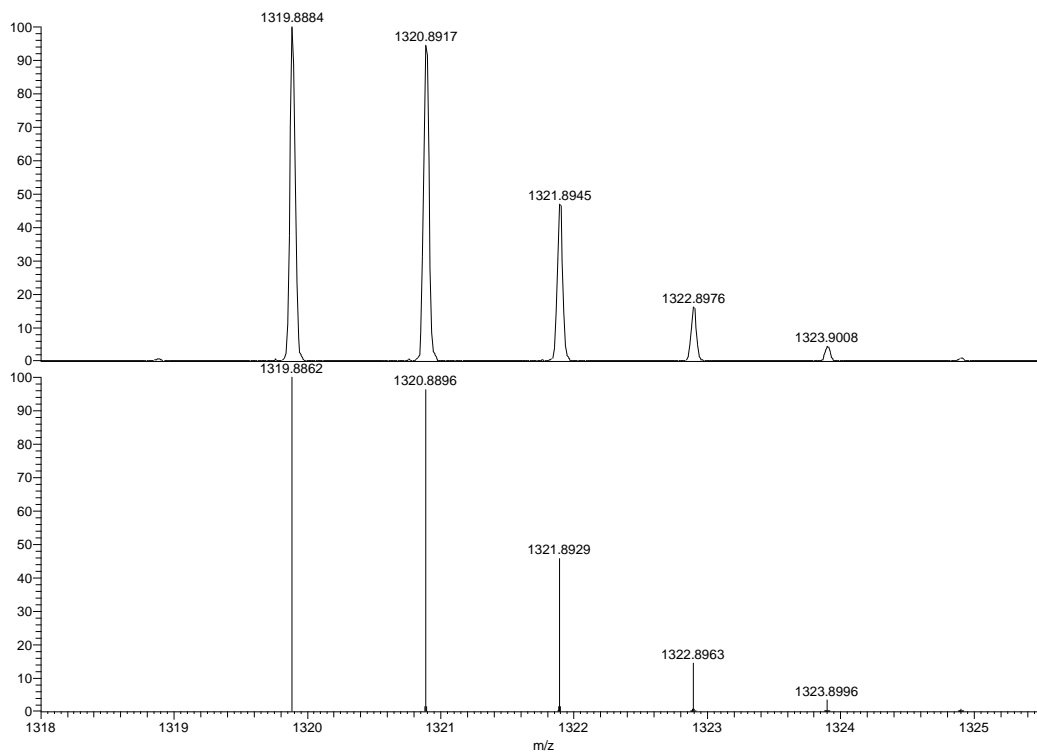
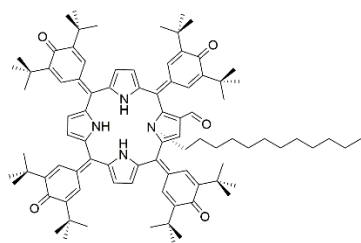
Mass spectrum of N₂₁-dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen OxP-DD-CHO

0deg_300min

Data: <Untitled> E10[c] 2 Jul 2019 17:38 Cal: 15 May 2006 11:45
Shimadzu Biotech Axima CFRplus 2.9.3.20110624: Mode linear, Power: 80
%Int. 1.0 mV[sum= 309 mV] Profiles 1-300 Unsmoothed



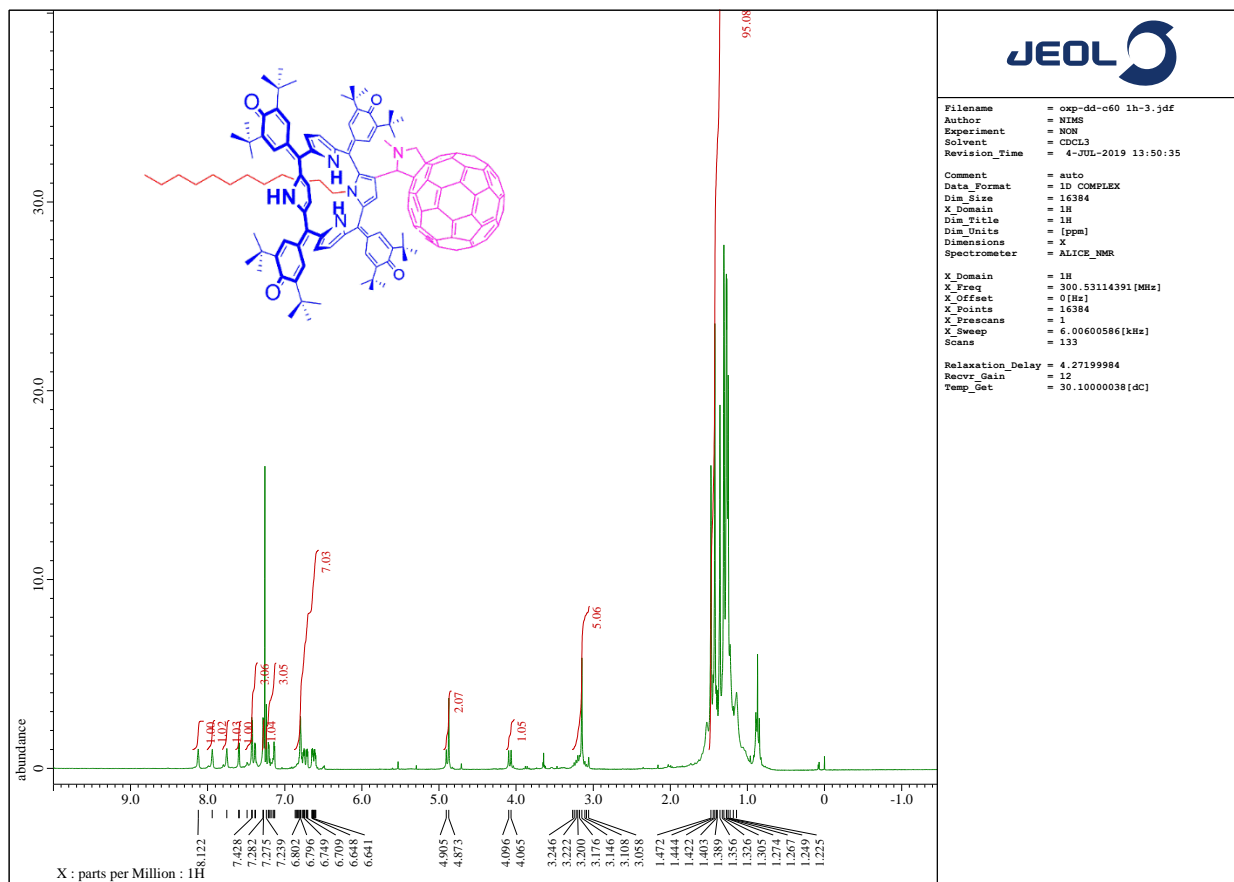
ESI-TOF-MS Spectrum of N_{21} -dodecyl-2-formyl-5,10,15,20-tetrakis(3,5-di-*tert*-butyl-4-oxo-cyclohexa-2,5-dienylidene)porphyrinogen **OxP-DD-CHO**



