

Supplementary Material

Synthesis of novel bisphosphorylimides based on Staudinger reaction

Lais Weber^a, Michael Weinert^b, Daniela Goedderz^a, Olaf Fuhr^c, and Manfred Döring^a

^aFraunhofer Institute for Structural Durability and System Reliability LBF, 64289 Darmstadt, Germany

^bFraunhofer Institute for Chemical Technology ICT, 76327 Pfinztal, Germany

^cInstitute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

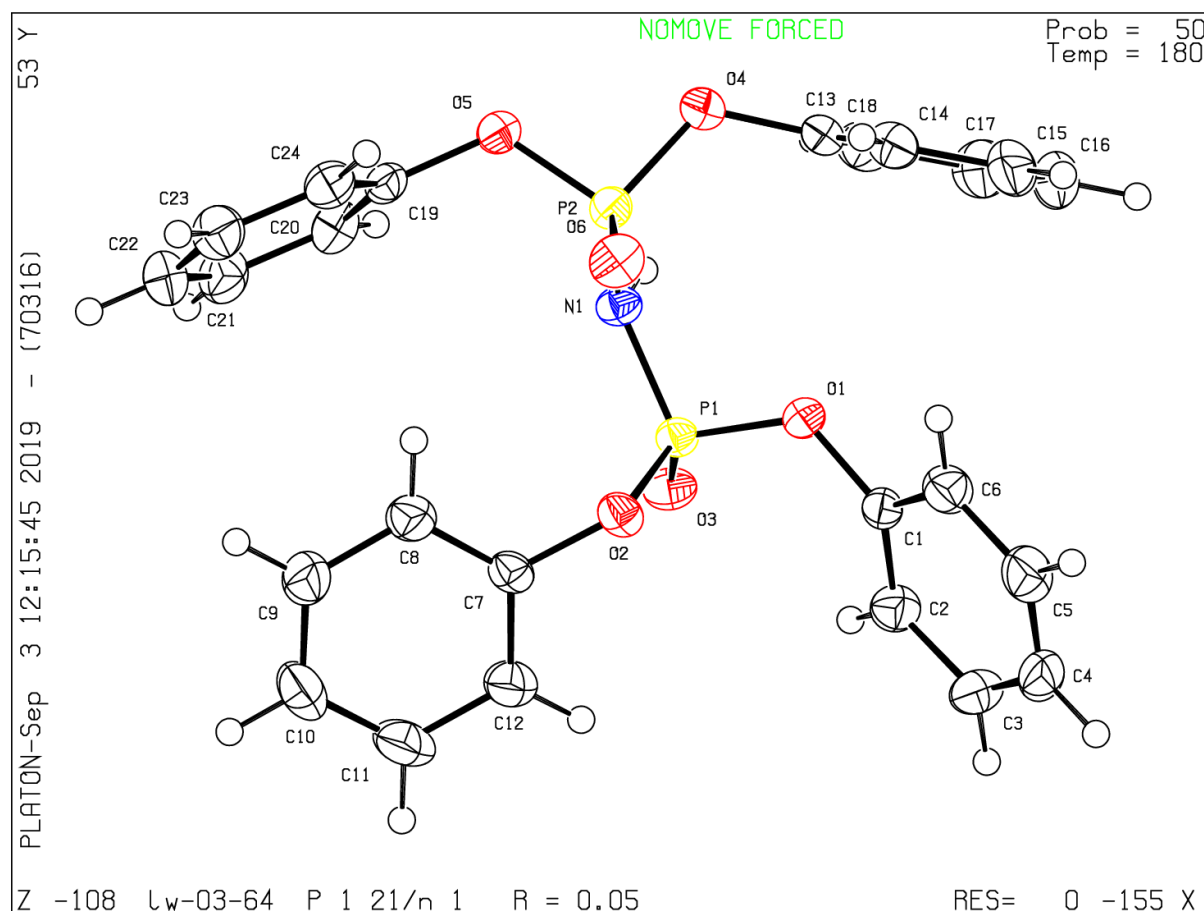
Email: manfred.doering@lbf.fraunhofer.de

