

Supplementary Material

Improved Access to Linear Tetrameric Hydroxamic Acids with Potential as Radiochemical Ligands for Zirconium(IV)-89 PET Imaging

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Electronic Supplementary Material

INDEX

Item	Title	Pg
Index	Index	1
Figure S1a	¹ H NMR spectrum of 2	2
Figure S1b	¹³ C NMR spectrum of 2	2
Figure S2a	¹ H NMR spectrum of 3	3
Figure S2b	¹³ C NMR spectrum of 3	3
Figure S2c	¹ H- ¹ H COSY NMR spectrum of 3	4
Figure S2d	¹ H- ¹³ C HSQC NMR spectrum of 3	4
Figure S2e	HRMS of 3	5
Figure S3a	¹ H NMR spectrum of 4	6
Figure S3b	¹³ C NMR spectrum of 4	6
Figure S3c	¹ H- ¹ H COSY NMR spectrum of 4	7
Figure S3d	¹ H- ¹³ C HSQC NMR spectrum of 4	7
Figure S3e	HRMS of 4	8
Figure S4a	¹ H NMR spectrum of 5	9
Figure S4b	¹³ C NMR spectrum of 5	9
Figure S4c	¹ H- ¹ H COSY NMR spectrum of 5	10
Figure S4d	¹ H- ¹³ C HSQC NMR spectrum of 5	10
Figure S4e	HRMS of 5	11
Scheme S1	Complexes between Fe(III) and 1–4	12

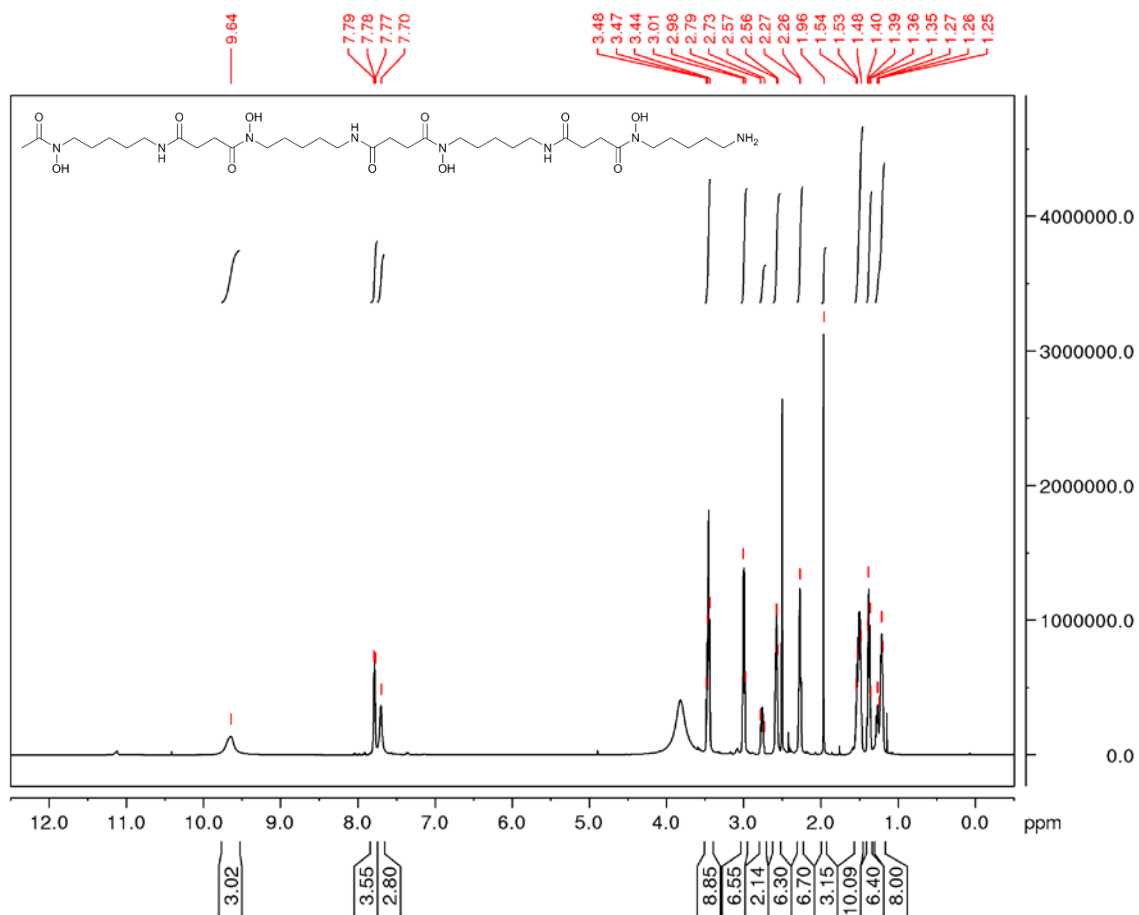


Figure S1a. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PBH (2).

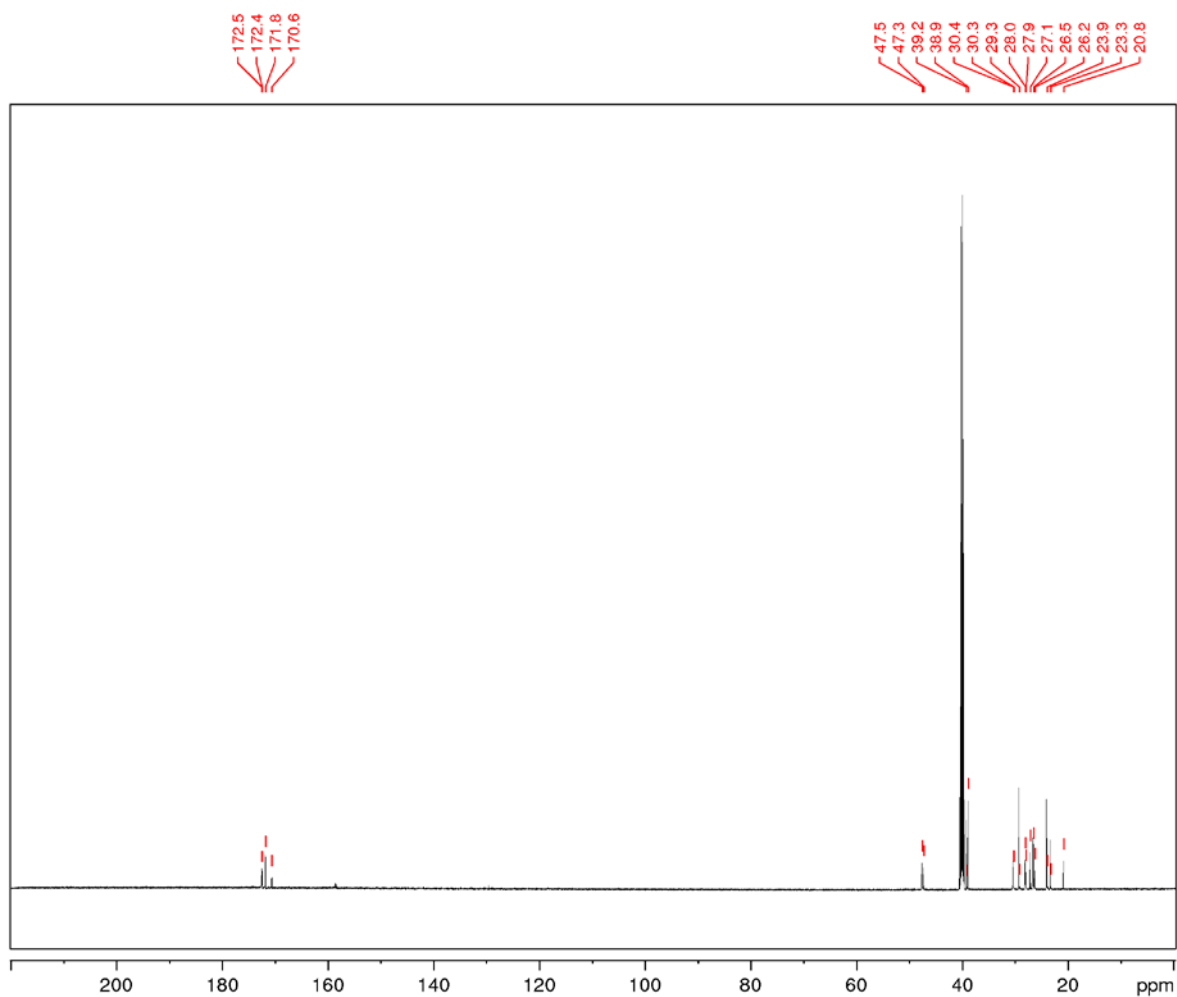


Figure S1b. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) for DFOB-PBH (2).

