

Supporting Information

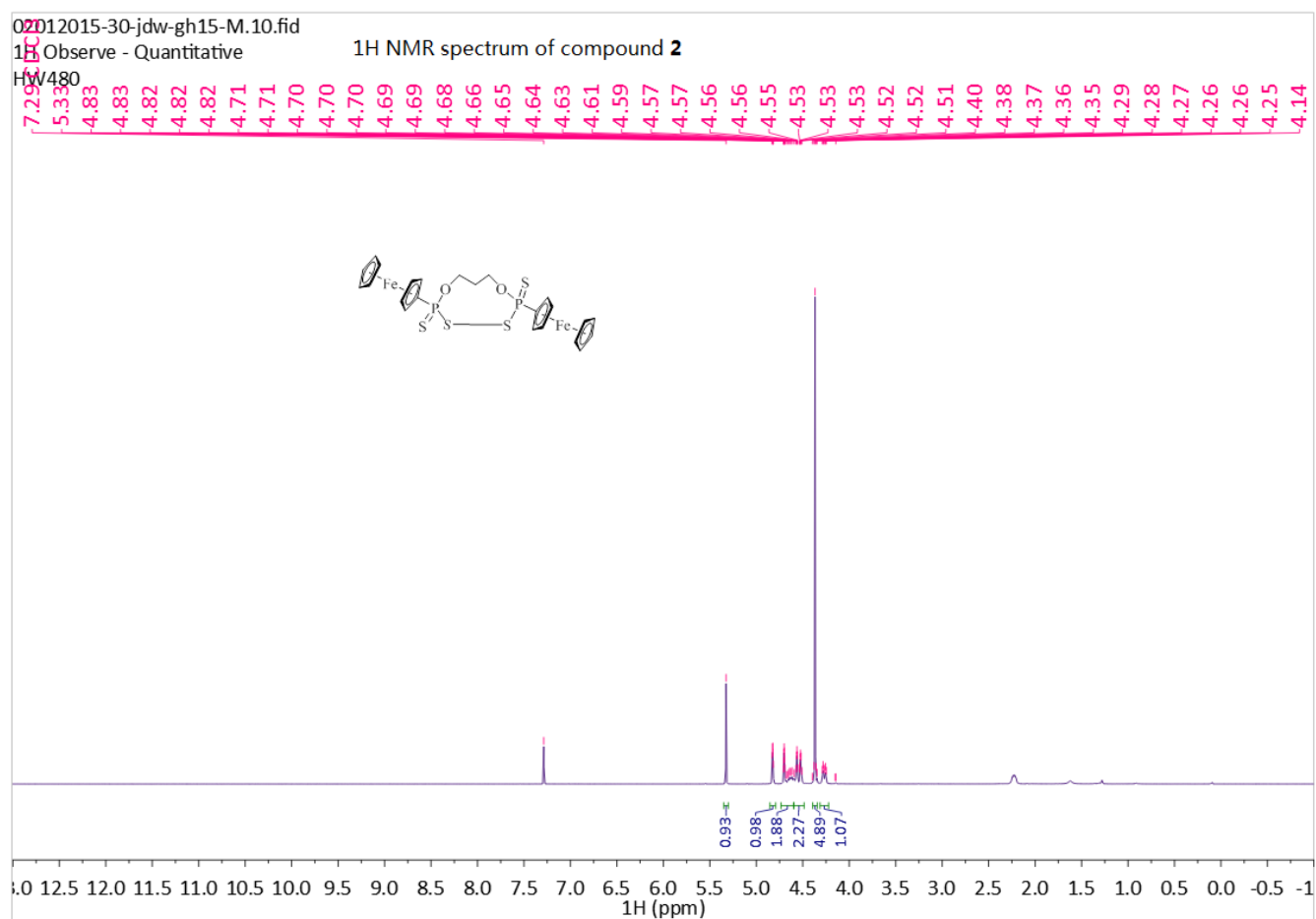
Phosphorus-Sulfur Heterocycles Incorporating with O-P(S)-O or O-P(S)-S-S-P(S)-O Scaffold: One-Pot Synthesis and Crystal Structural Study

Guoxiong Hua, Kate Davidson, David B. Cordes, Junyi Du, Alexandra M. Z. Slawin and J. Derek Woollins*

School of Chemistry, University of St Andrews, Fife, KY16 9ST, UK

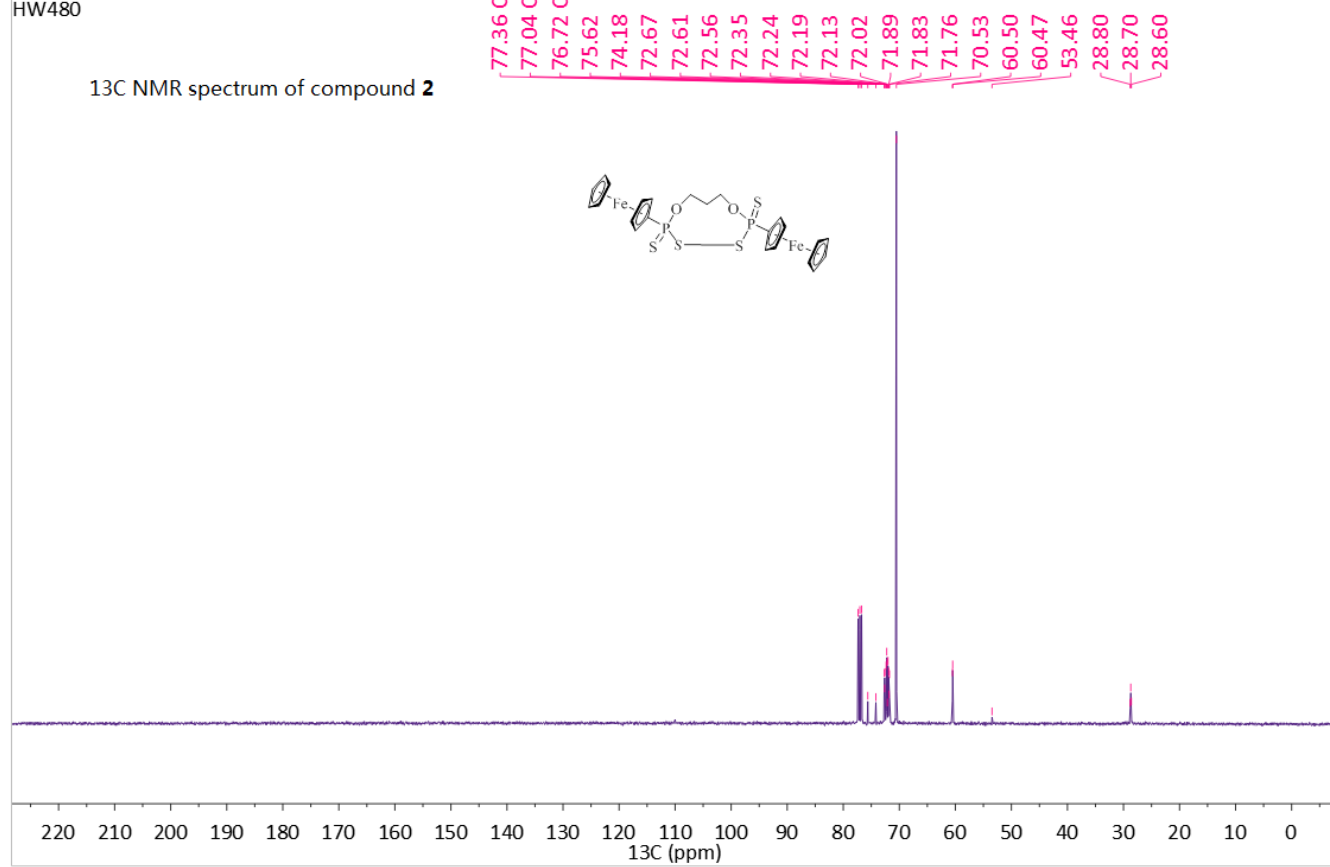
*Corresponding author. Tel.: (+44)-1334-463384; email: jdww3@st-and.ac.uk