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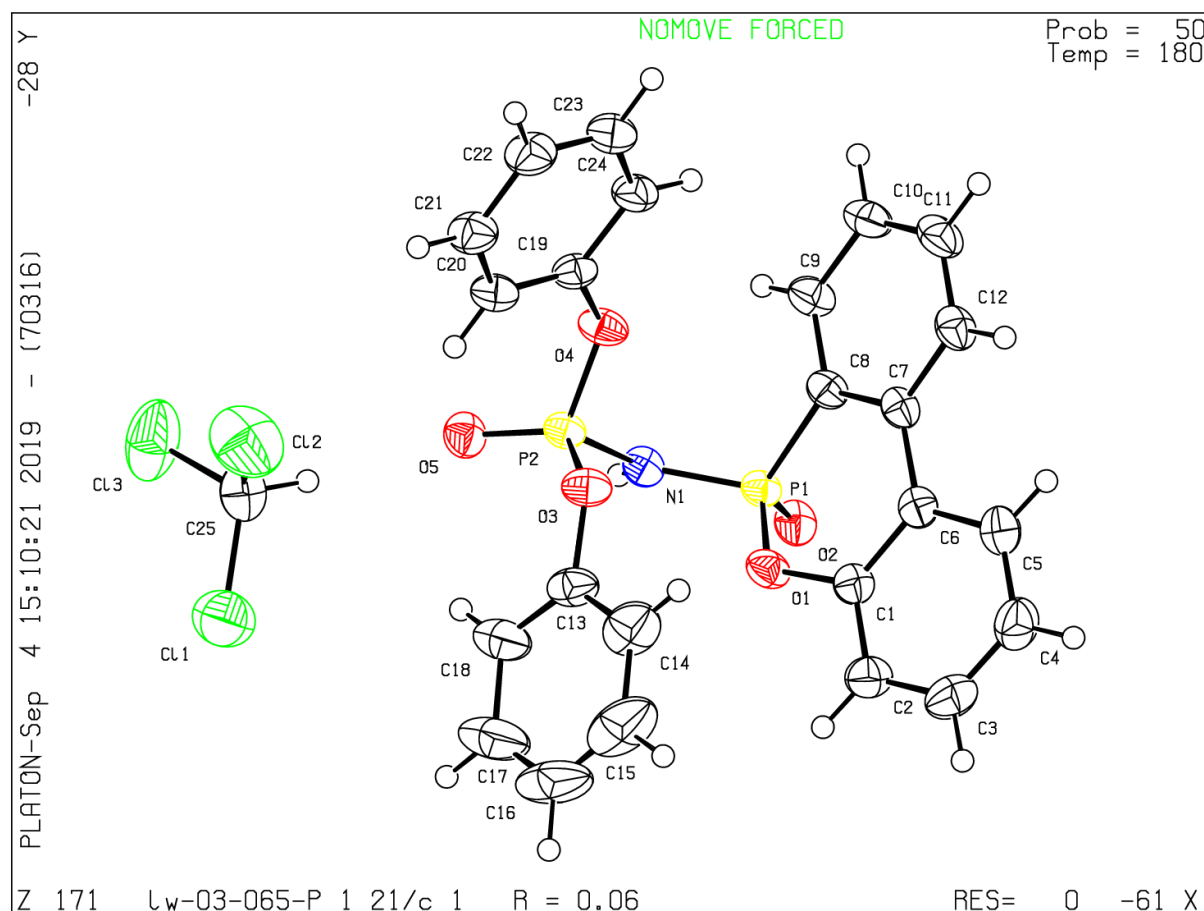
Crystallographic data of DPP-NH-DPP

Crystal Data for $C_{24}H_{21}NO_6P_2$ ($M = 481.36$ g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a = 11.8530(8)$ Å, $b = 12.2459(11)$ Å, $c = 16.1055(12)$ Å, $\beta = 96.619(6)^\circ$, $V = 2322.1(3)$ Å³, $Z = 4$, $T = 180$ K, $\mu(\text{MoK}\alpha) = 0.228$ mm⁻¹, $D_{\text{calc}} = 1.377$ g/cm³, 14338 reflections measured ($4.8^\circ \leq 2\theta \leq 59.992^\circ$), 6637 unique ($R_{\text{int}} = 0.0370$, $R_{\text{sigma}} = 0.0596$) which were used in all calculations. The final R_1 was 0.0505 ($I > 2\sigma(I)$) and wR_2 was 0.1303 (all data).