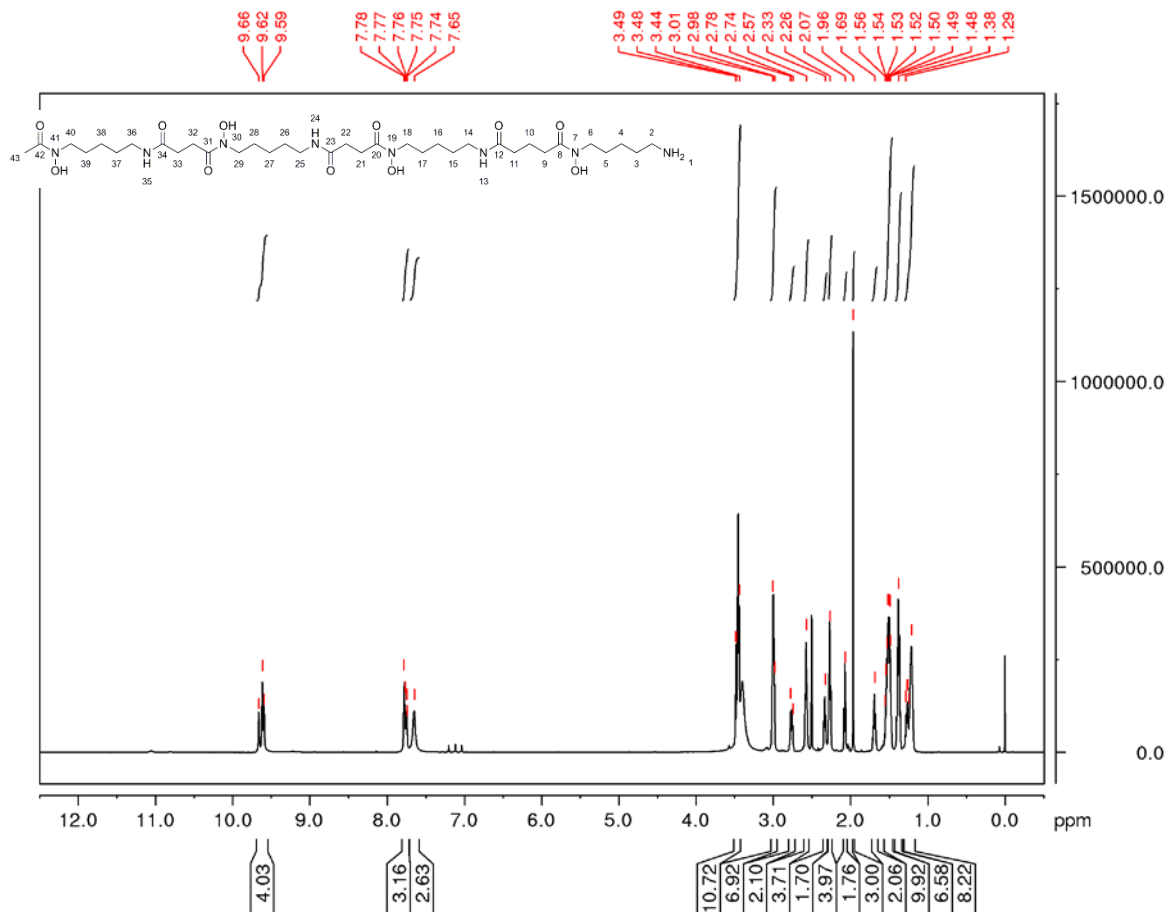


Figure S2a. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH (3).

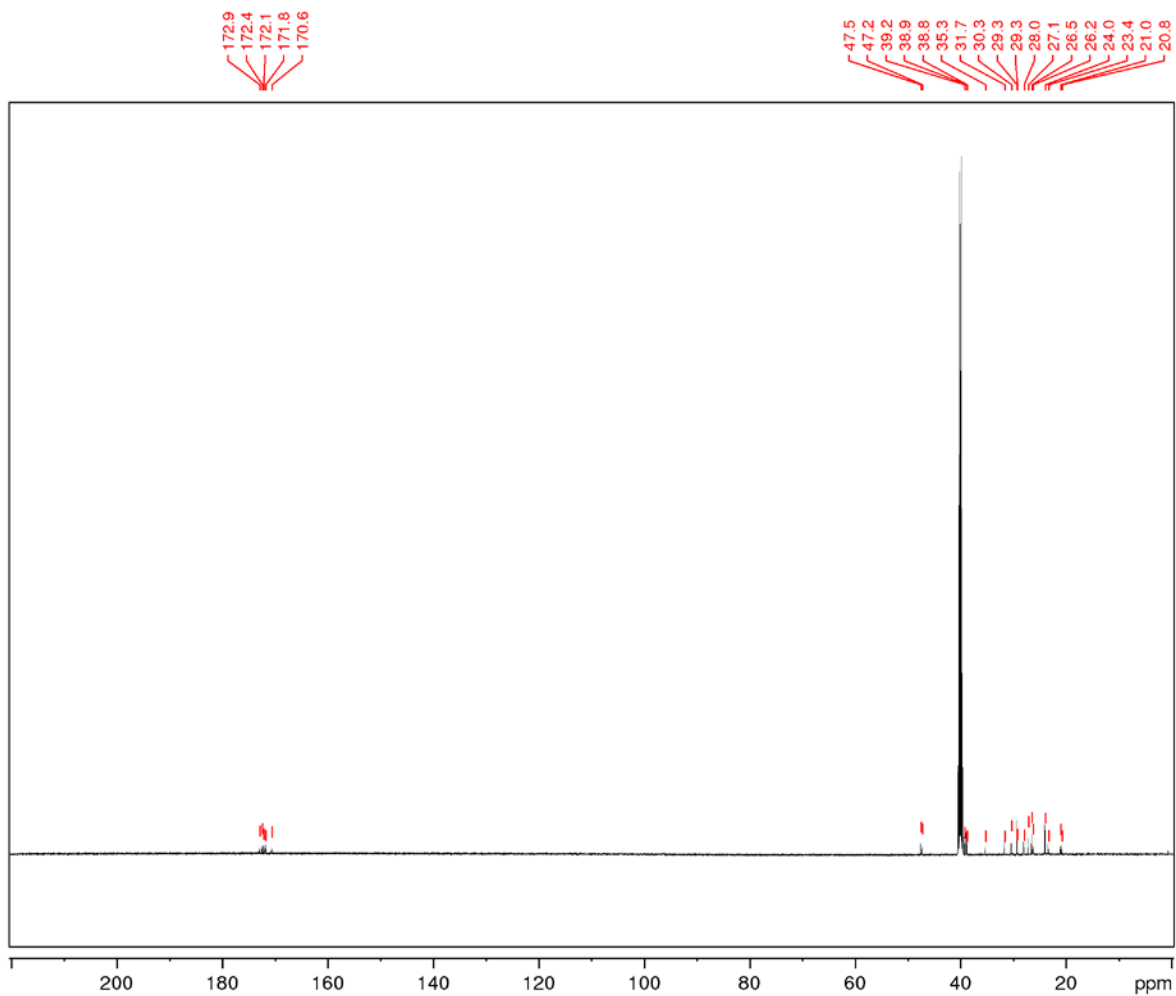


Figure S2b. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) for DFOB-PPH (3).