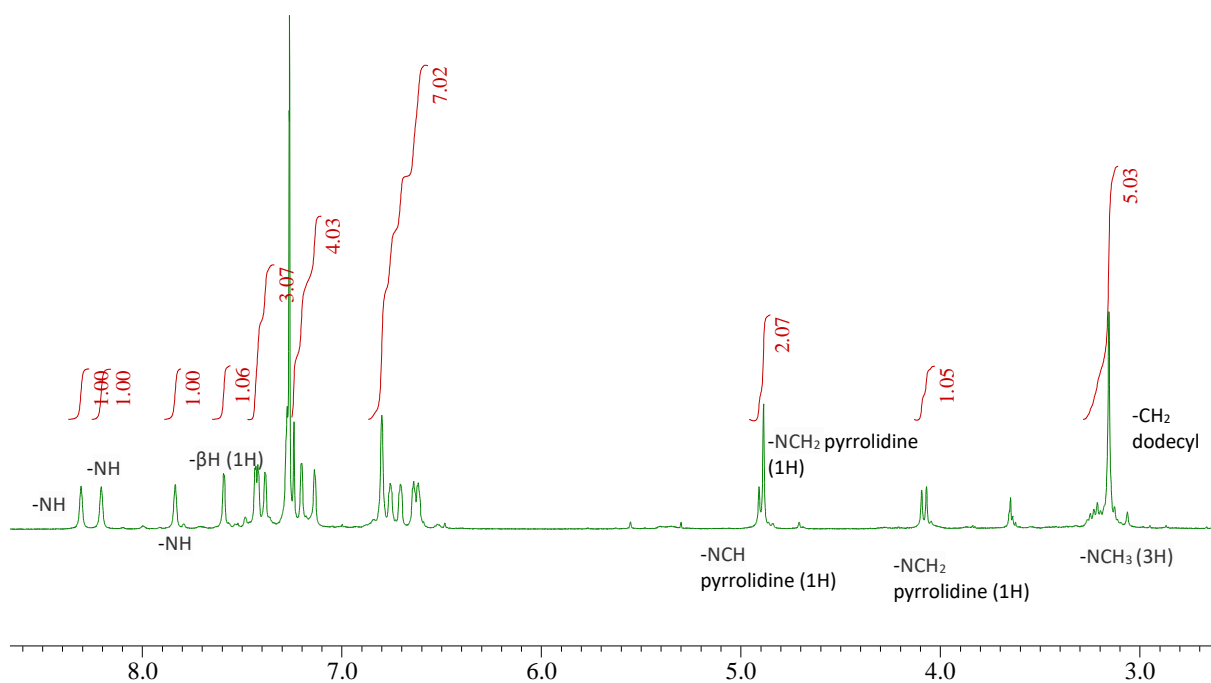
NL:
1.91E7
DDOxPCHO neg#1
RT: 0.04 AV: 1 T:
FTMS - p ESI Full
ms
[300.0000-
4000.0000]

NL:
3.69E5
C₈₉H₁₁₅O₅N₄:
C₈₉H₁₁₅O₅N₄
pa Chrg 1

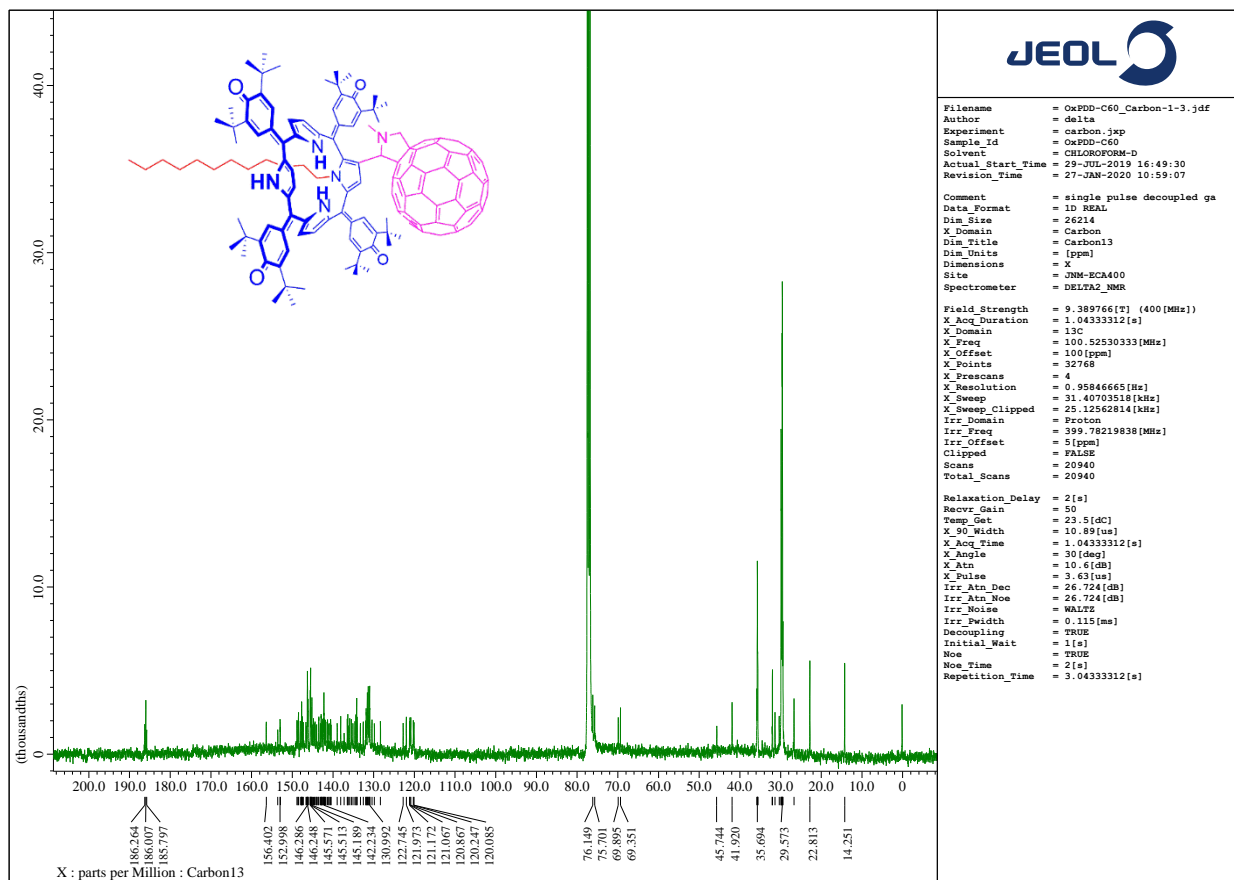
¹H NMR spectrum of Oxp-DD-C₆₀ Dyad



Expansion of low field region:



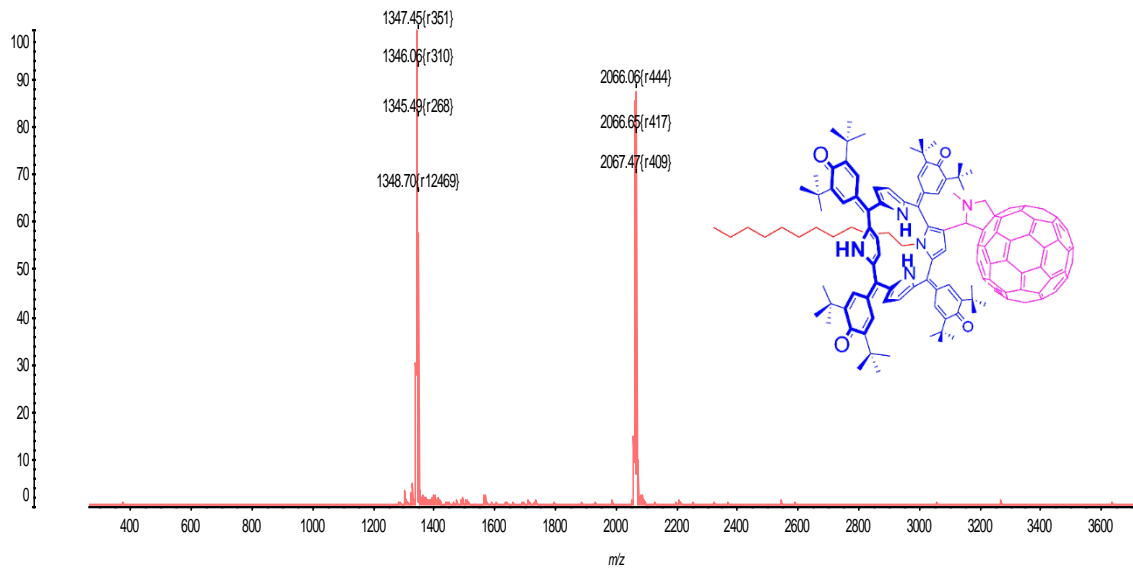
¹³C NMR spectrum of OxP-DD-C₆₀ Dyad



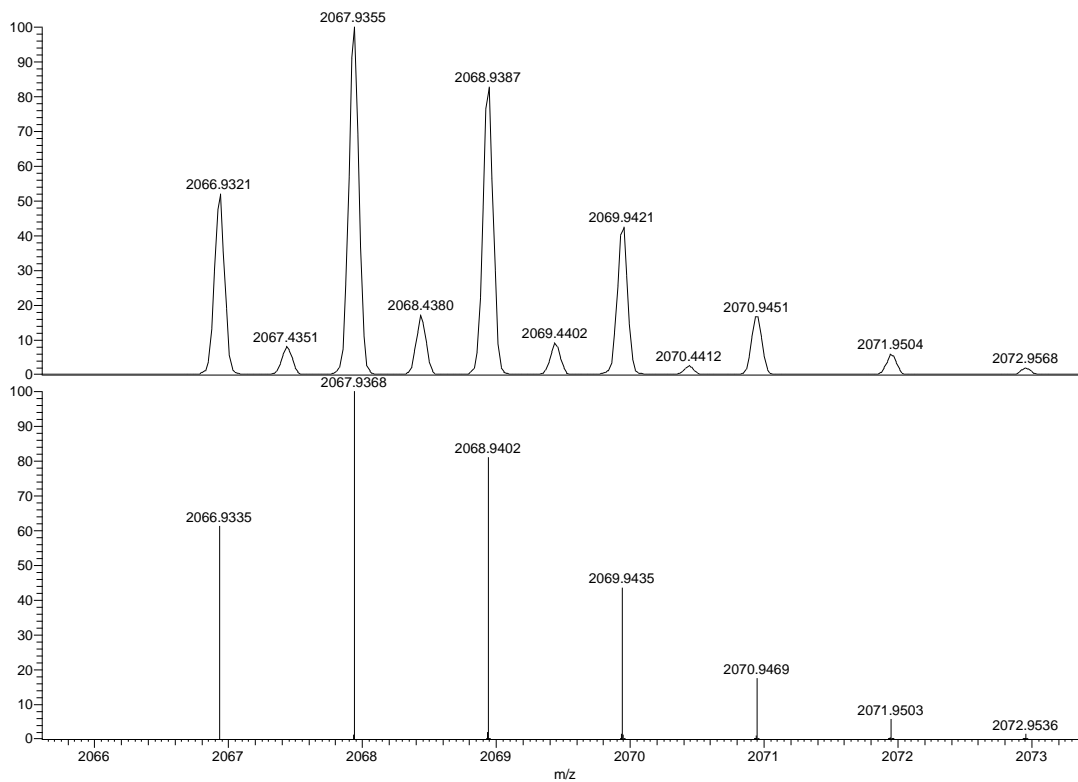
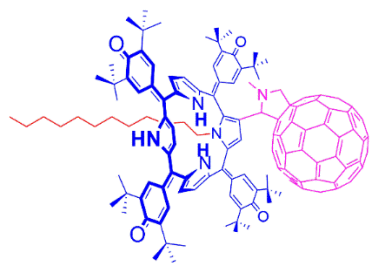
Mass spectrum of **OxP-DD-C₆₀** Dyad

0deg_300min

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%Int. 1.8 mV[sum= 287 mV] Profiles 1-161 Unsmoothed