1. ^1H and ^{13}C NMR spectra of compounds **2-4**, **6**, **8-12**



02012015-30-jdw-gh15-M.12.fid
13C Observe with 1H decoupling - UDEFT
HW480

13C NMR spectrum of compound **2**

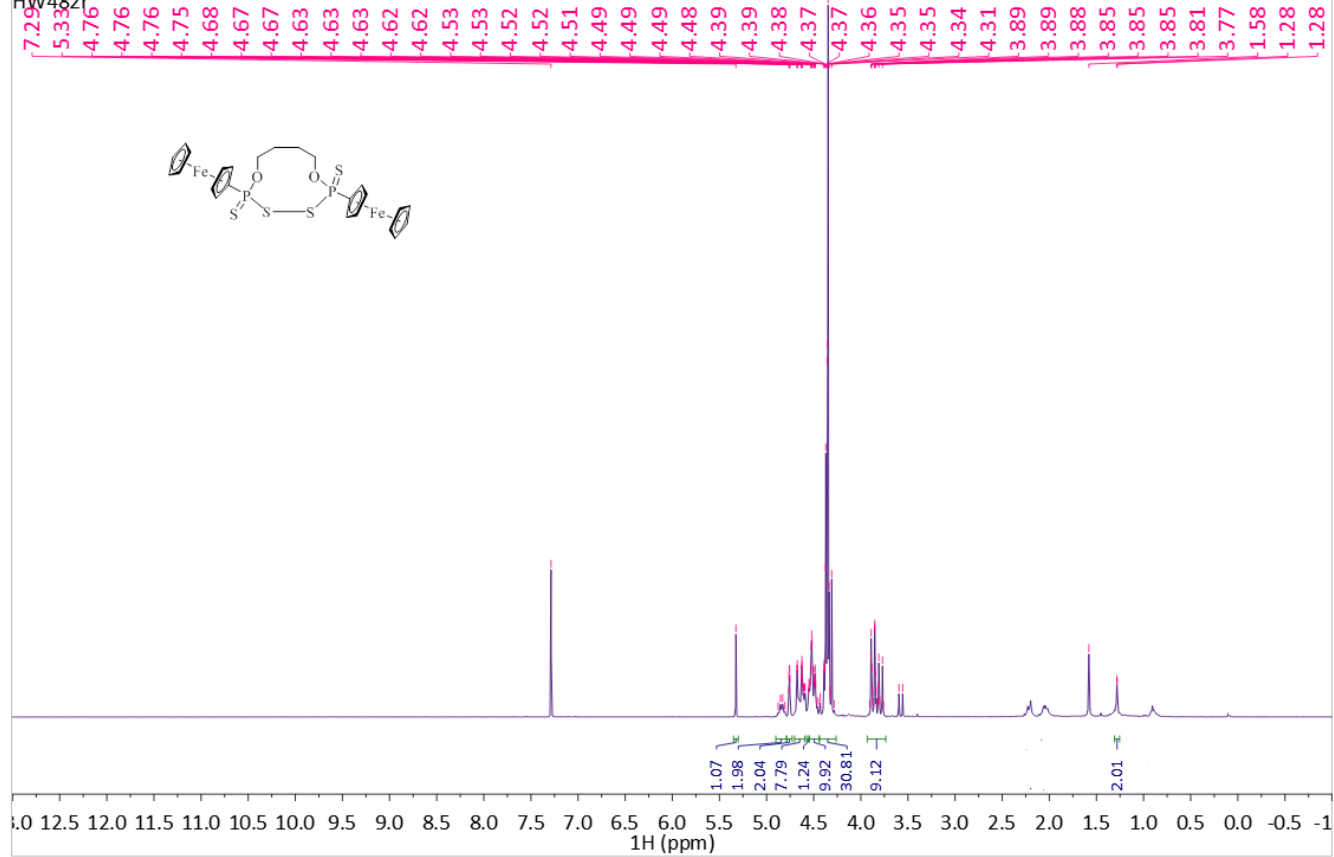


02062015-14-jdw-gh15-M.10.fid

1H Observe - Quantitative

1H NMR spectrum of compound **3**

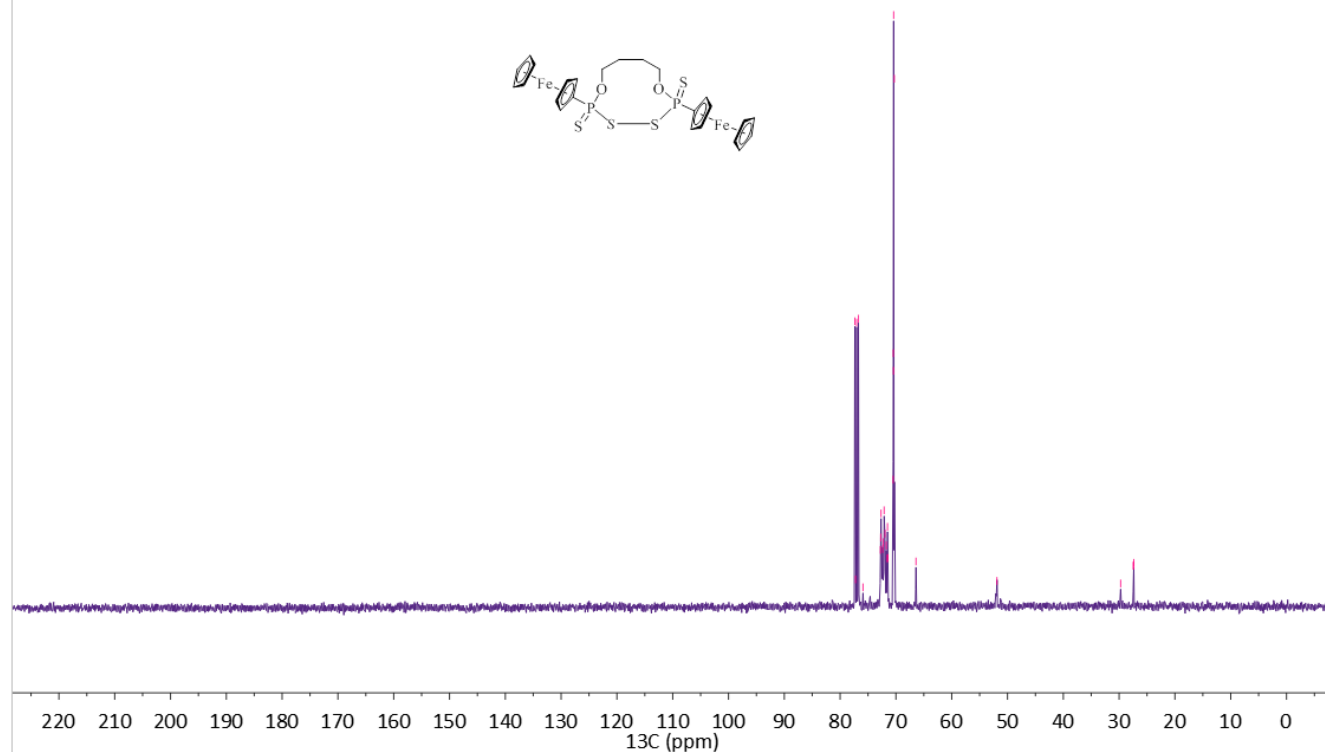
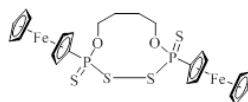
Hw482r