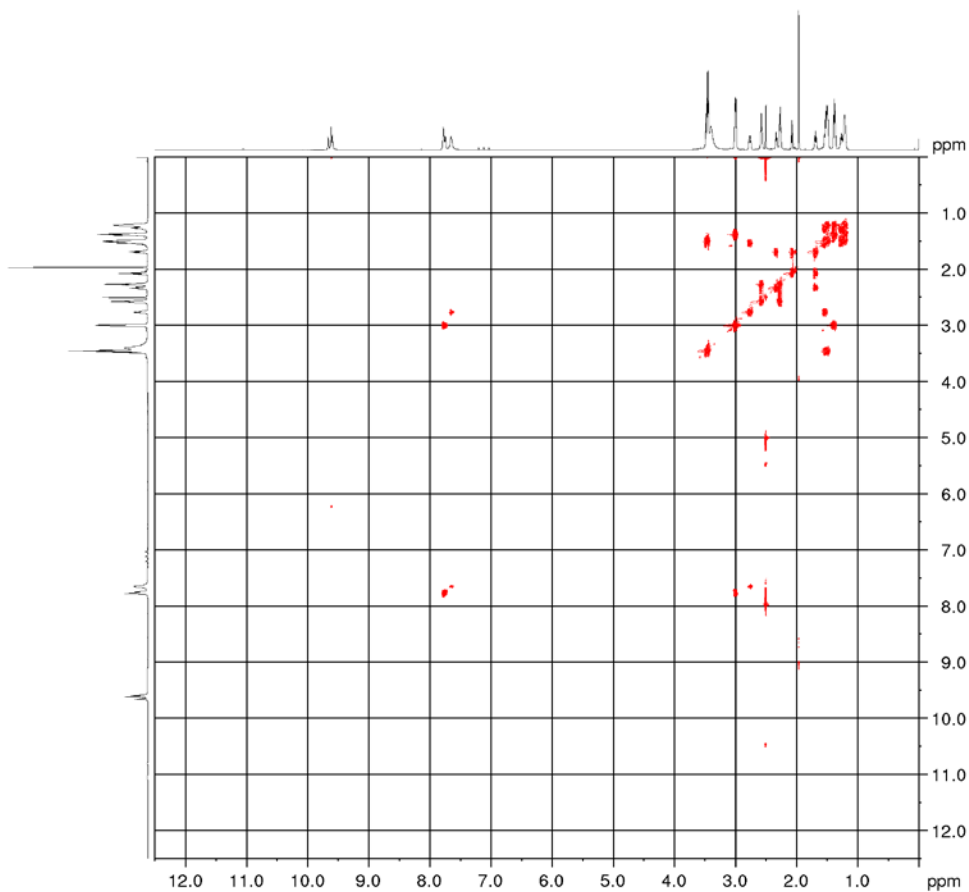


Figure S2c. ¹H-¹H COSY NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH (**3**).

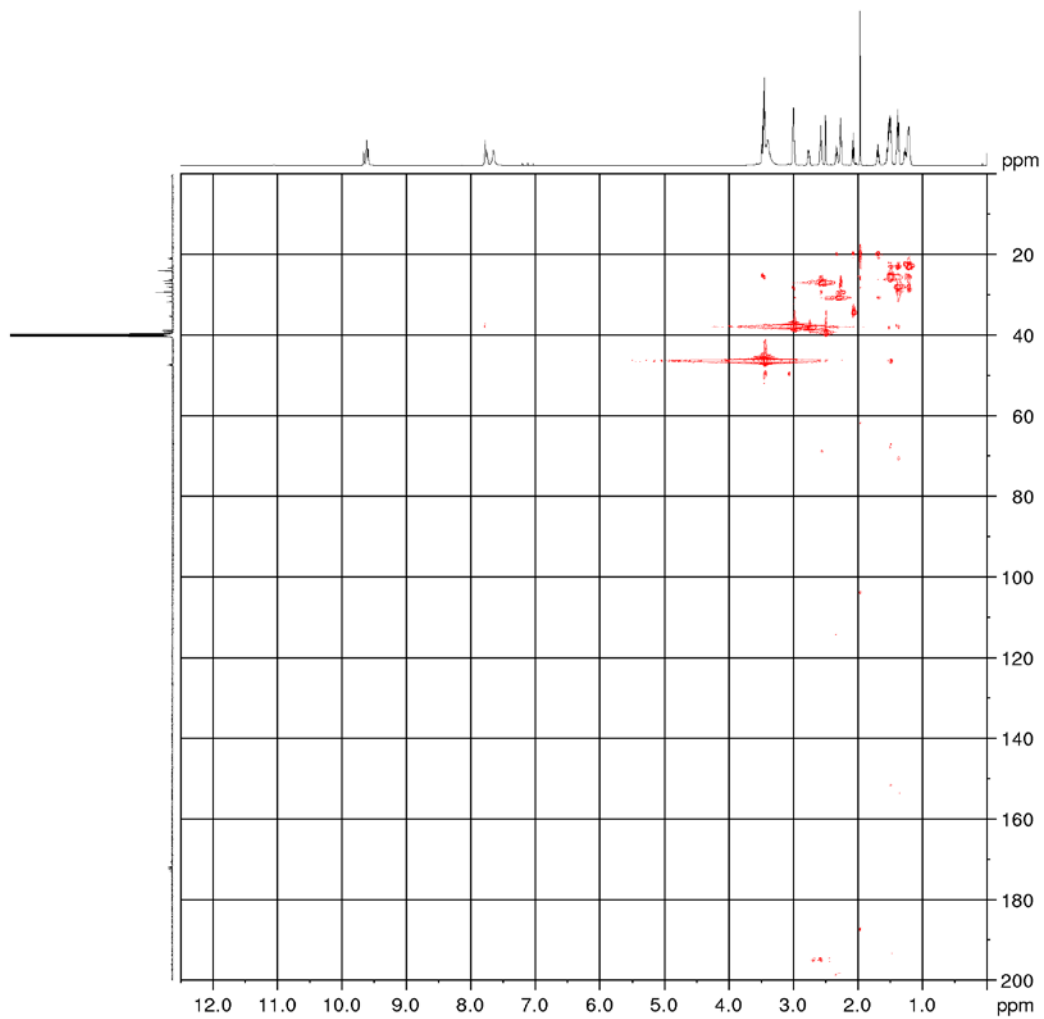
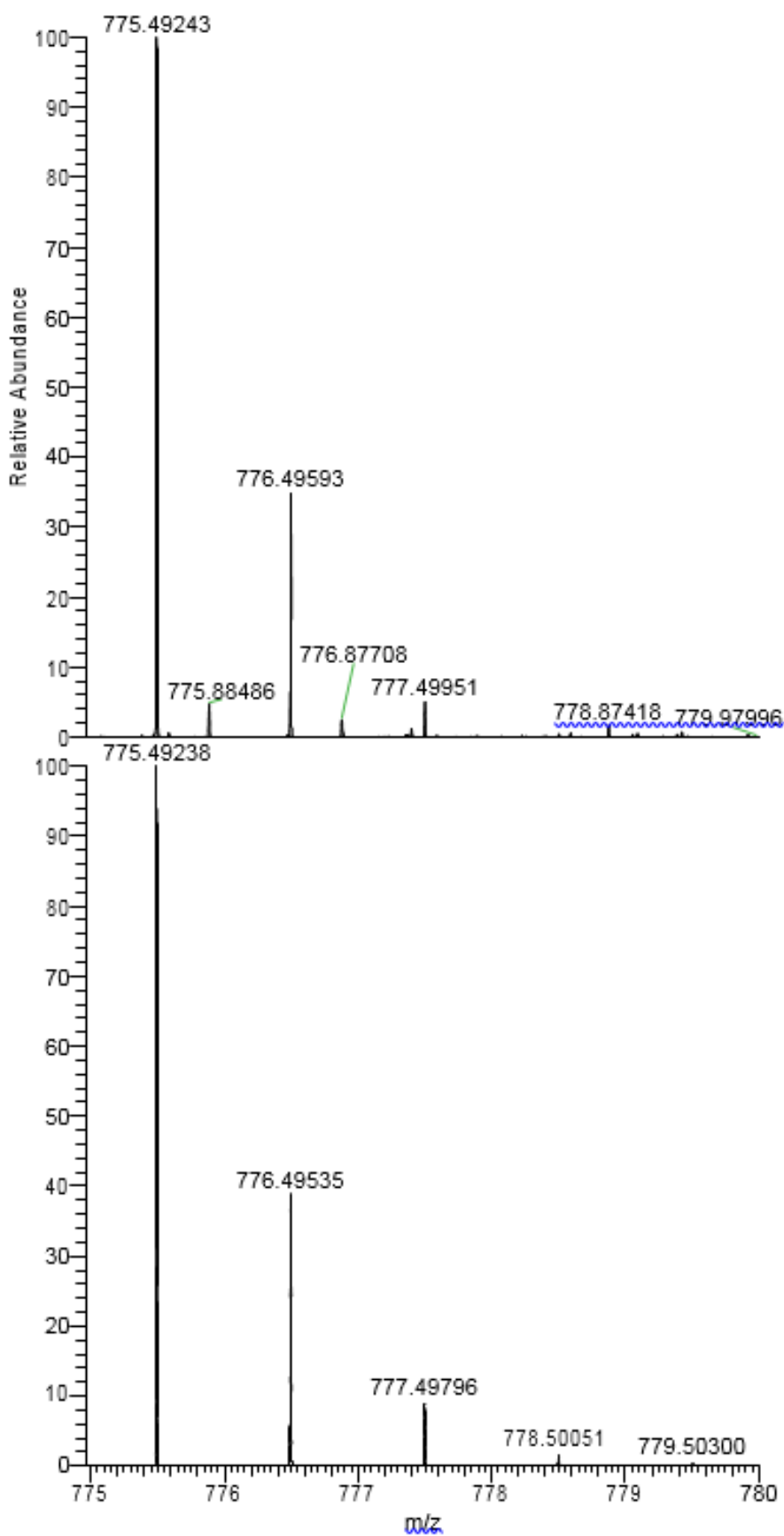


Figure S2d. ¹H-¹³C HSQC NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH (**3**).