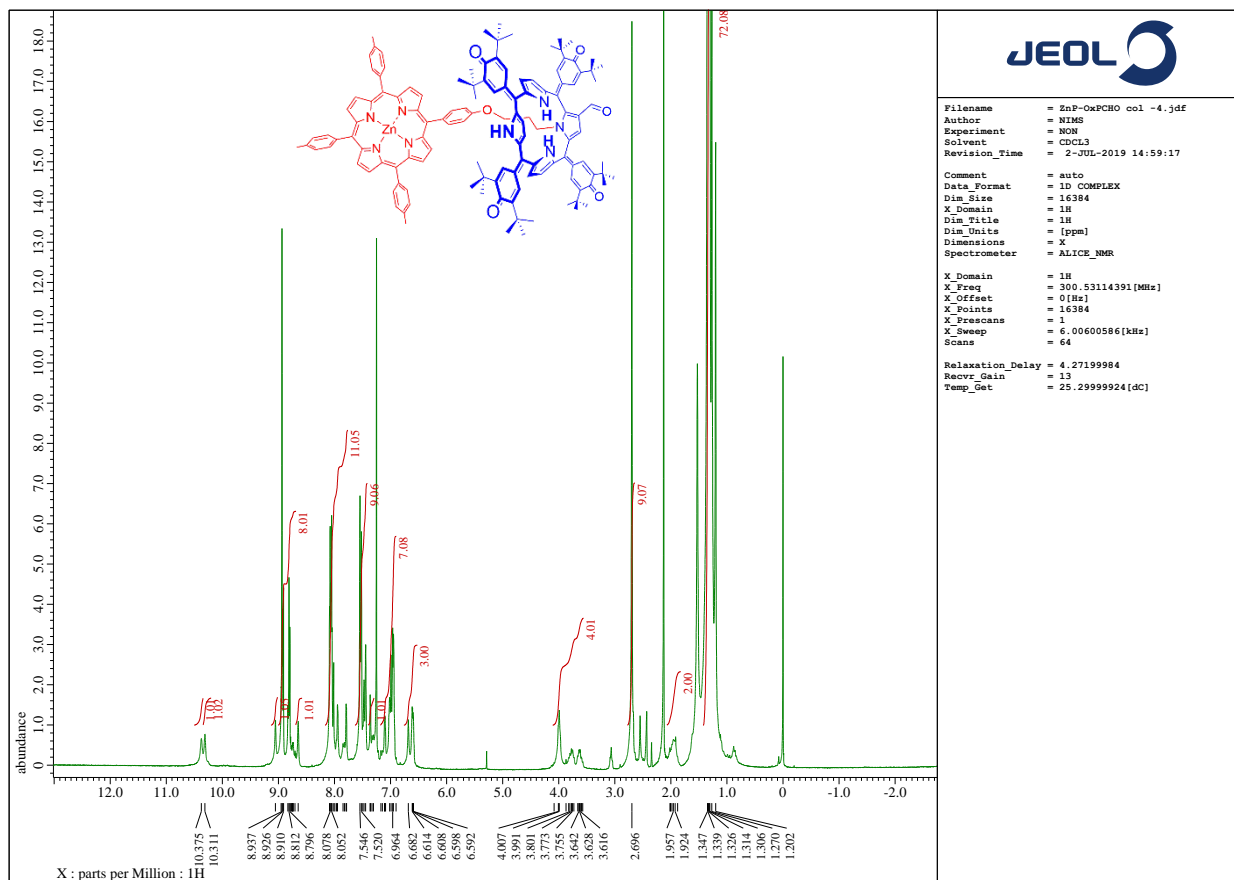
ESI-TOF-MS spectrum of **OxP-DD-C₆₀ Dyad**



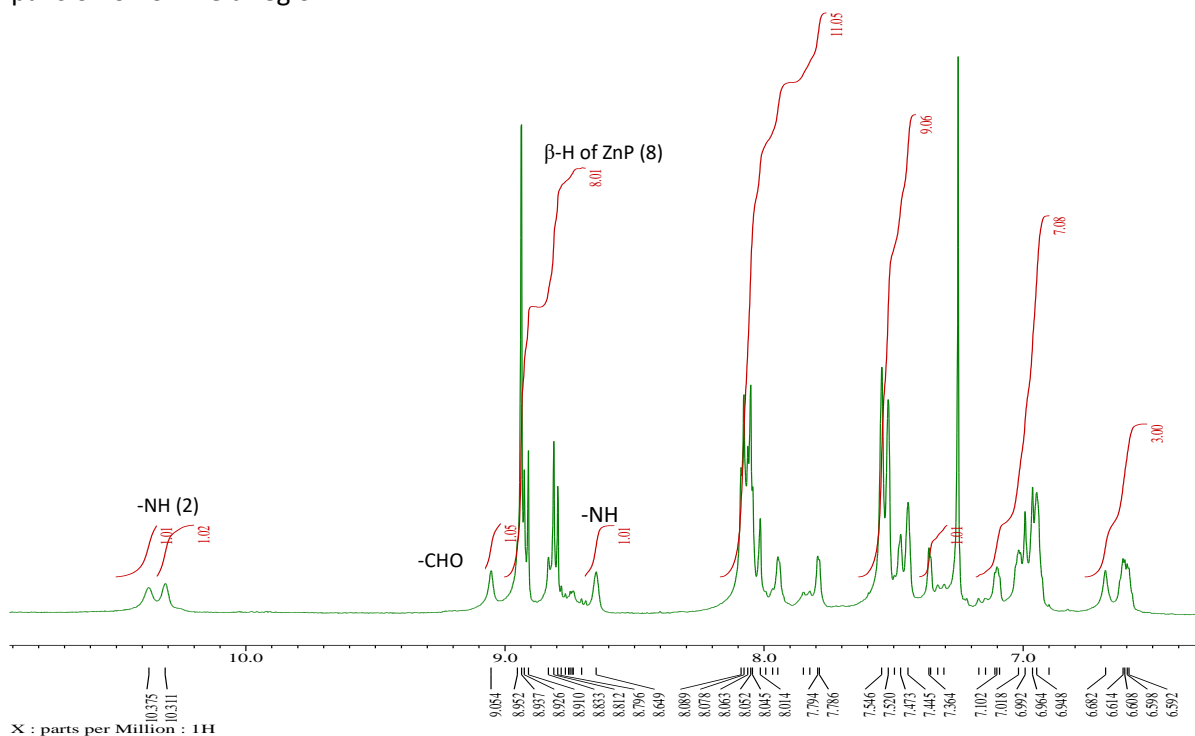
NL:
1.86E6
DDOxPC60 Neg#1
RT: 0.04 AV: 1 T:
FTMS - p ESI Full
ms
[300.0000-
4000.0000]