02062015-14-jdw-gh15-M.11.fid
 13C Observe with 1H decoupling - UDEFT
 HW482r

73.35 73.24 77.04 76.72 75.90 72.78 72.72 72.67 72.34 72.25 72.11 71.95 71.73 71.57 71.51 71.44 70.50 70.47 70.44 70.40 70.29 66.40 51.90 29.72 27.45 27.41 27.37

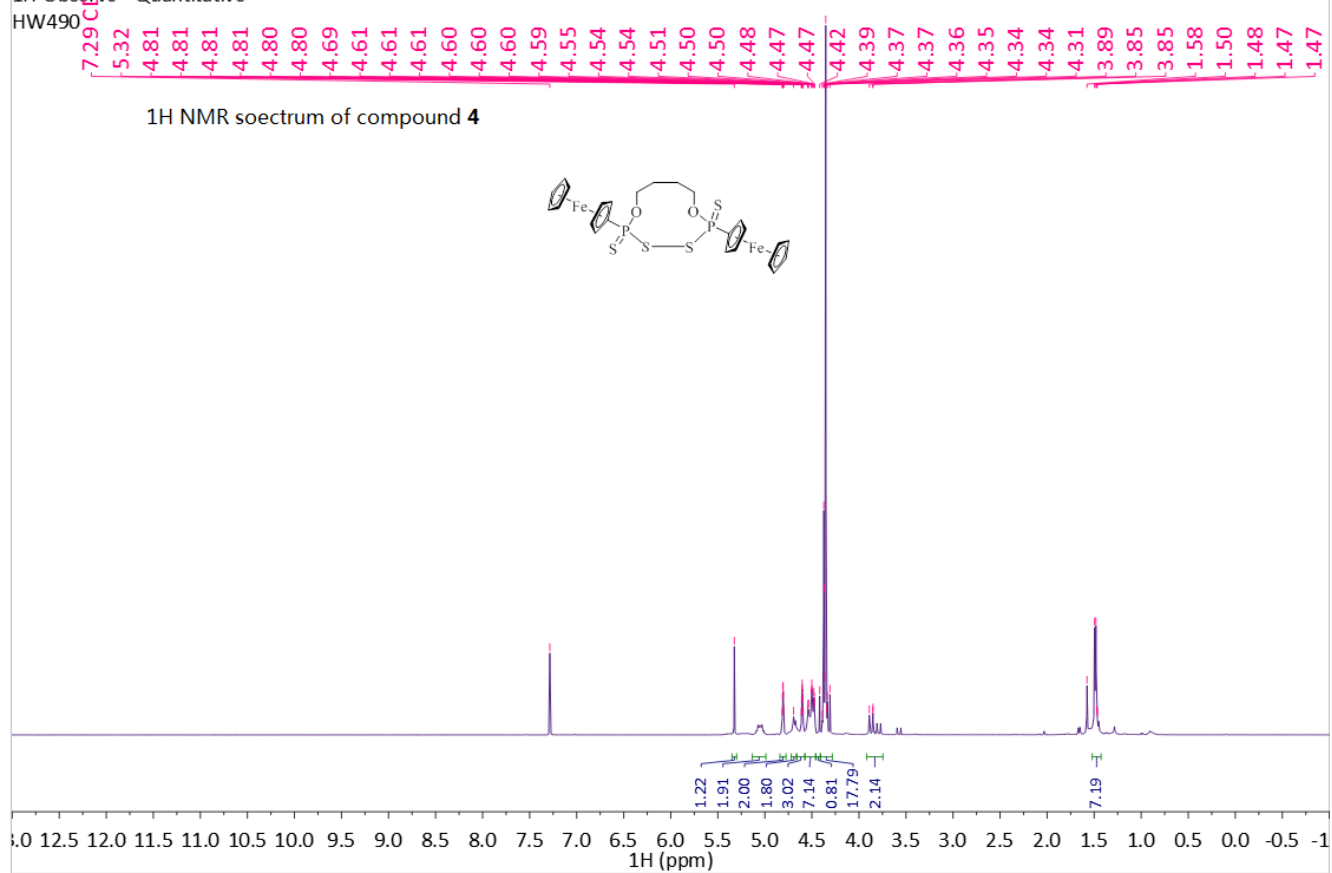
13C NMR spectrum of compound **3**



02232015-17-jdw-gh15-M.10.fid

1H Observed - Quantitative

HW490

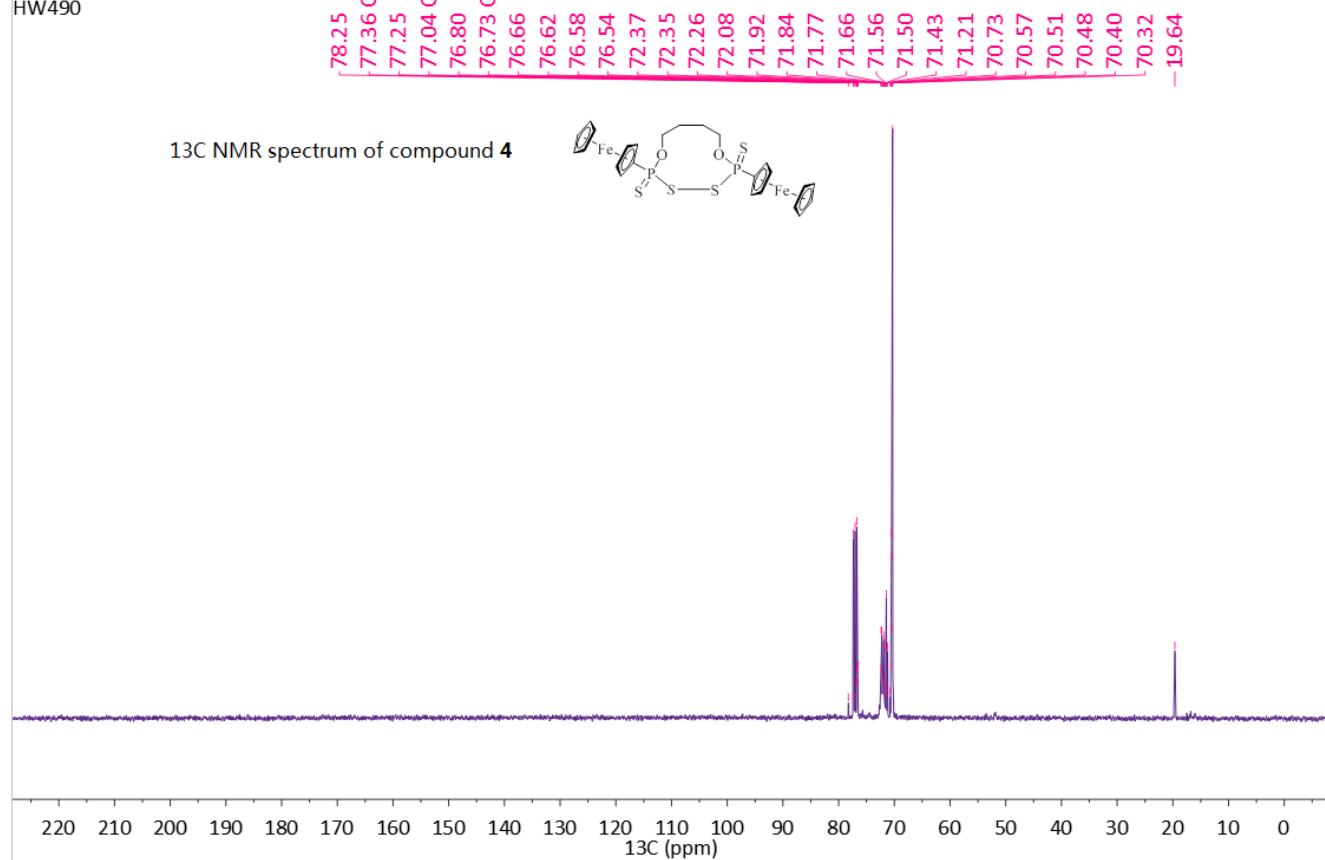
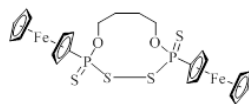