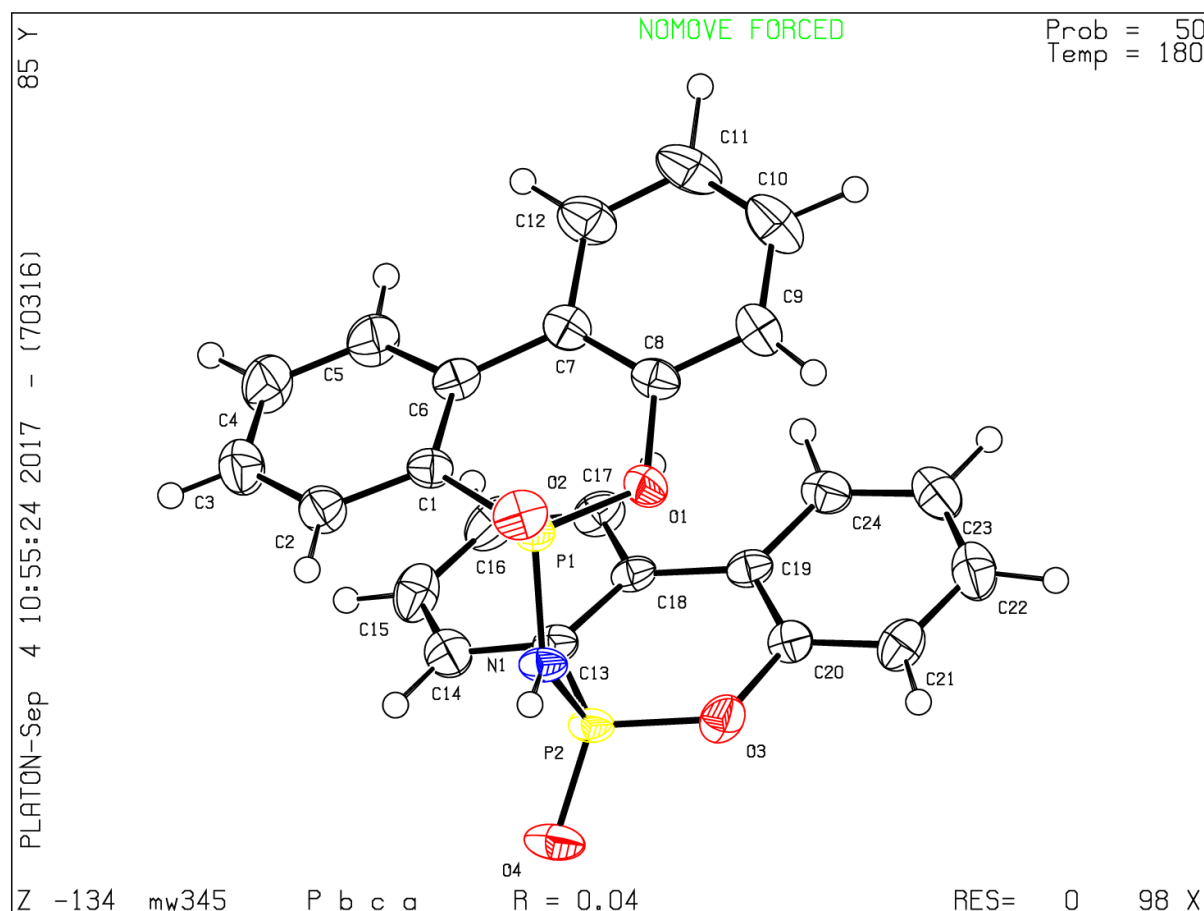
Crystallographic data of DPP-NH-DOPO

Crystal Data for $C_{25}H_{20}Cl_3NO_5P_2$ ($M = 582.71$ g/mol): monoclinic, space group $P2_1/c$ (no. 14), $a = 9.7473(4)$ Å, $b = 26.3609(15)$ Å, $c = 10.2662(4)$ Å, $\beta = 99.553(4)^\circ$, $V = 2601.3(2)$ Å³, $Z = 4$, $T = 180$ K, $\mu(\text{MoK}\alpha) = 0.513$ mm⁻¹, $D_{\text{calc}} = 1.488$ g/cm³, 18699 reflections measured ($4.31^\circ \leq 2\theta \leq 60^\circ$), 7471 unique ($R_{\text{int}} = 0.0477$, $R_{\text{sigma}} = 0.0519$) which were used in all calculations. The final R_1 was 0.0630 ($I > 2\sigma(I)$) and wR_2 was 0.1874 (all data).