NL:
3.09E5
C₁₅₁ H₁₂₀ N₅ O₄
C₁₅₁ H₁₂₀ N₅ O₄
pa Chrg 1

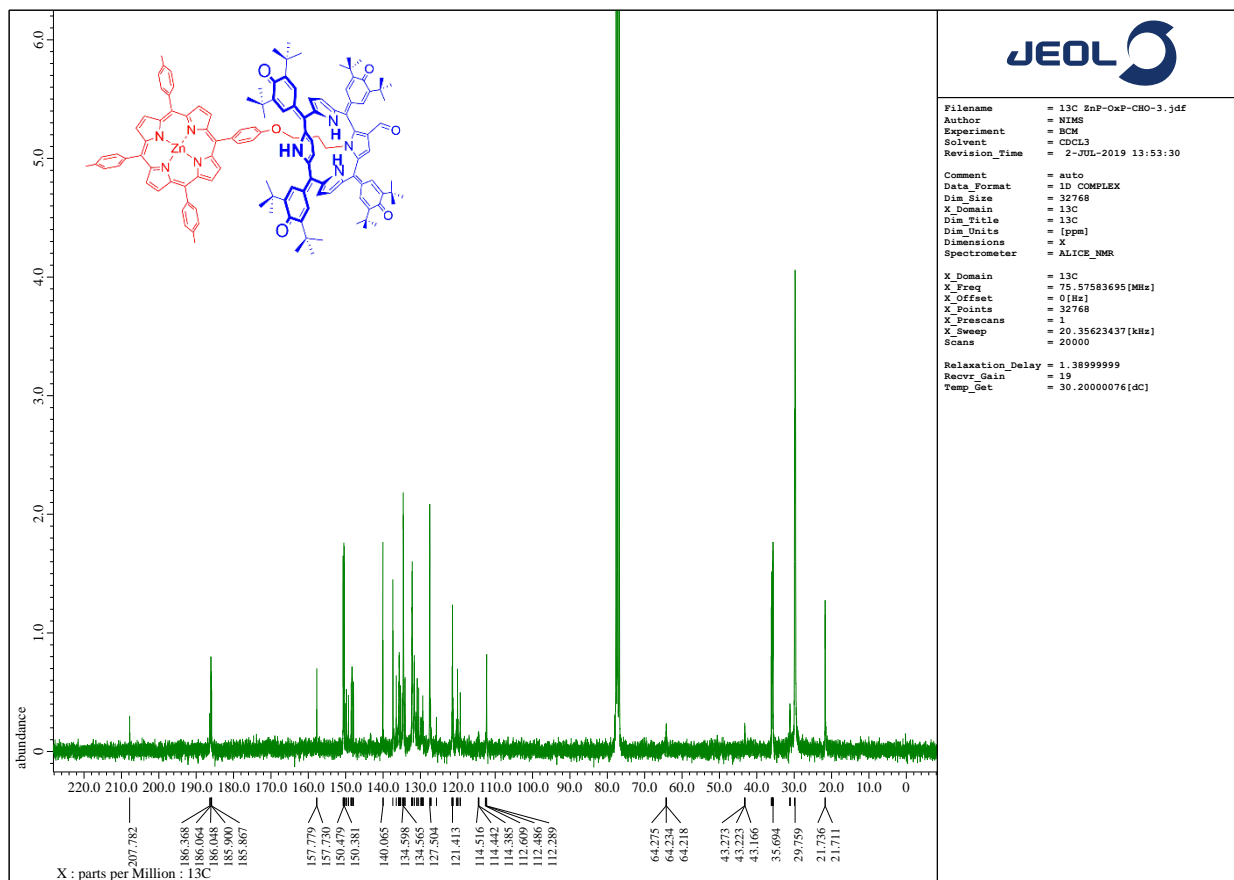
¹H NMR spectrum of ZnP-OxP-CHO Dyad



Expansion of low field region:



¹³C NMR spectrum of ZnP-OxP-CHO Dyad

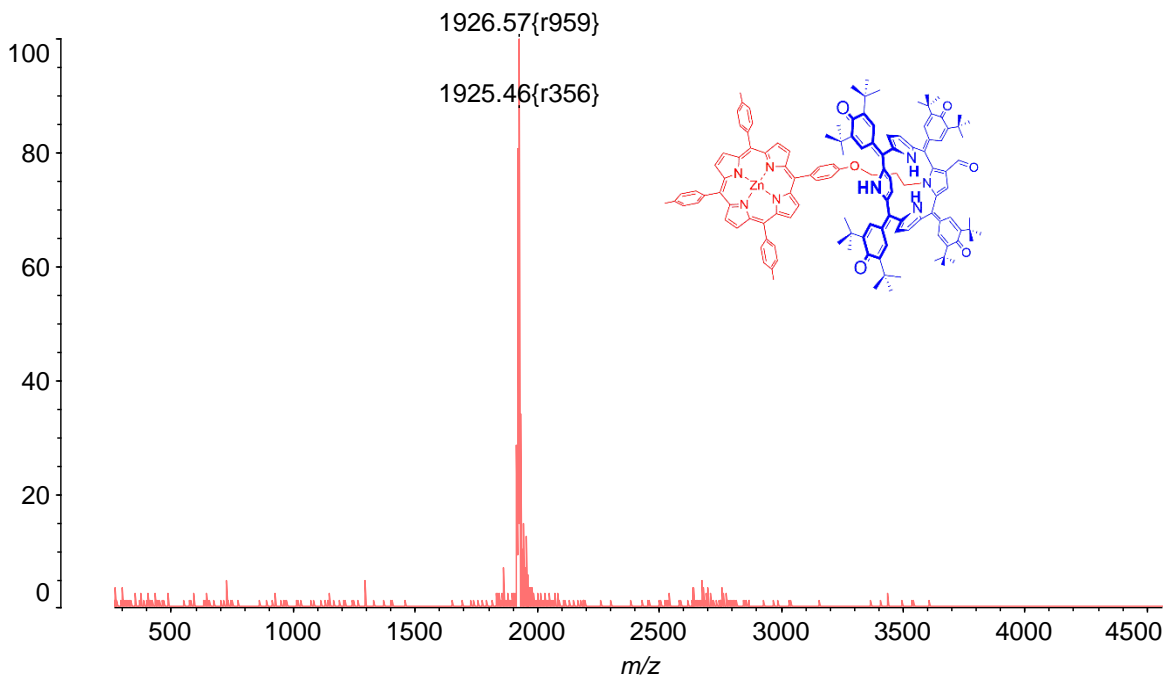


Filename = 13C ZnP-OxP-CHO-3.jdf
Author = NIMS
Experiment = BCM
Solvent = CDCl3
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Comment = auto
Data_Format = 1D_COMPLEX
Dim_Size = 32768
X_Domain = 13C
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Dim_Units = [ppm]
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X_Domain = 13C
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X_Offset = 0[Hz]
X_Points = 32768
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Recvr_Gain = 19
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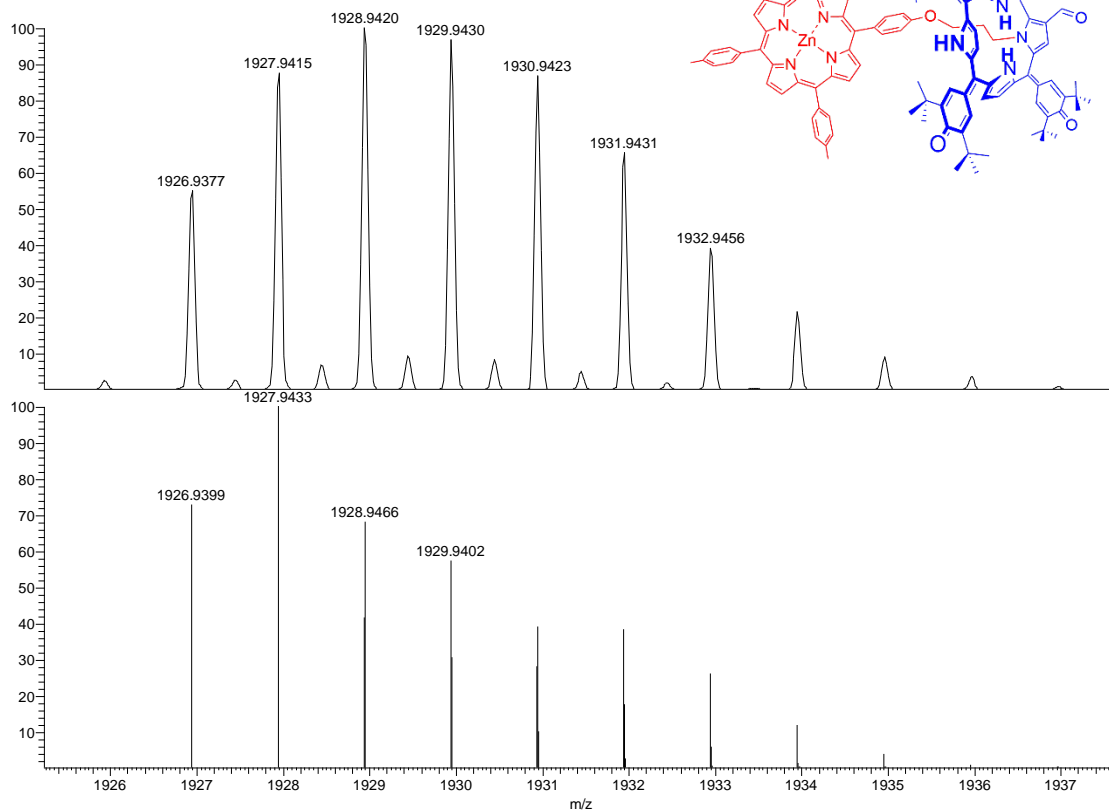
Mass spectrum of ZnP-OxP-CHO Dyad

0deg_300min

Data: <Untitled>.H7[c] 24 Aug 2018 17:24 Cal: 15 May 2006 11:45
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%Int. 0.8 mV[sum= 138 mV] Profiles 1-166 Unsmoothed