02232015-17-jdw-gh15-M.11.fid

13C Observe with 1H decoupling - UDE

HW490

13C NMR spectrum of compound **4**

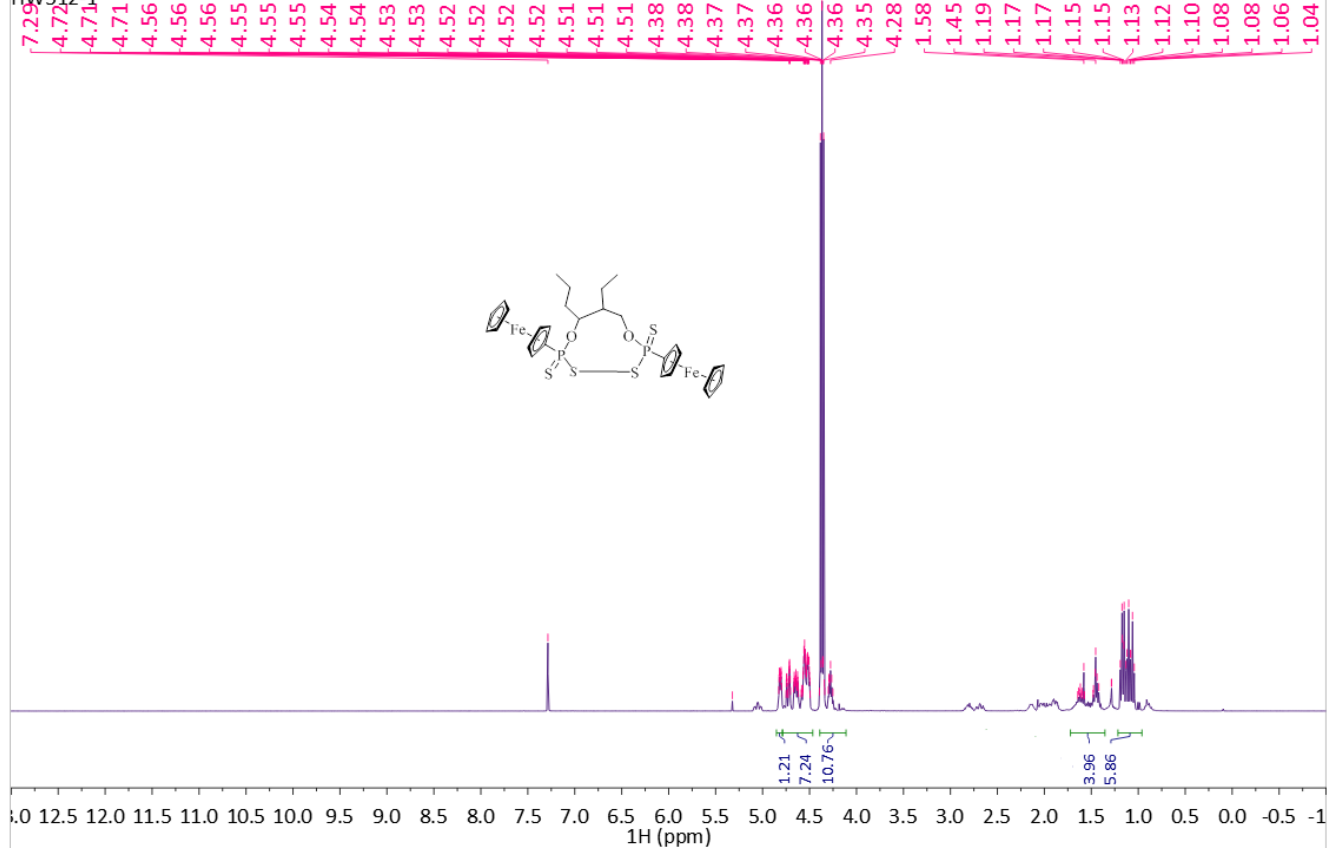


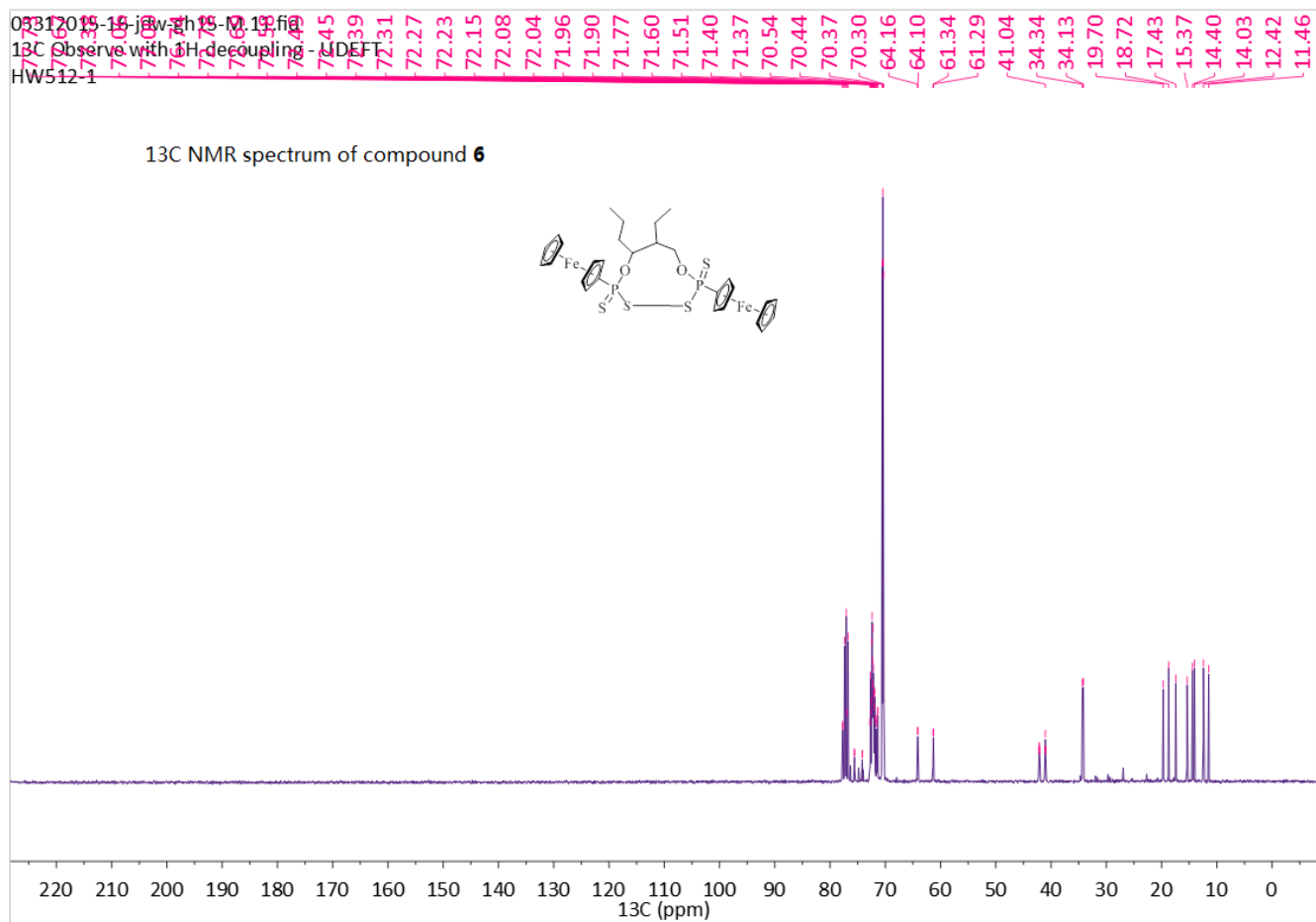
0312015-16-jdw-gh15-M.10.fid