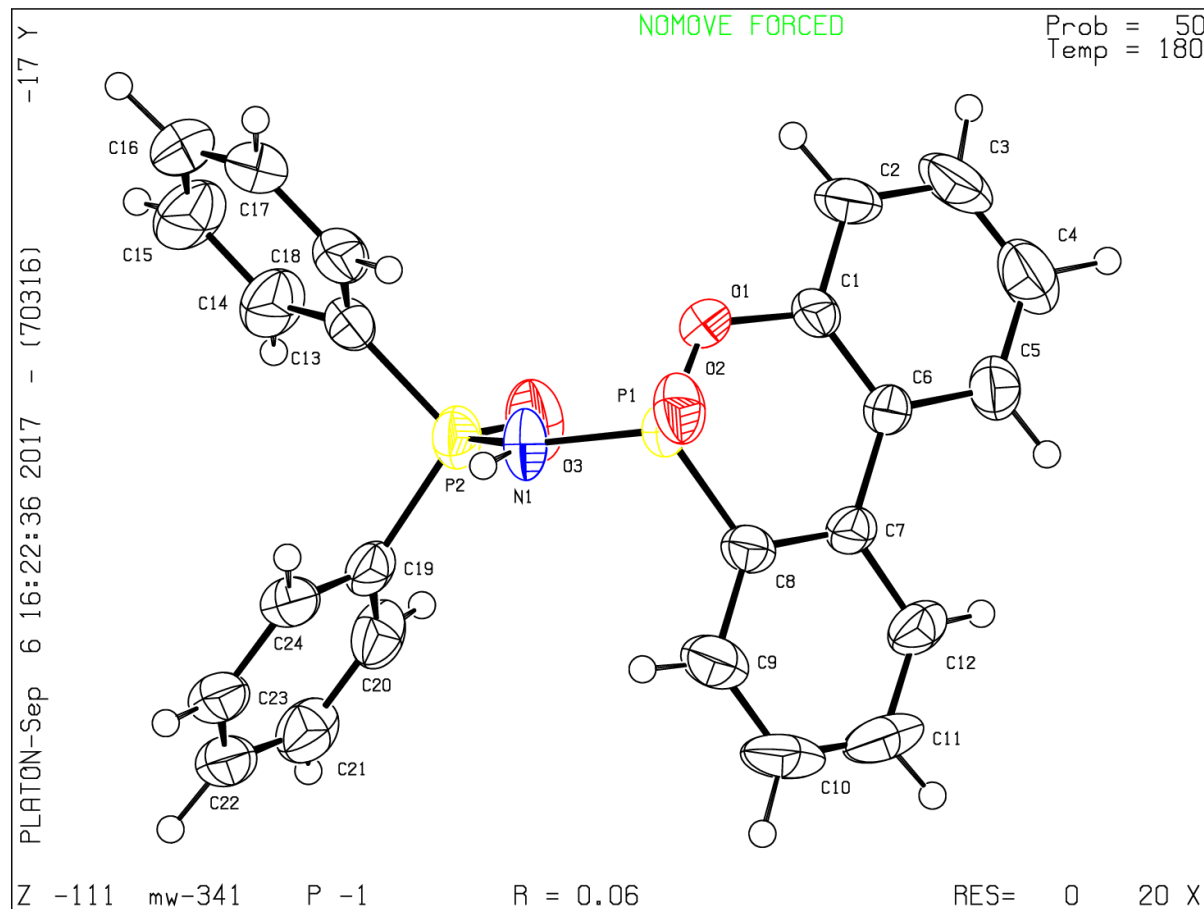
Crystallographic data of DOPO-NH-DOPO

Crystal Data for $C_{24}H_{17}NO_4P_2$ ($M = 445.32$ g/mol): orthorhombic, space group $Pbca$ (no. 61), $a = 15.5440(5)$ Å, $b = 13.7055(4)$ Å, $c = 18.7987(7)$ Å, $V = 4004.8(2)$ Å³, $Z = 8$, $T = 180.15$ K, $\mu(\text{MoK}\alpha) = 0.251$ mm⁻¹, $D_{\text{calc}} = 1.477$ g/cm³, 35005 reflections measured ($4.334^\circ \leq 2\theta \leq 53.622^\circ$), 4248 unique ($R_{\text{int}} = 0.0535$, $R_{\text{sigma}} = 0.0318$) which were used in all calculations. The final R_1 was 0.0398 ($I > 2\sigma(I)$) and wR_2 was 0.1035 (all data).