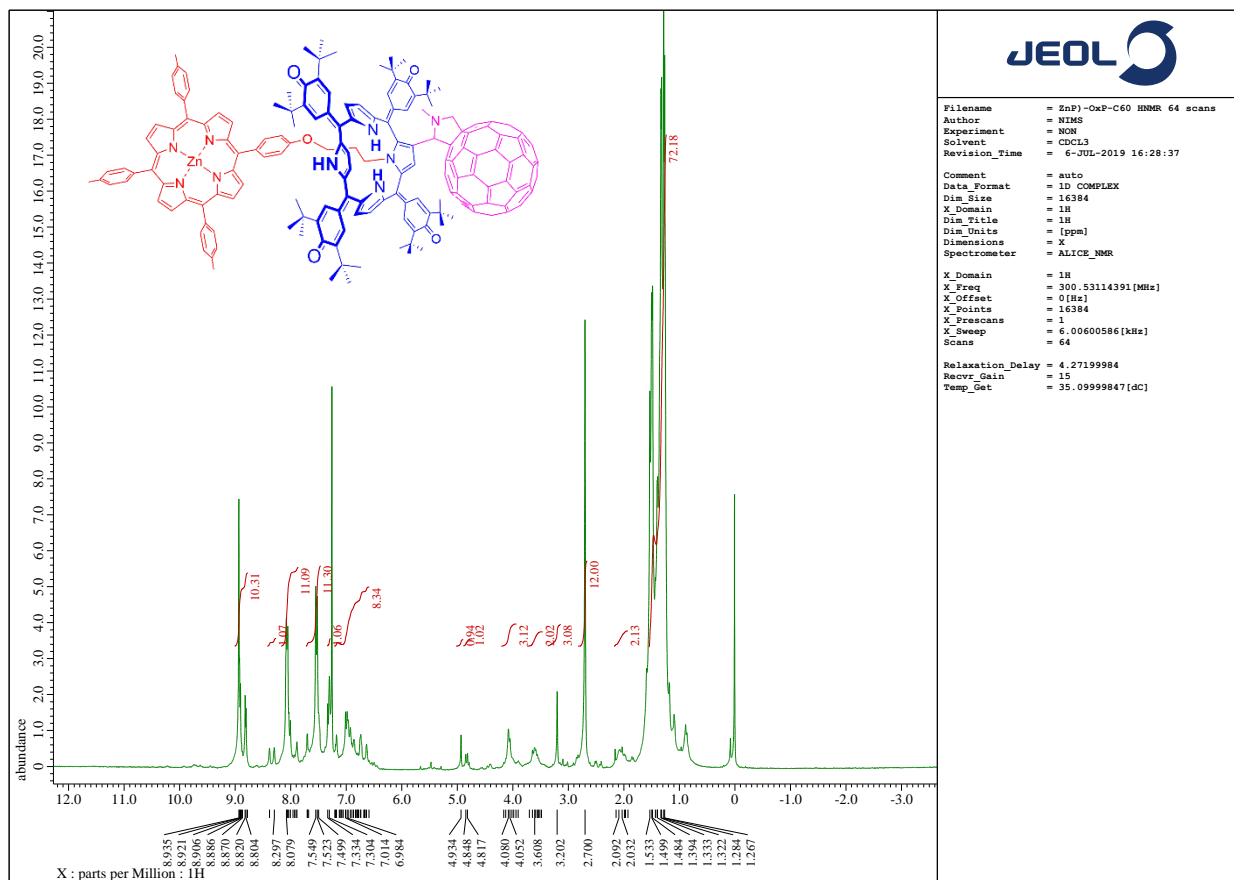
ESI-TOF-MS spectrum of ZnP-OxP-CHO Dyad



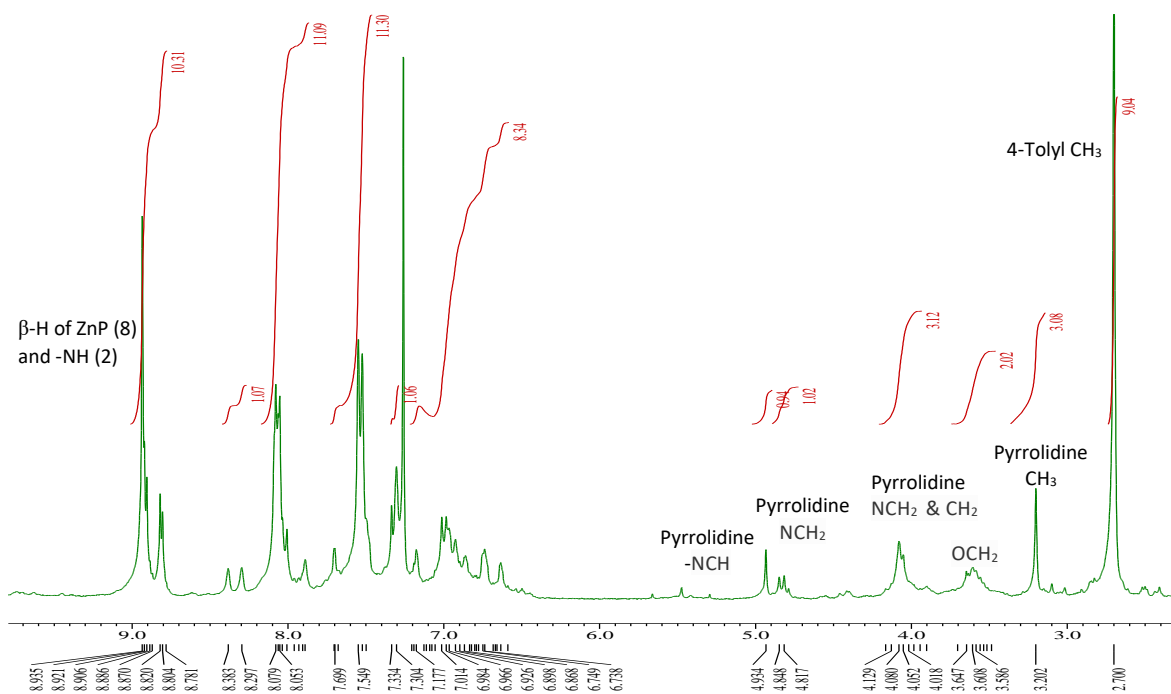
NL:
1.55E6
ZnPoxPCHO Pos#1
RT: 0.04 AV: 1 T:
FTMS + p ESI Full ms
[400.0000-
5000.0000]

NL:
1.61E5
C 127 H 130 O 6 N 8 Zn:
C 127 H 130 O 6 N 8 Zn 1
pa Chrg 1

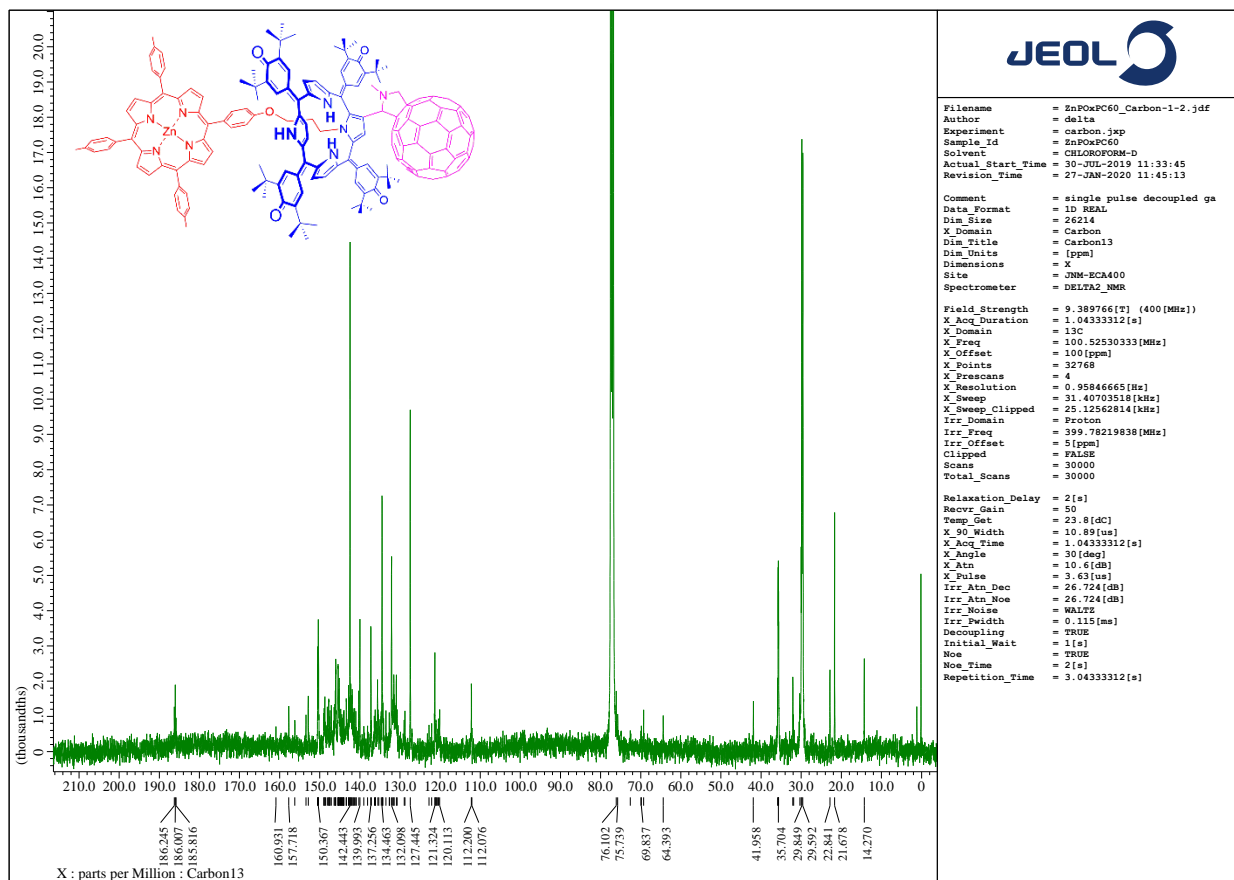
¹H NMR spectrum of ZnP-OxP-C₆₀ Triad



Expansion of low field region:



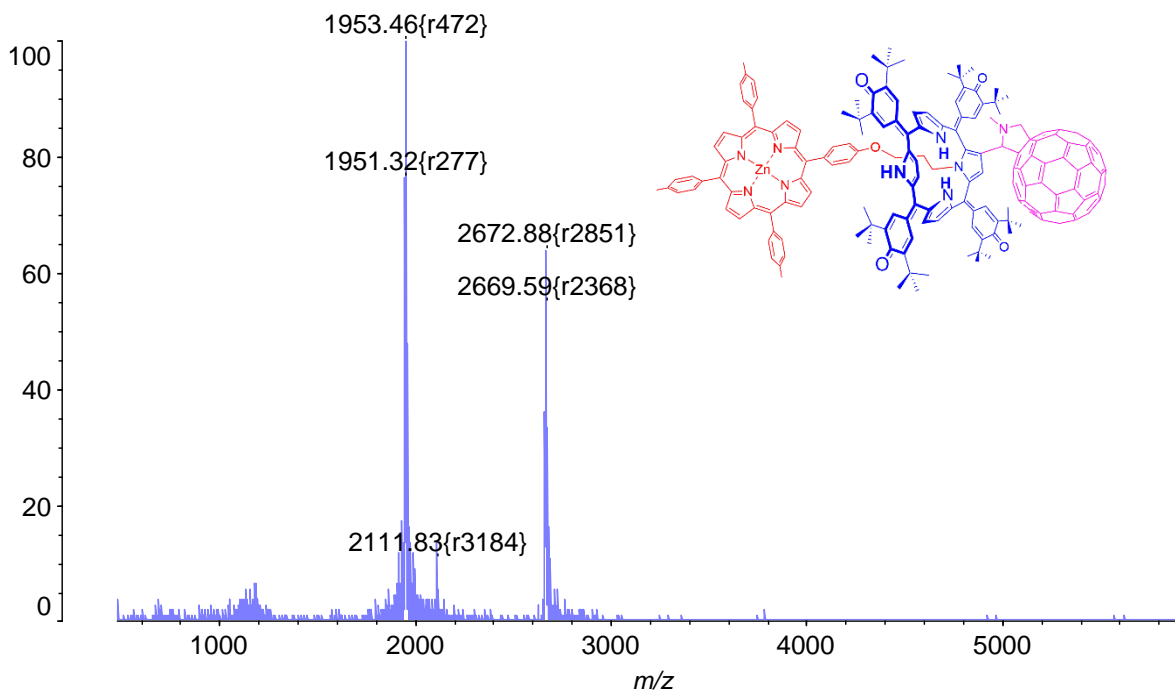
¹³C NMR spectrum of ZnP-OxP-C₆₀ Triad



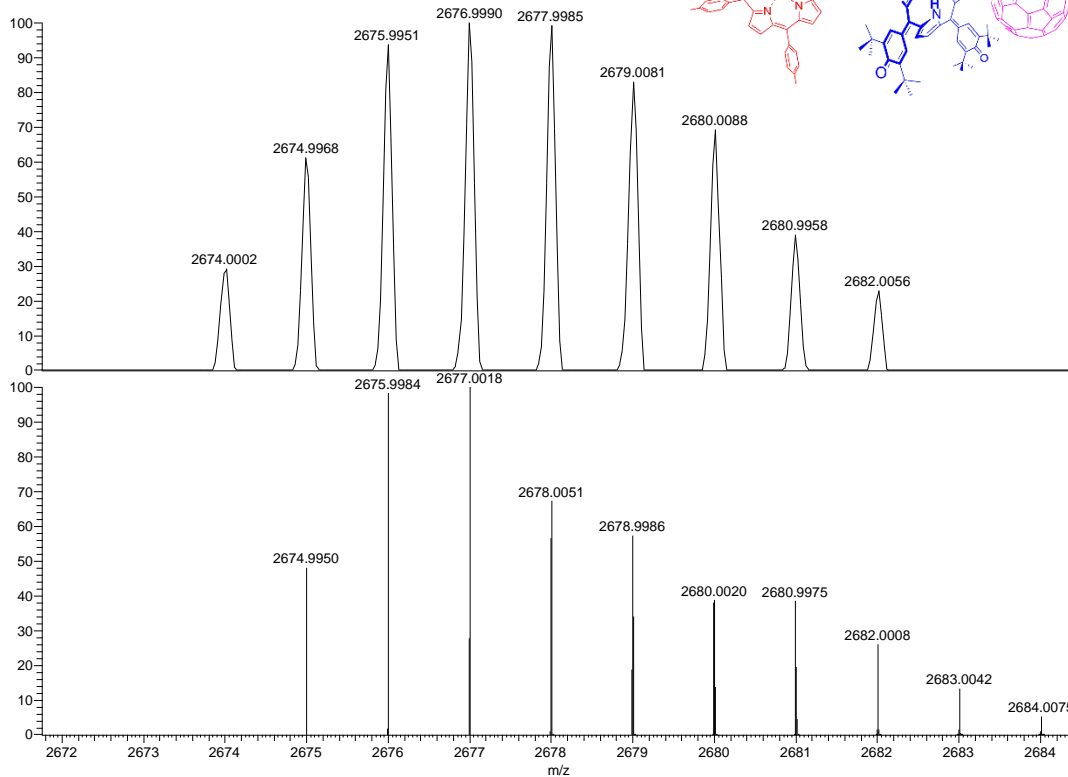
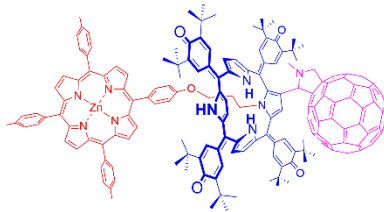
Mass spectrum of ZnP-OxP-C₆₀ Triad

Odeg_300min

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Shimadzu Biotech Axima CFRplus 2.9.3.20110624: Mode linear, Power: 80
%Int. 0.8 mV[sum= 174 mV] Profiles 1-210 Unsmoothed



ESI-TOF-MS spectrum of ZnP-OxP-C₆₀ Triad



NL:
1.29E5
ZnP-OxP-C60 Pos#1
RT: 0.04 AV: 1 T:
FTMS+ p ESI Full ms
[400.0000-
5000.0000]

NL:
1.24E5
C₁₈₉ H₁₃₆ N₉ O₅ Zn:
C₁₈₉ H₁₃₆ N₉ O₅ Zn₁
pa Chrg 1

Overlaid ^{13}C NMR spectra of **ZnP-OxP-C₆₀** Triad and **ZnP-OxP-CHO** Dyad (Shows reaction of 2-formyl group)