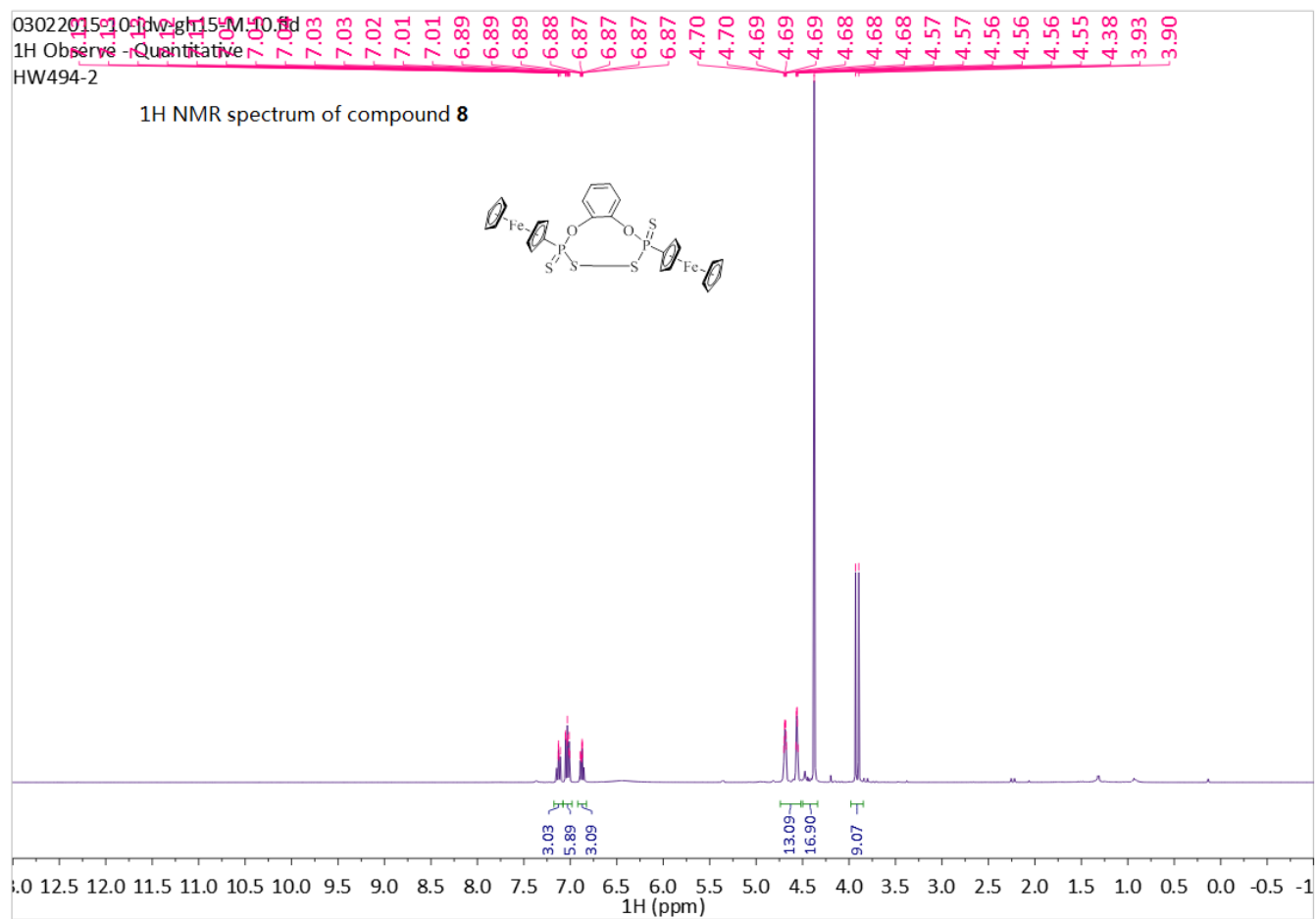
1H Observe - Quantitative

1H NMR spectrum of compound **6**

HW512-1





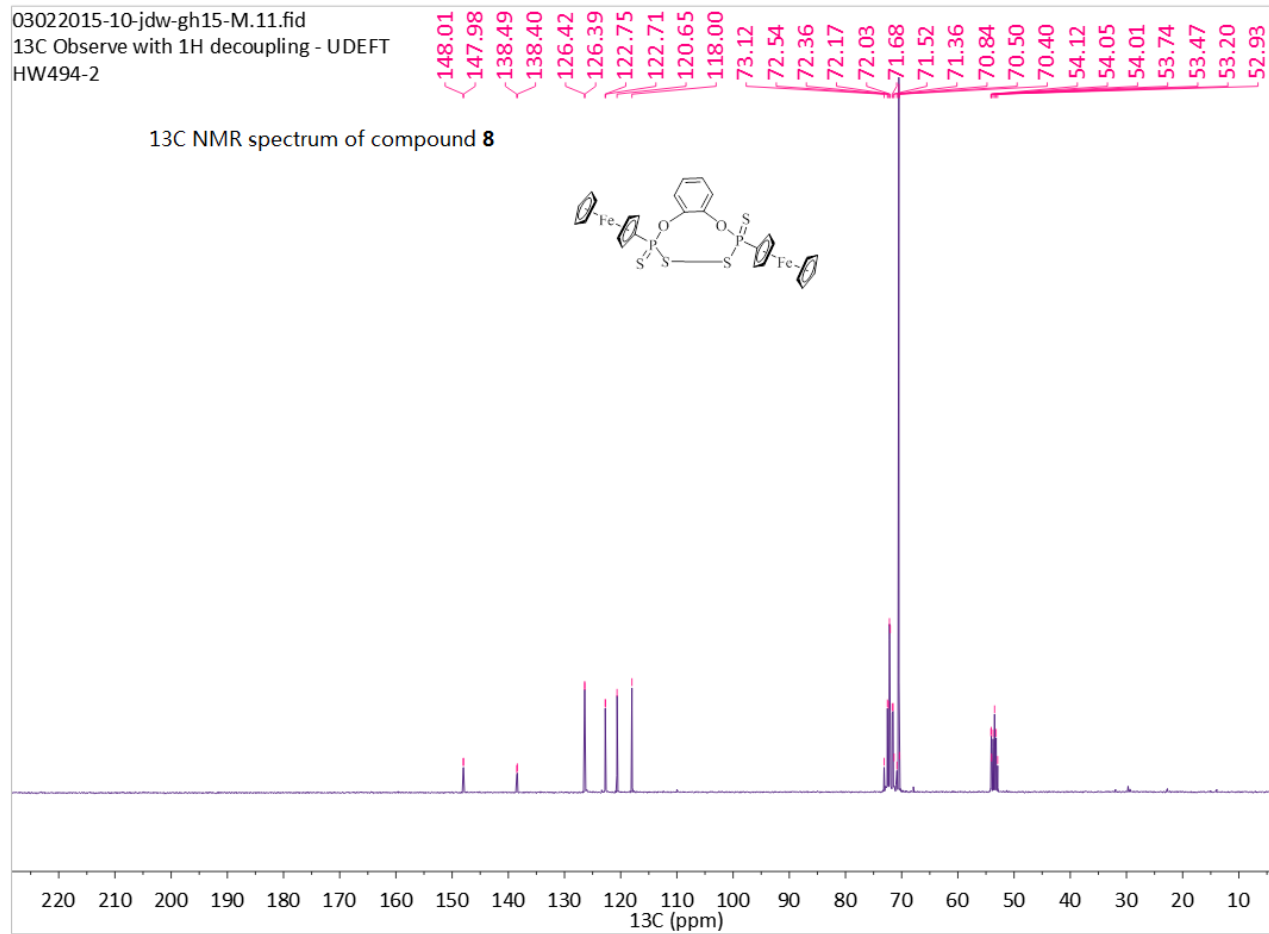
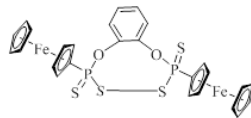