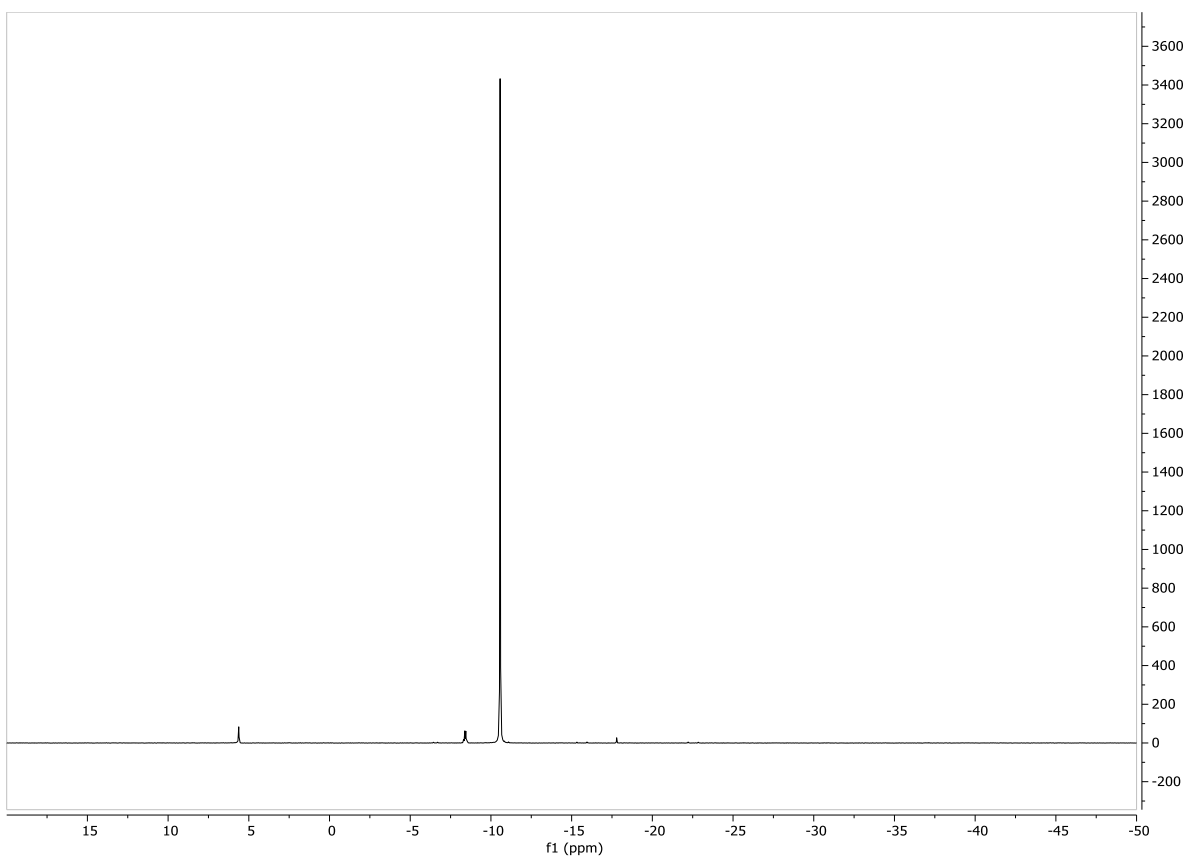
Crystallographic data of DOPO-NH-DPhPO

Crystal Data for $C_{24}H_{19}NO_3P_2$ ($M=431.34$ g/mol): triclinic, space group P-1 (no. 2), $a = 8.6769(8)$ Å, $b = 10.2292(7)$ Å, $c = 11.9908(12)$ Å, $\alpha = 80.721(7)^\circ$, $\beta = 83.260(8)^\circ$, $\gamma = 77.540(6)^\circ$, $V = 1021.84(16)$ Å³, $Z = 2$, $T = 180.15$ K, $\mu(\text{MoK}\alpha) = 0.240$ mm⁻¹, $D_{\text{calc}} = 1.402$ g/cm³, 8486 reflections measured ($4.826^\circ \leq 2\theta \leq 53.724^\circ$), 4256 unique ($R_{\text{int}} = 0.0598$, $R_{\text{sigma}} = 0.0659$) which were used in all calculations. The final R_1 was 0.0613 ($I > 2\sigma(I)$) and wR_2 was 0.1742 (all data).