NL:
5.51E5
20191014_Velos_NP_DFOB-
PPH#73-87 RT: 2.08-2.45 AV:
15 T: FTMS + p ESI Full ms.
[100.00-2000.00]

NL:
1.51E4
C₃₅H₆₆N₈O₁₁ +H:
C₃₅H₆₇N₈O₁₁
p (gss, s /p:40) Chrg 1
R: 125255 Res. Pwr. @FWHM

Figure S2e. Experimental (top) and calculated (bottom) isotope patterns for the [M+H]⁺ adduct of DFOB-PPH (3).

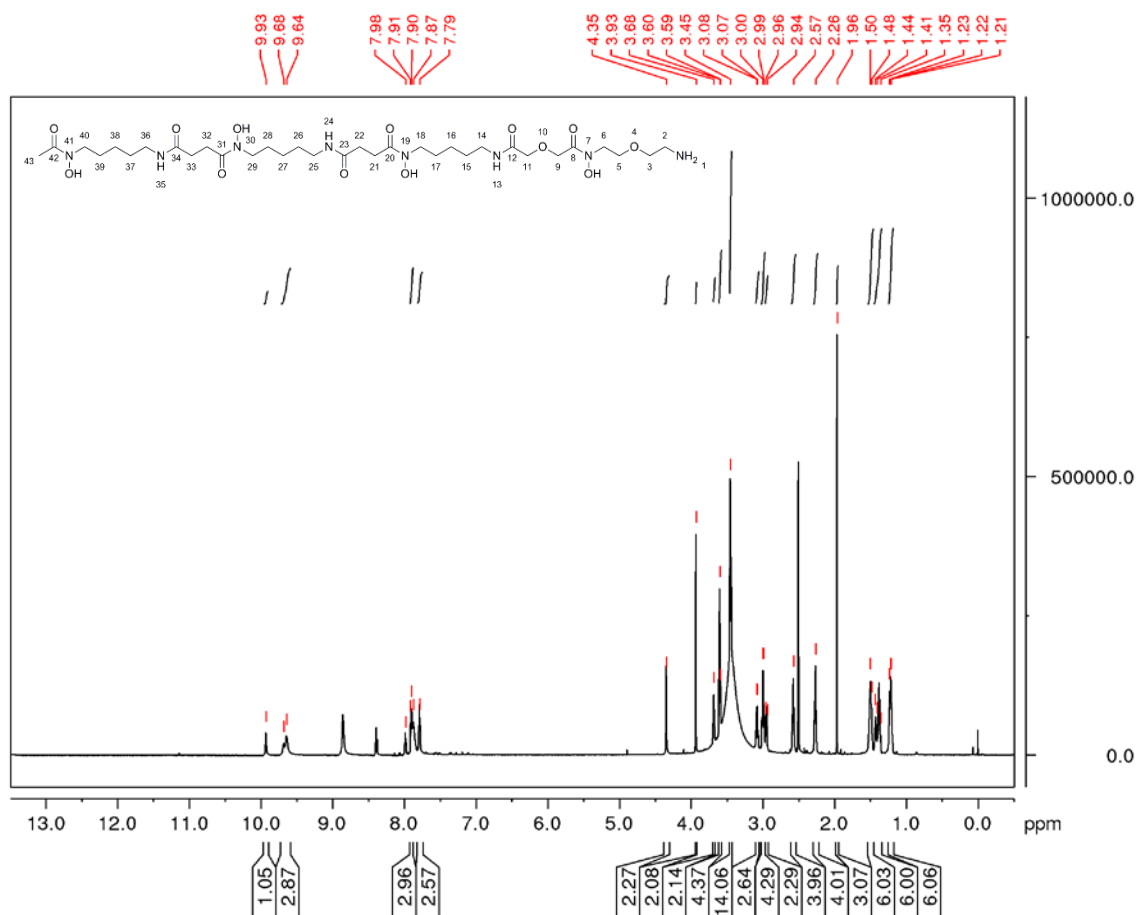


Figure S3a. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH^NO^CO (4).

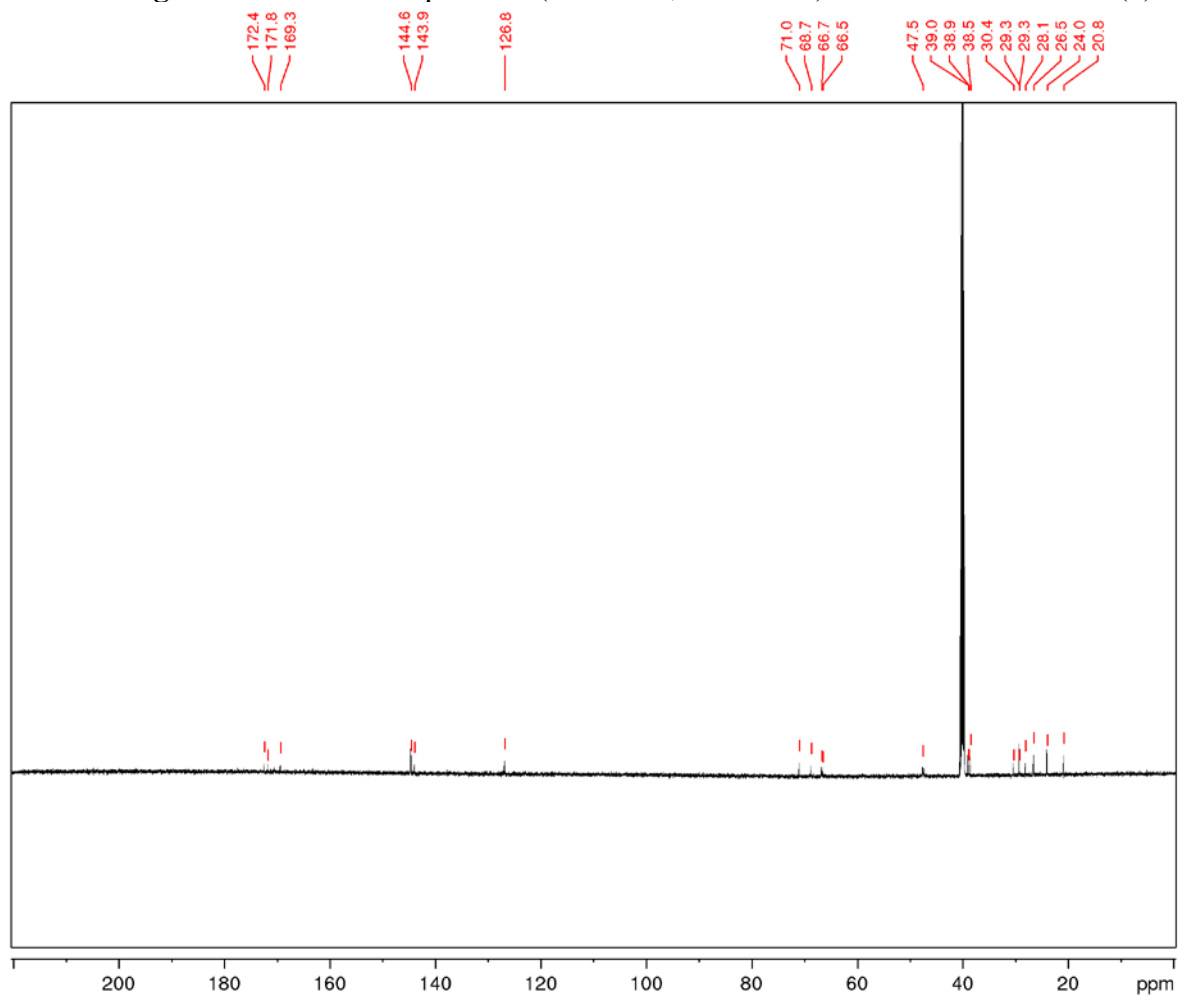


Figure S3b. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) for DFOB-PPH^NO^CO (4).