03022015-10-jdw-gh15-M.11.fid

¹³C Observe with ¹H decoupling - UDEFT

HW494-2

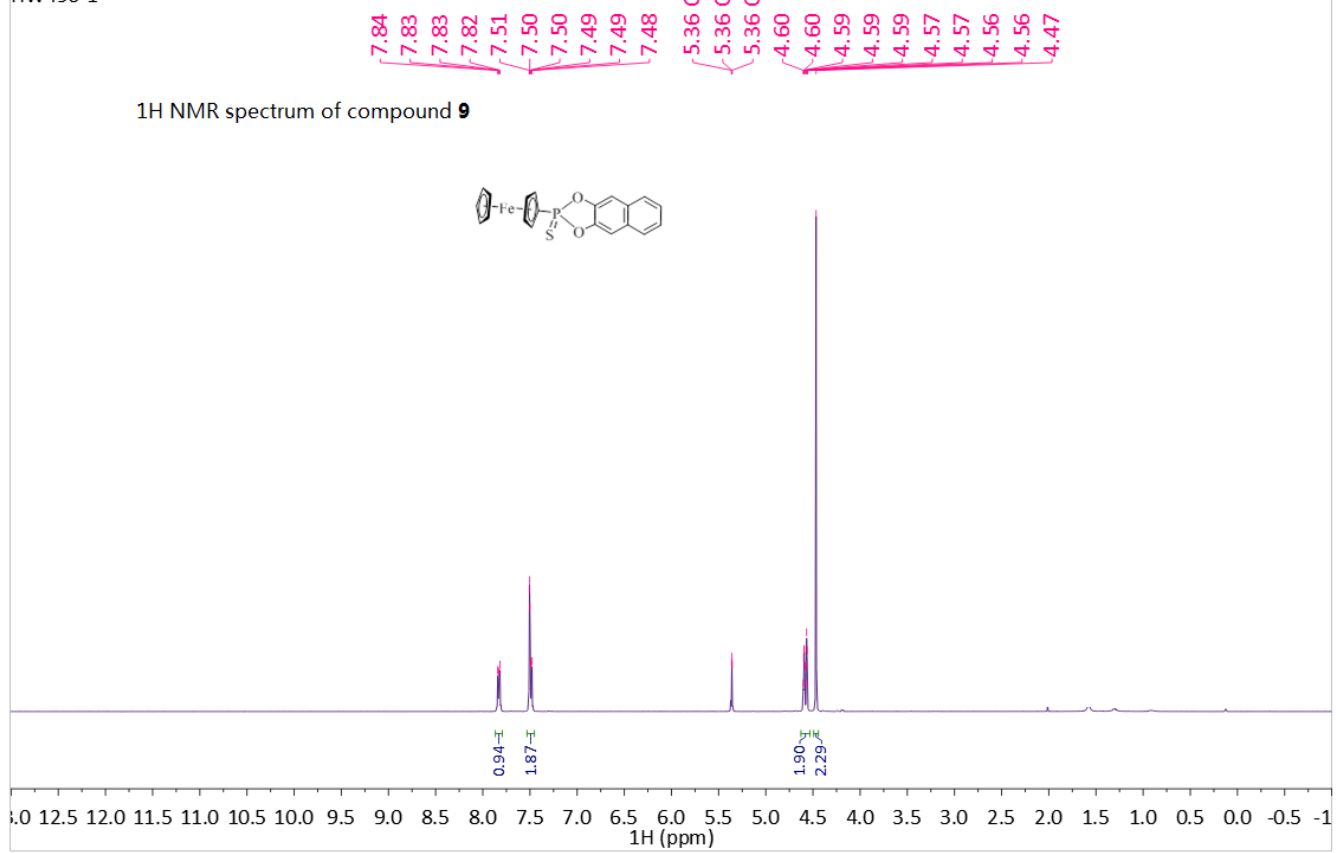
¹³C NMR spectrum of compound **8**



03032015-12-jdw-gh15-M.10.fid

1H Observe - Quantitative

HW496-1



03032015-12-jdw-gh15-M.11.fid

¹³C Observe with ¹H decoupling - UDEFT

HW496-1

144.82

130.32

127.39

125.48

108.48

108.38

73.35

73.21

72.60

72.42

71.05

53.97

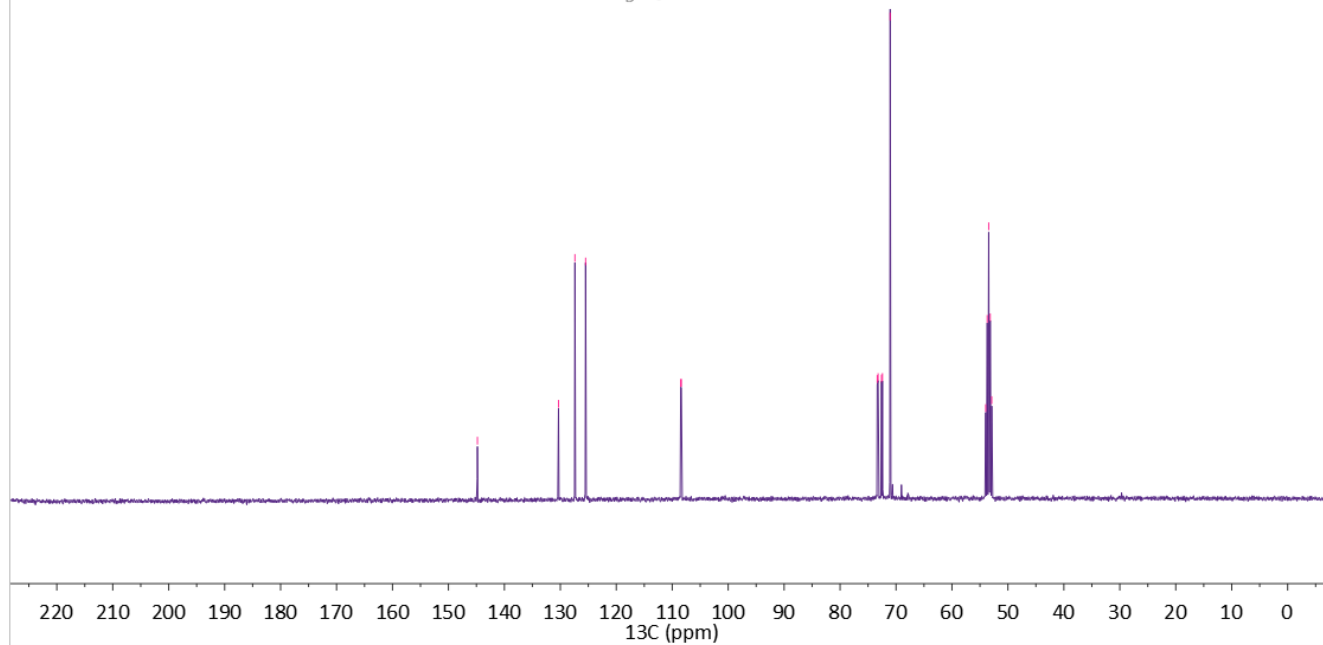
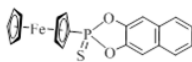
53.70