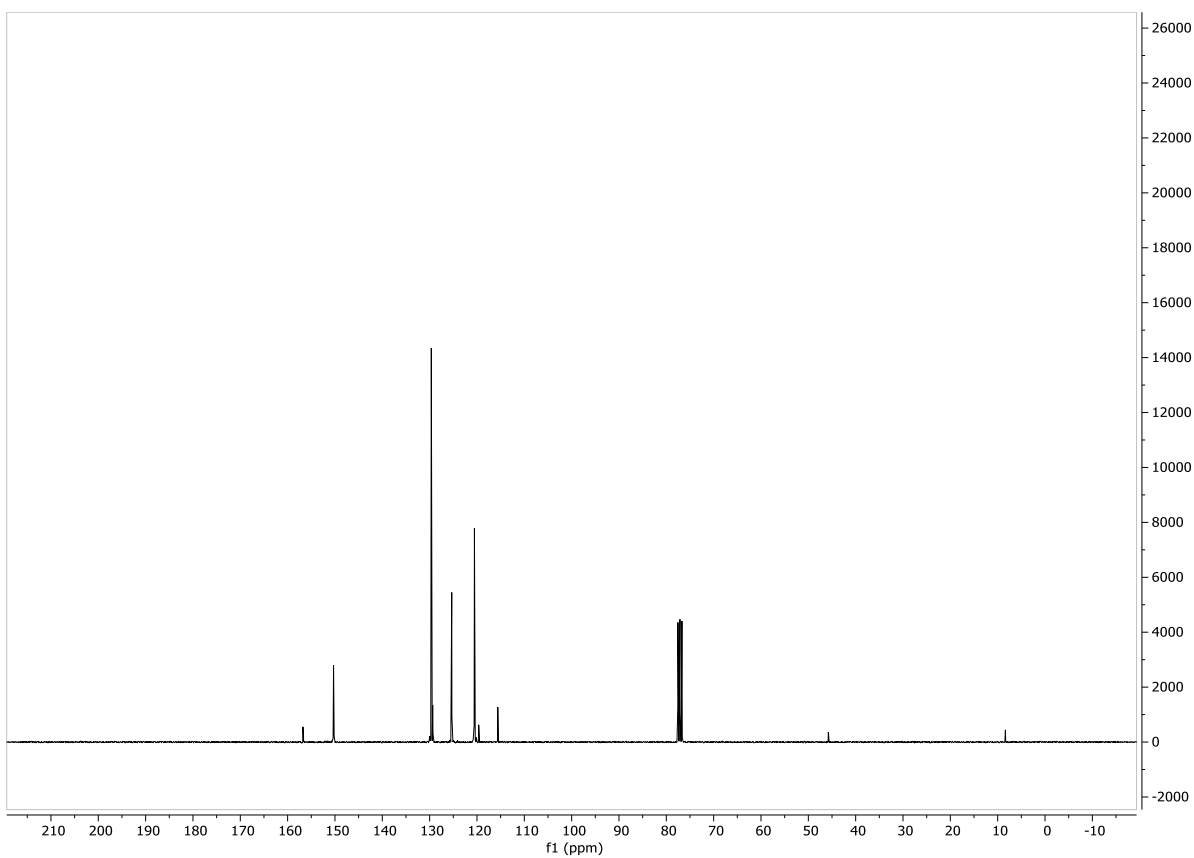


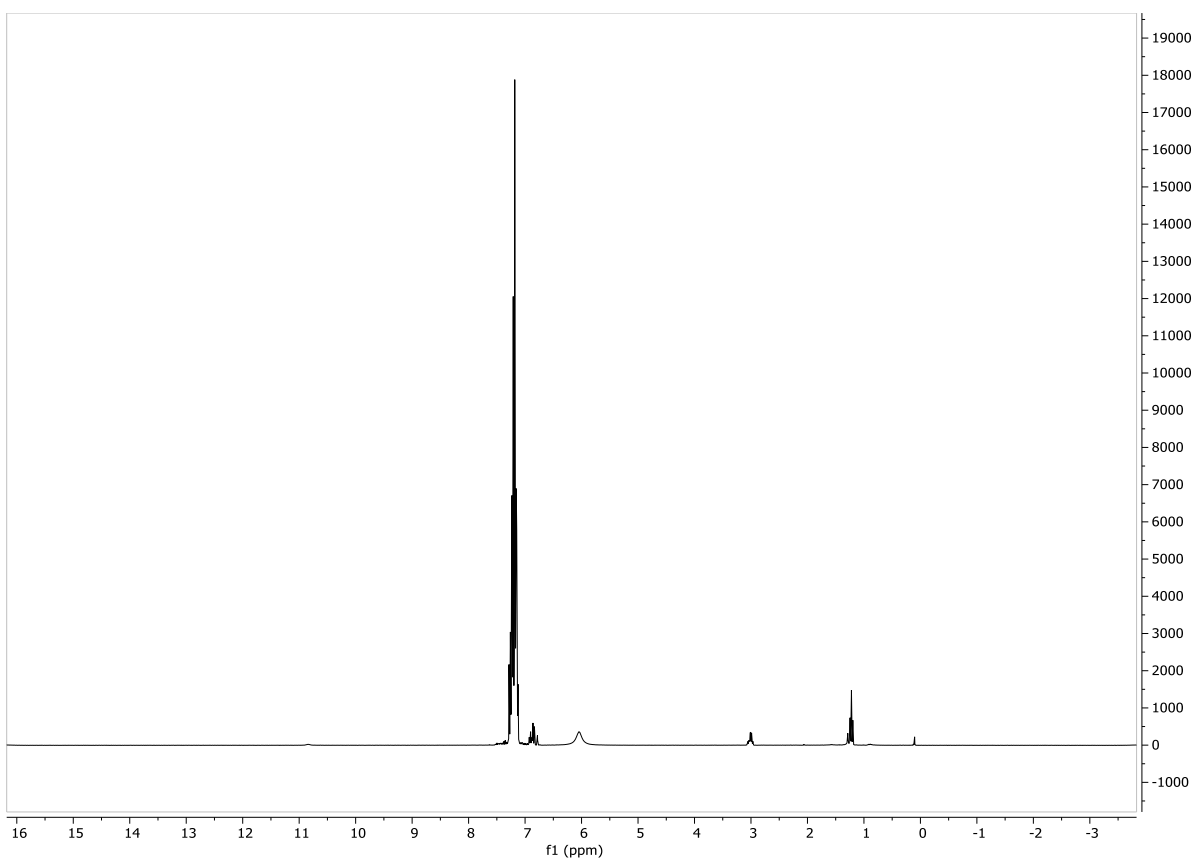
Nuclear magnetic resonance spectra of DPP-NH-DPP