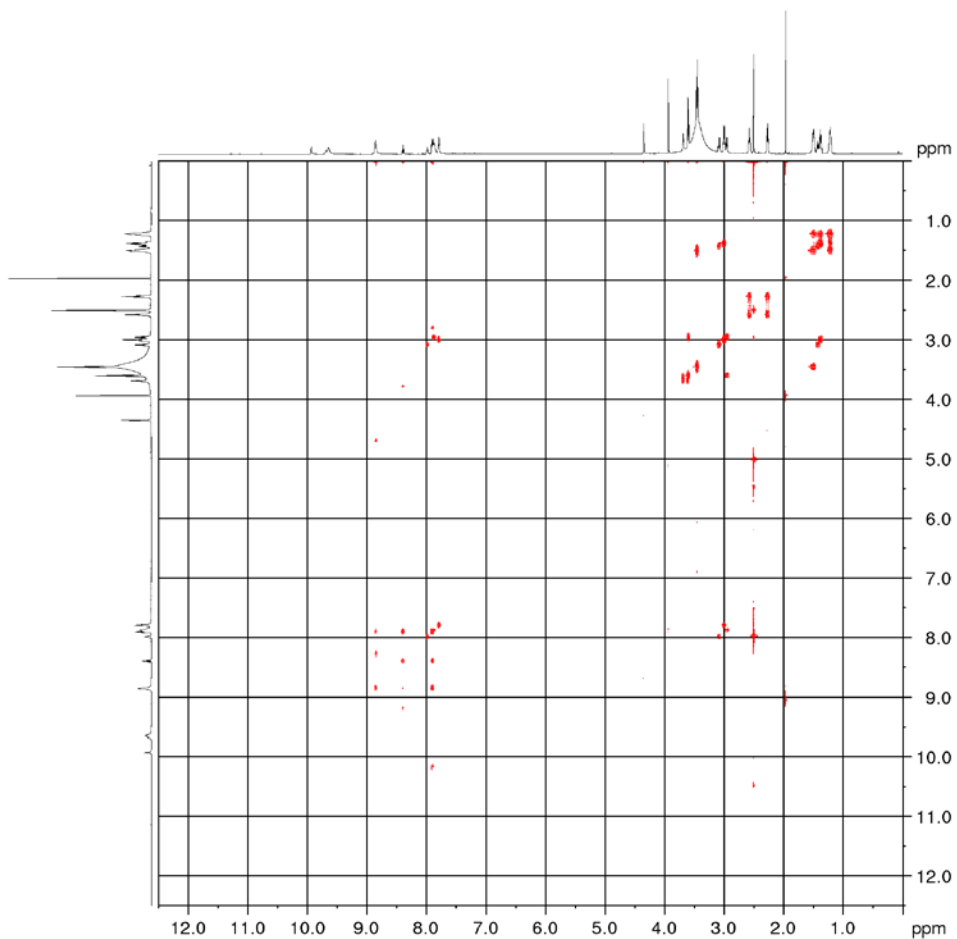


Figure S3c. ^1H - ^1H COSY NMR spectrum (600 MHz, $\text{DMSO-}d_6$) for DFOB-PPH $^{\text{NO}}$ C $^{\text{O}}$ (**4**).

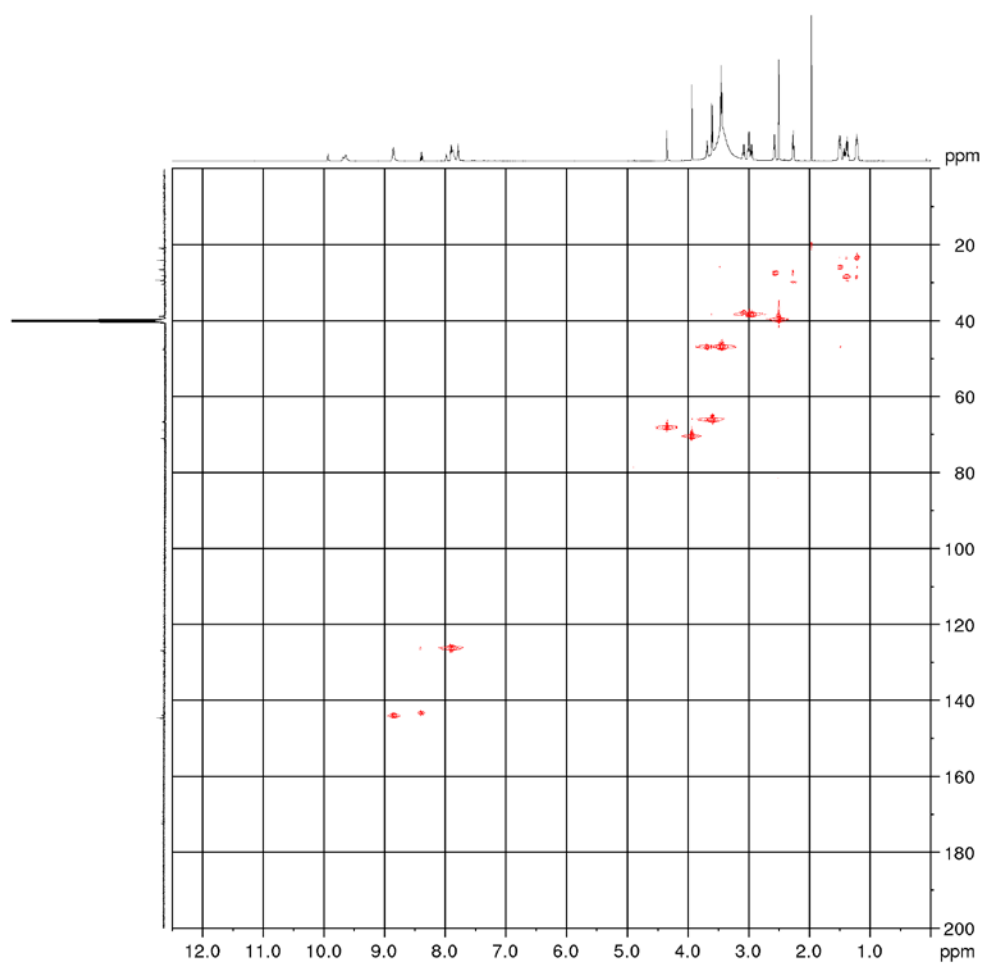


Figure S3d. ^1H - ^{13}C HSQC NMR spectrum (600 MHz, $\text{DMSO-}d_6$) for DFOB-PPH $^{\text{NO}}$ C $^{\text{O}}$ (**4**).