53.43

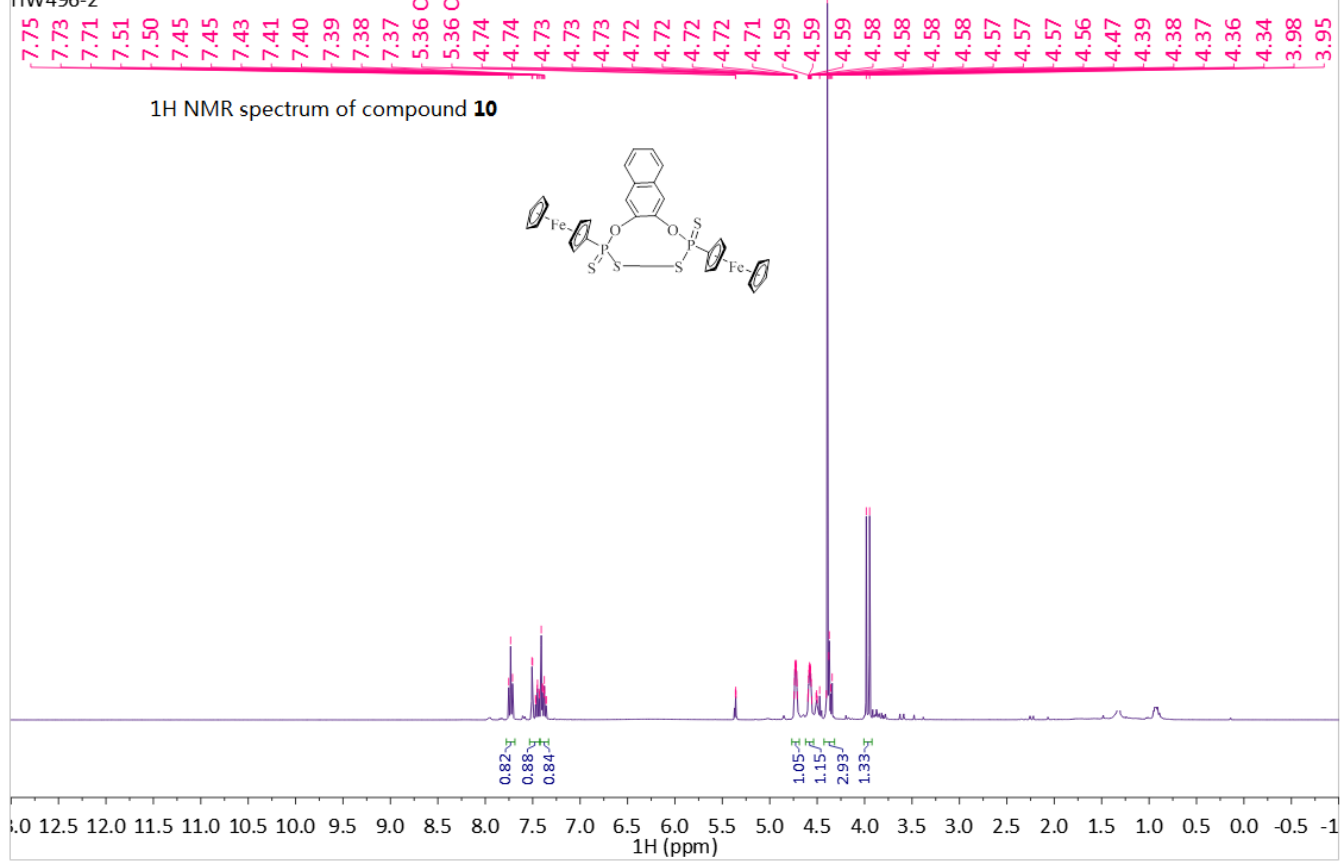
53.16

52.89

¹³C NMR spectrum of compound **9**



HW496-2



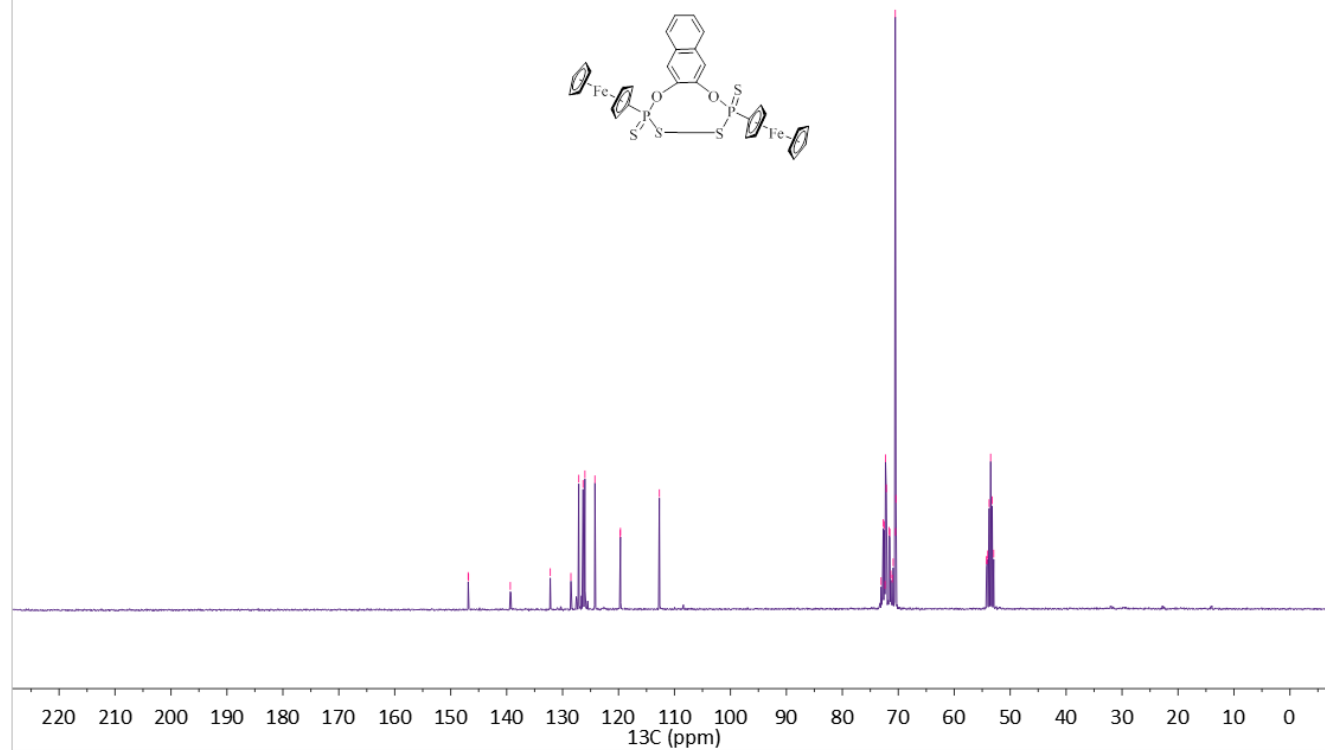
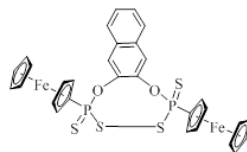
03032015-13-jdw-gh-15-M-11.fid