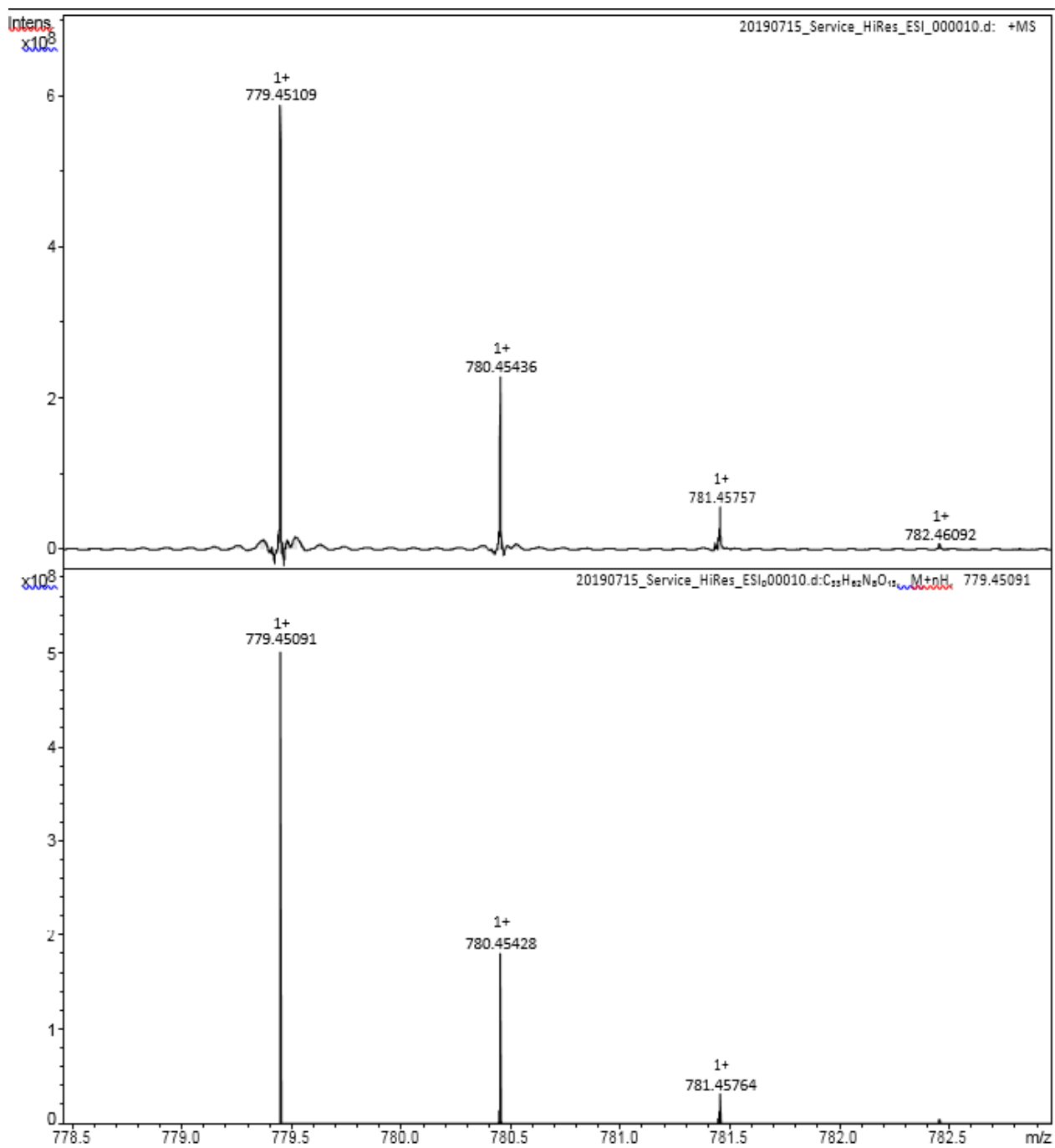


Figure S3e. Experimental (top) and calculated (bottom) isotope patterns for the $[M+H]^+$ adduct of DFOB-PPH^NO^CO (**4**).

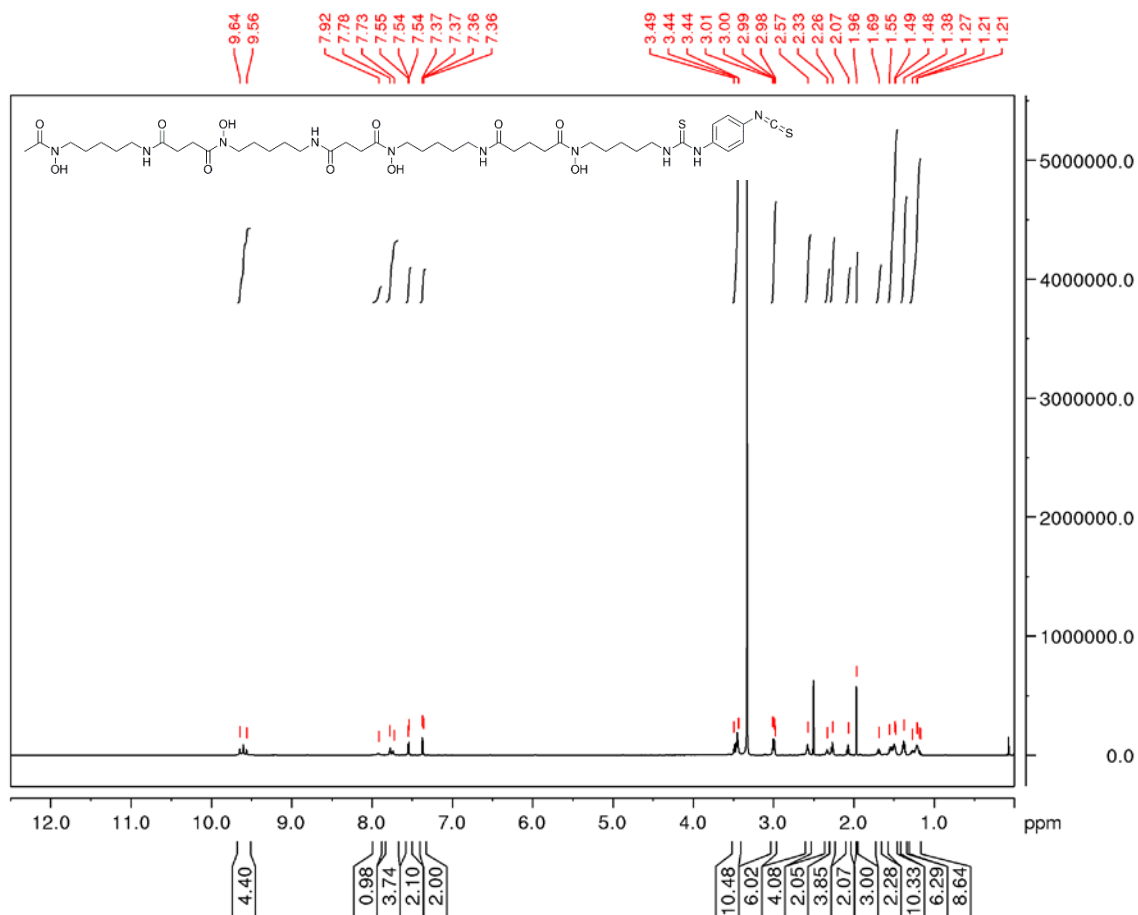


Figure S4a. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH-*p*-Bn-SCN (5).

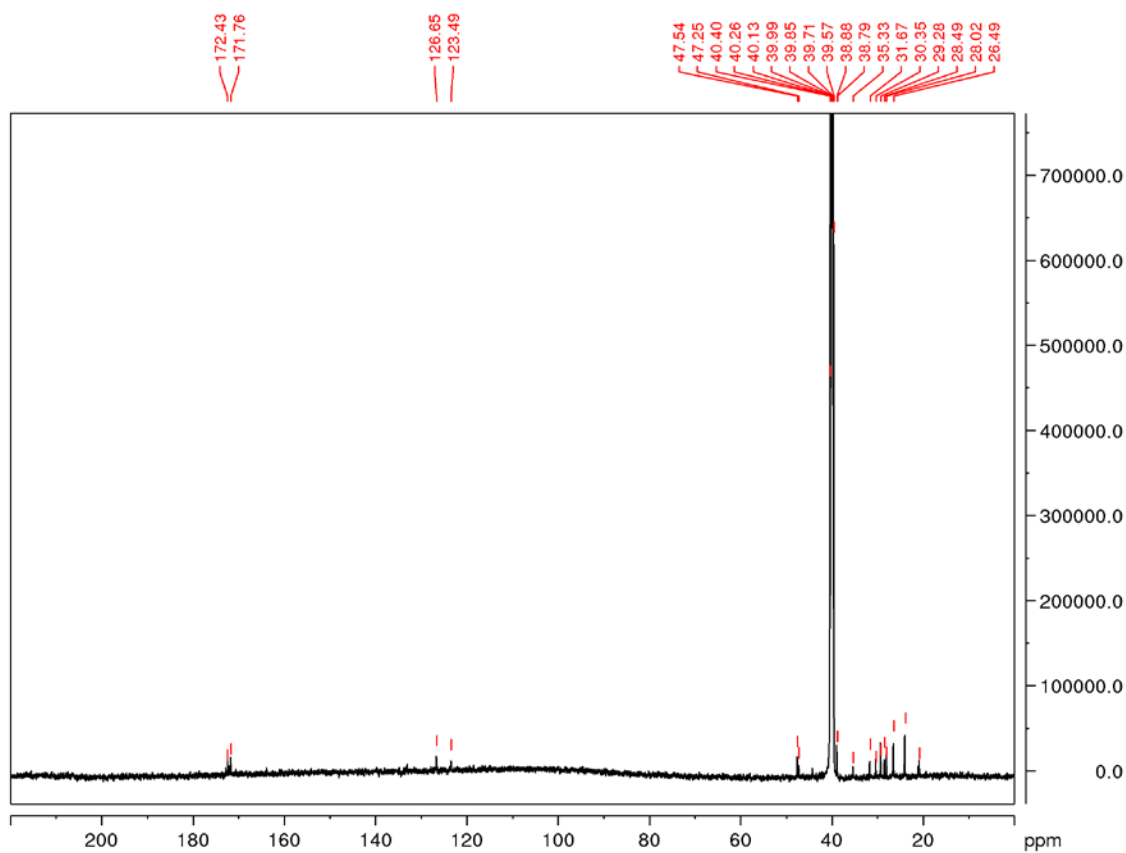


Figure S4b. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) for DFOB-PPH-*p*-Bn-SCN (5).

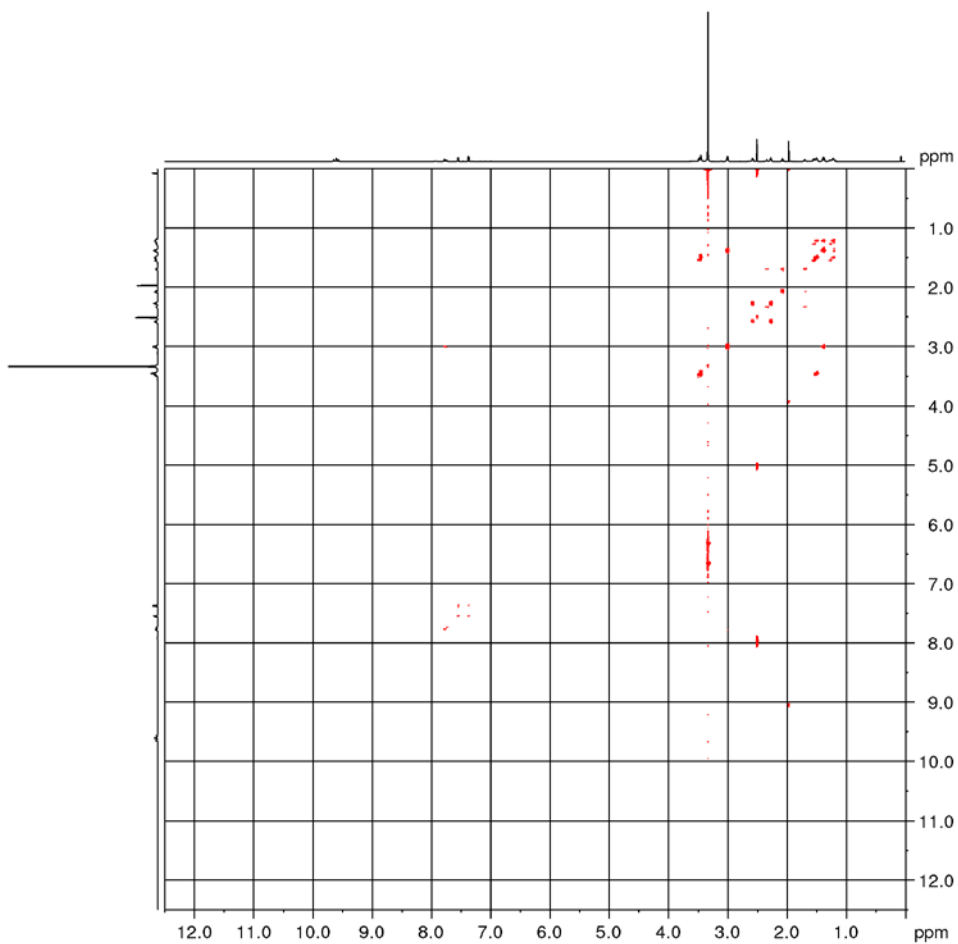


Figure S4c. ¹H-¹H COSY NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH-*p*-Bn-SCN (**5**).

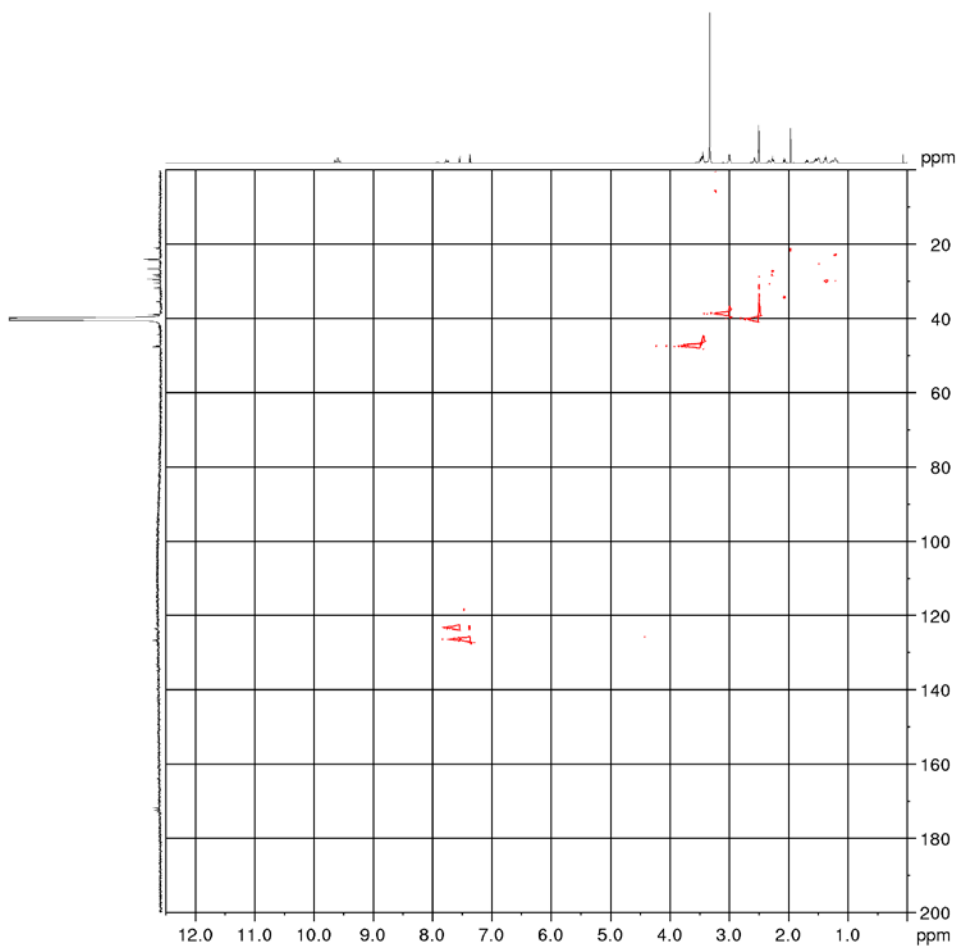
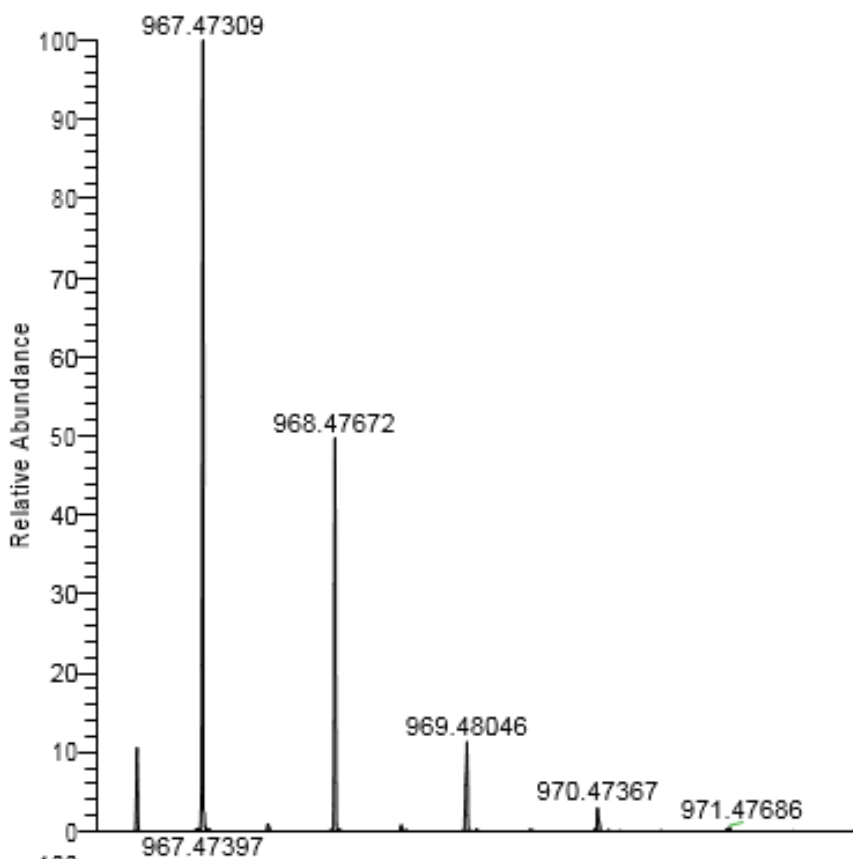
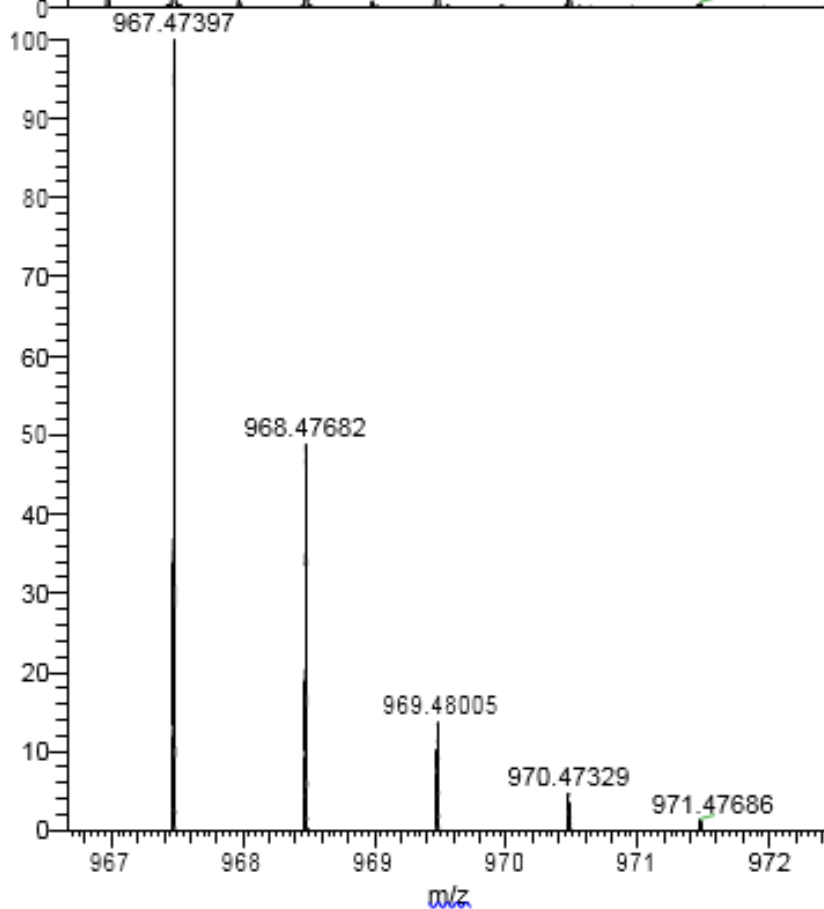