13C Observe with 1H decoupling - UDF-F

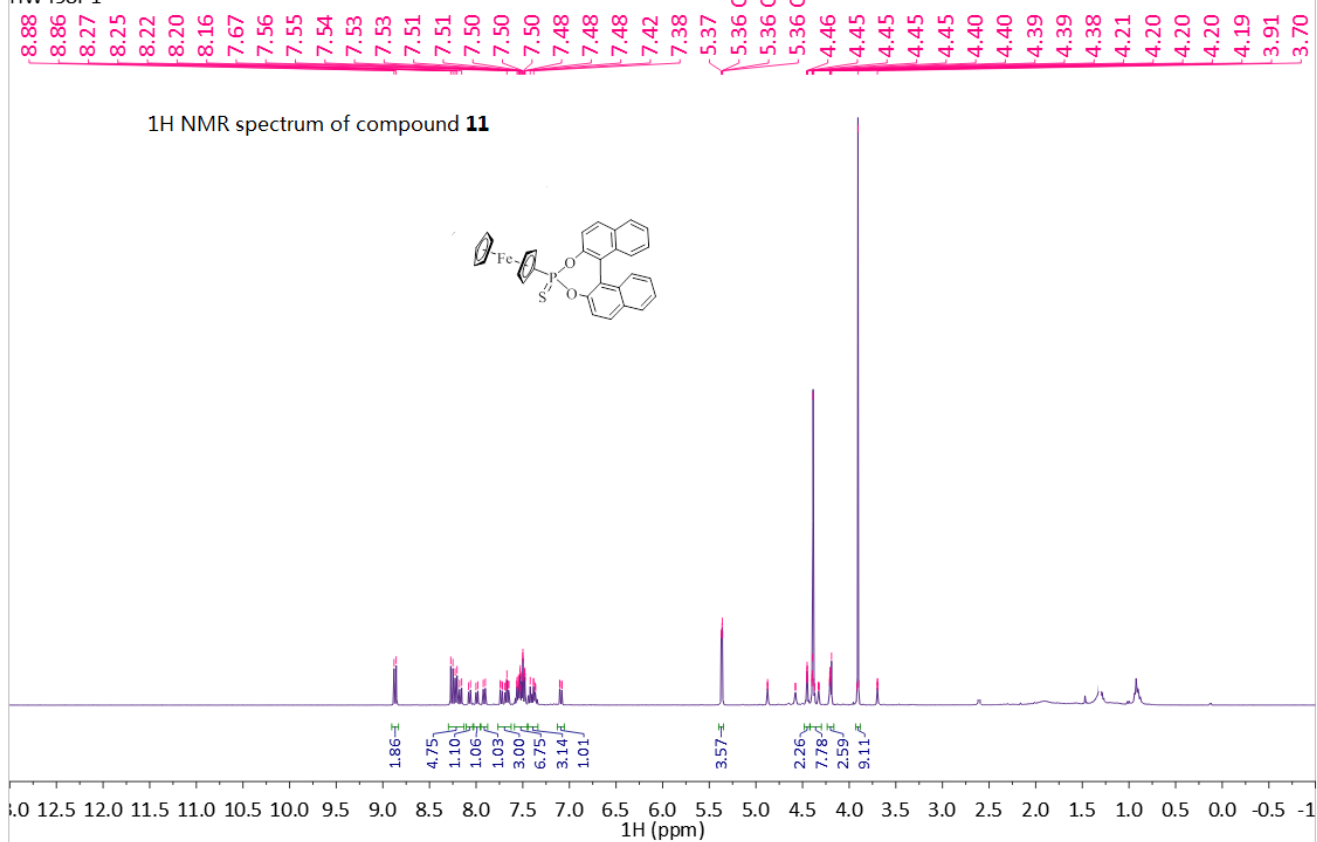
HW496-2

145.87, 145.81, 145.75, 137.71, 137.55, 127.12, 126.34, 126.01, 124.22, 119.71, 119.66, 112.71, 73.08, 72.68, 72.50, 72.36, 72.28, 72.14, 71.65, 71.50, 71.31, 71.08, 70.91, 70.54, 70.50, 70.41, 54.22, 54.16, 54.03, 53.76, 53.49, 53.22, 52.95

13C NMR spectrum of compound **10**

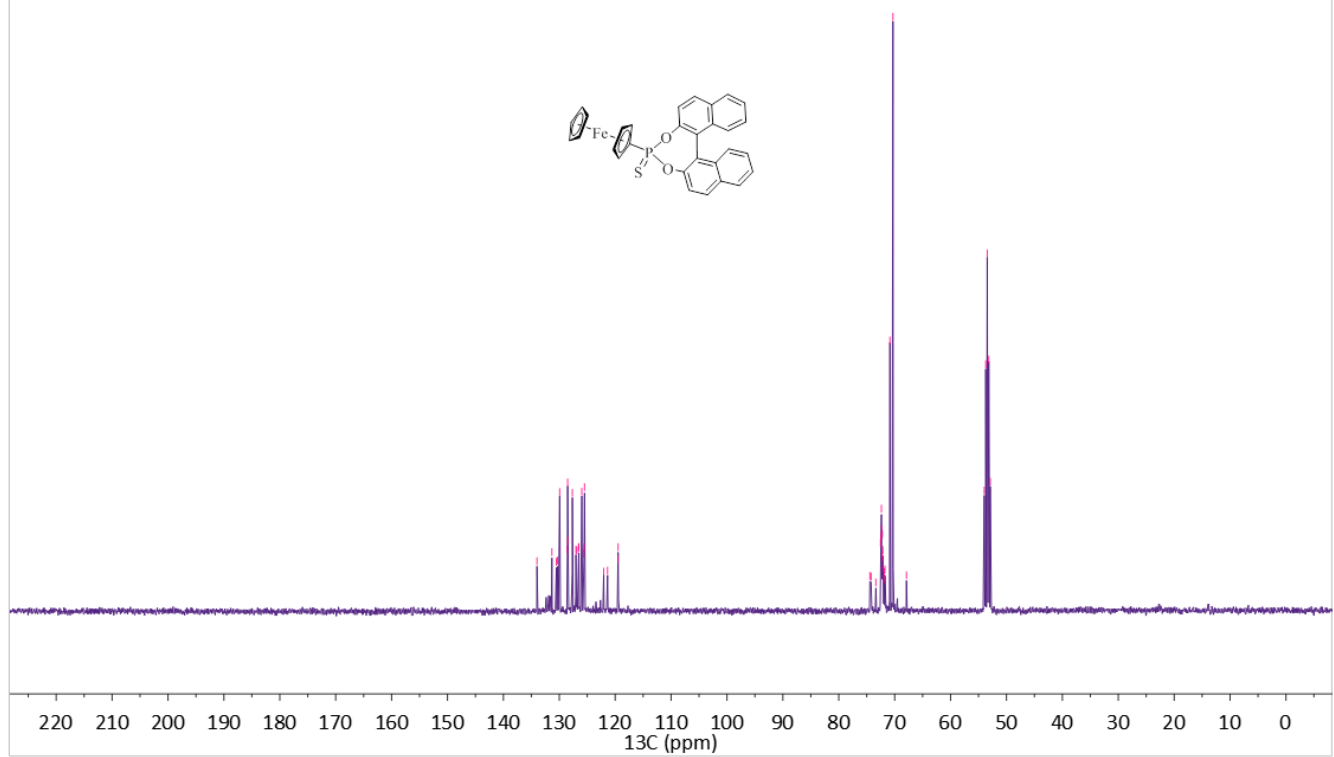


HW498r-1



HW498r-1

72.53
72.45
72.37
72.34
72.29
72.25
72.20
72.12
72.05
71.85
71.75
70.85
70.31
67.89
53.98
53.71
53.44
53.17
52.90



03192015-11-jdw-gh15-M.10.fid

1H Observe - Quantitative

HW498r-2