Figure S4d. ¹H-¹³C HSQC NMR spectrum (600 MHz, DMSO-*d*₆) for DFOB-PPH-*p*-Bn-SCN (**5**).

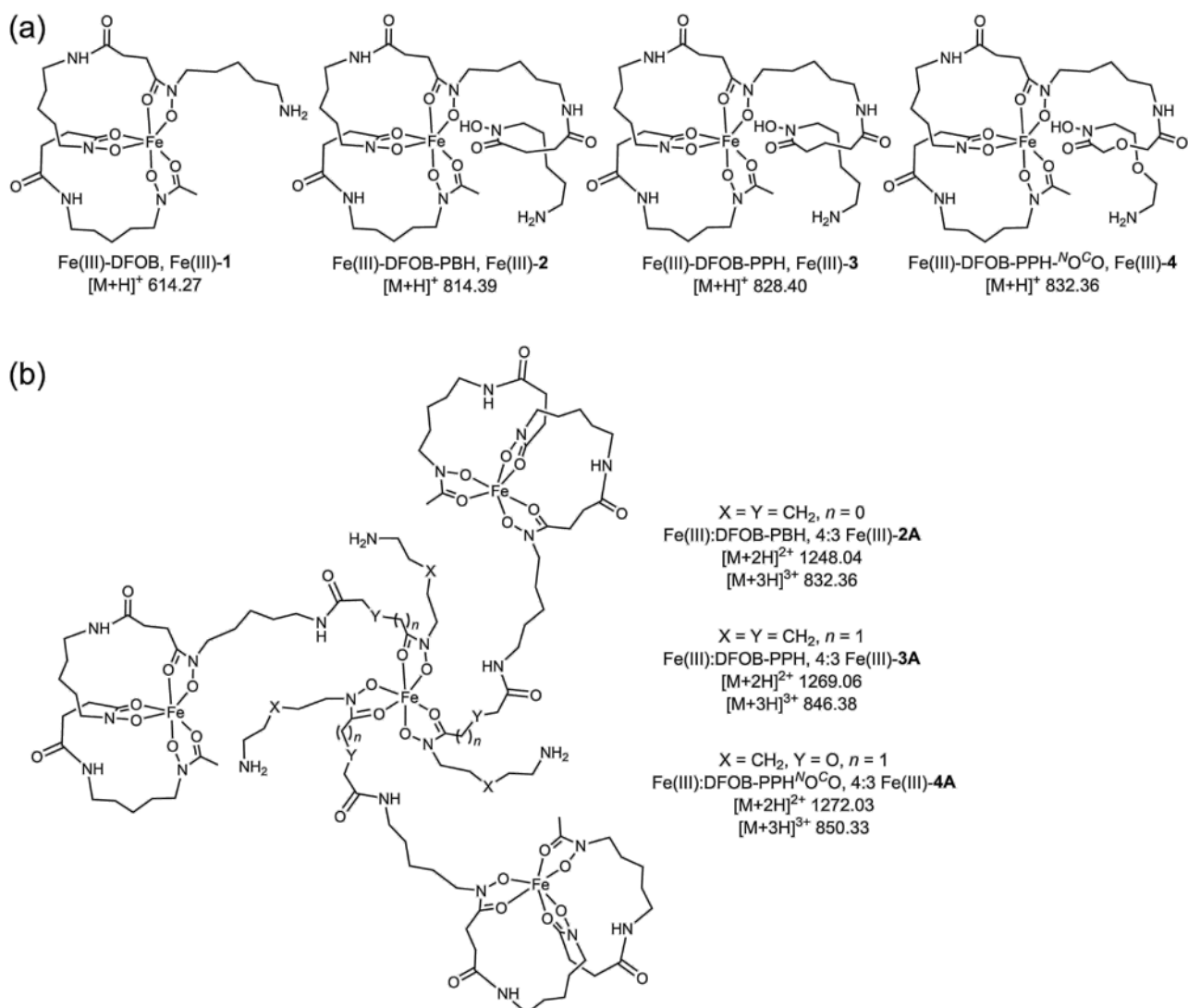


NL:
5.02E6
20191014_Velos_NP_DFOB-
PPM-NCS_a#38-44 RT:
1.01-1.17 AV: 7 T: FTMS + p
ESI Full ms [200.00-2000.00]



NL:
1.24E4
C₄₃ H₇₀ N₁₀ O₁₁ S₂ +H:
C₄₃ H₇₁ N₁₀ O₁₁ S₂
p (qss, s /p:40) Chrg 1
R: 125255 Res. Pw. @FWHM

Figure S4e. Experimental (top) and calculated (bottom) isotope patterns for the $[M+H]^+$ adduct of DFOB-PPH-*p*-Bn-SCN (**5**).



Scheme S1. Complexes between Fe(III) and **1–4** as formed in a metal:ligand stoichiometry of (a) 1:1 or (b) 4:3.