³¹P-NMR



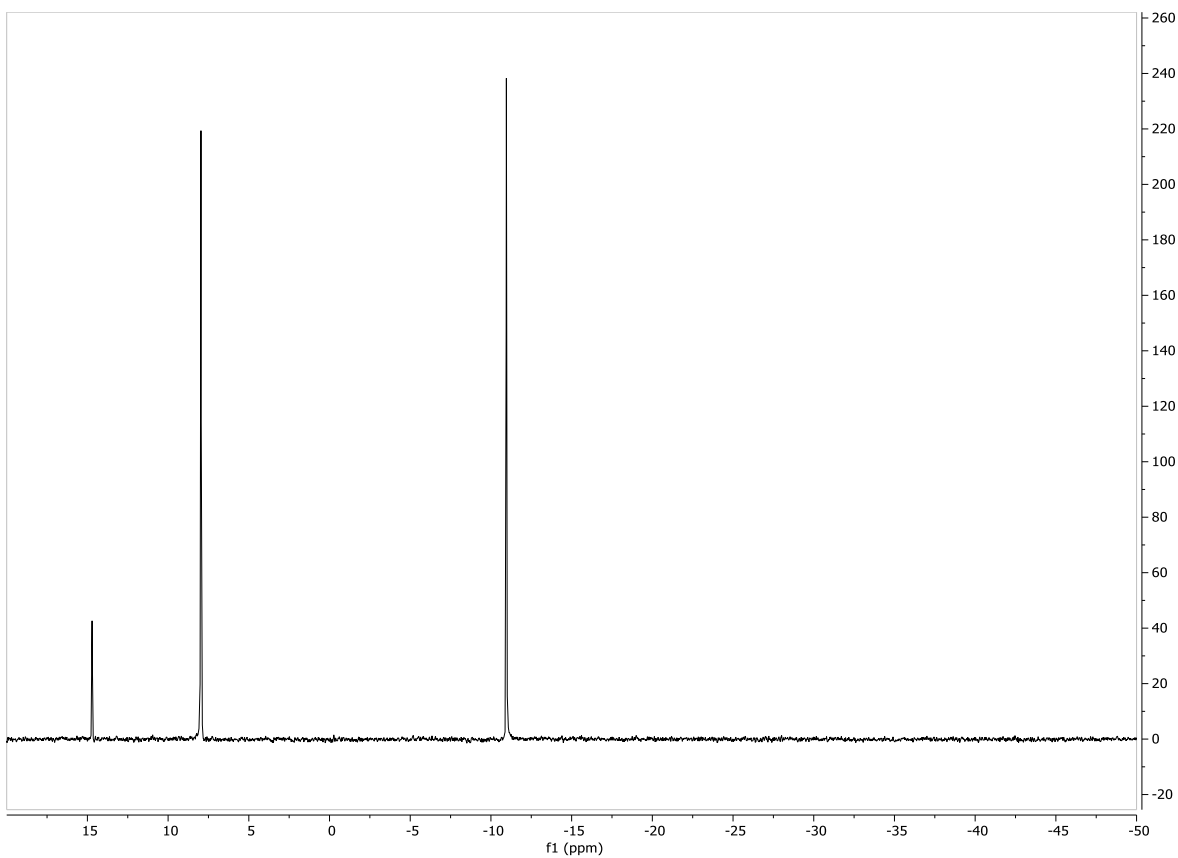
¹³C-NMR



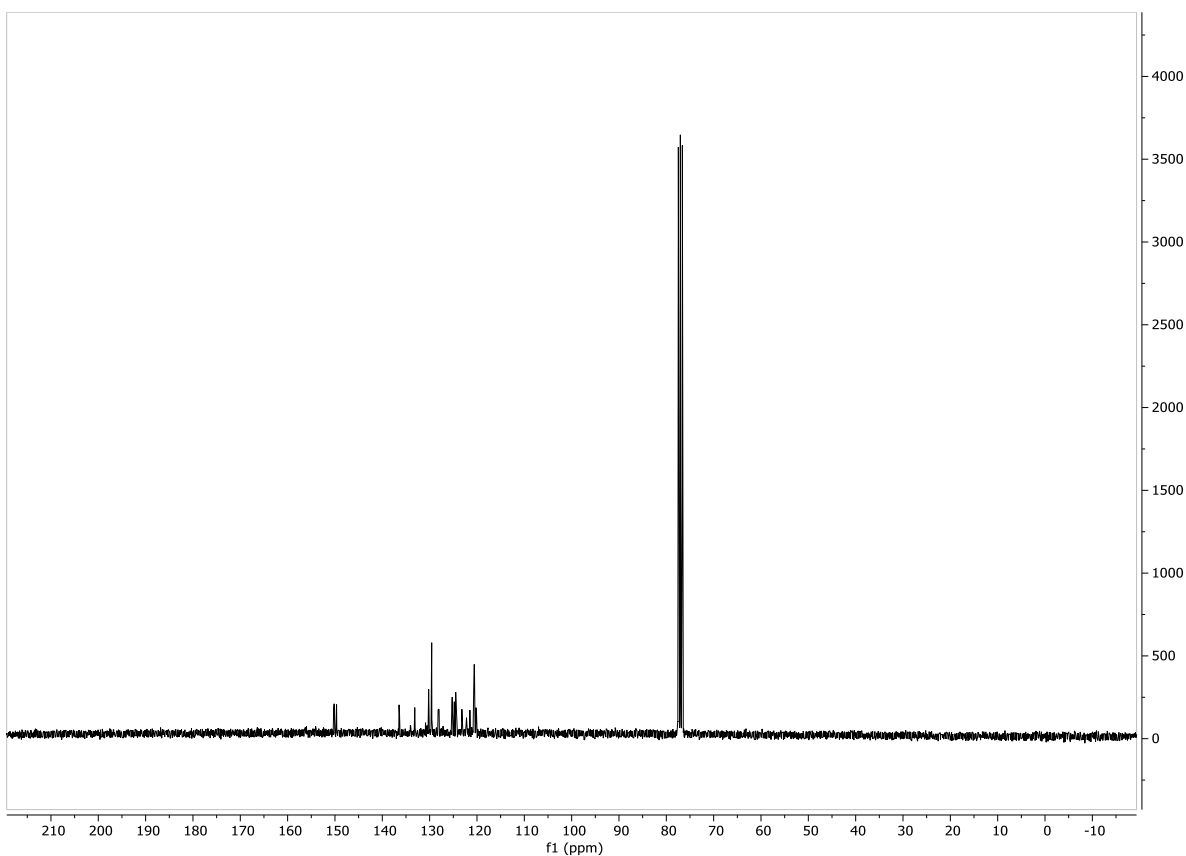
^1H -NMR

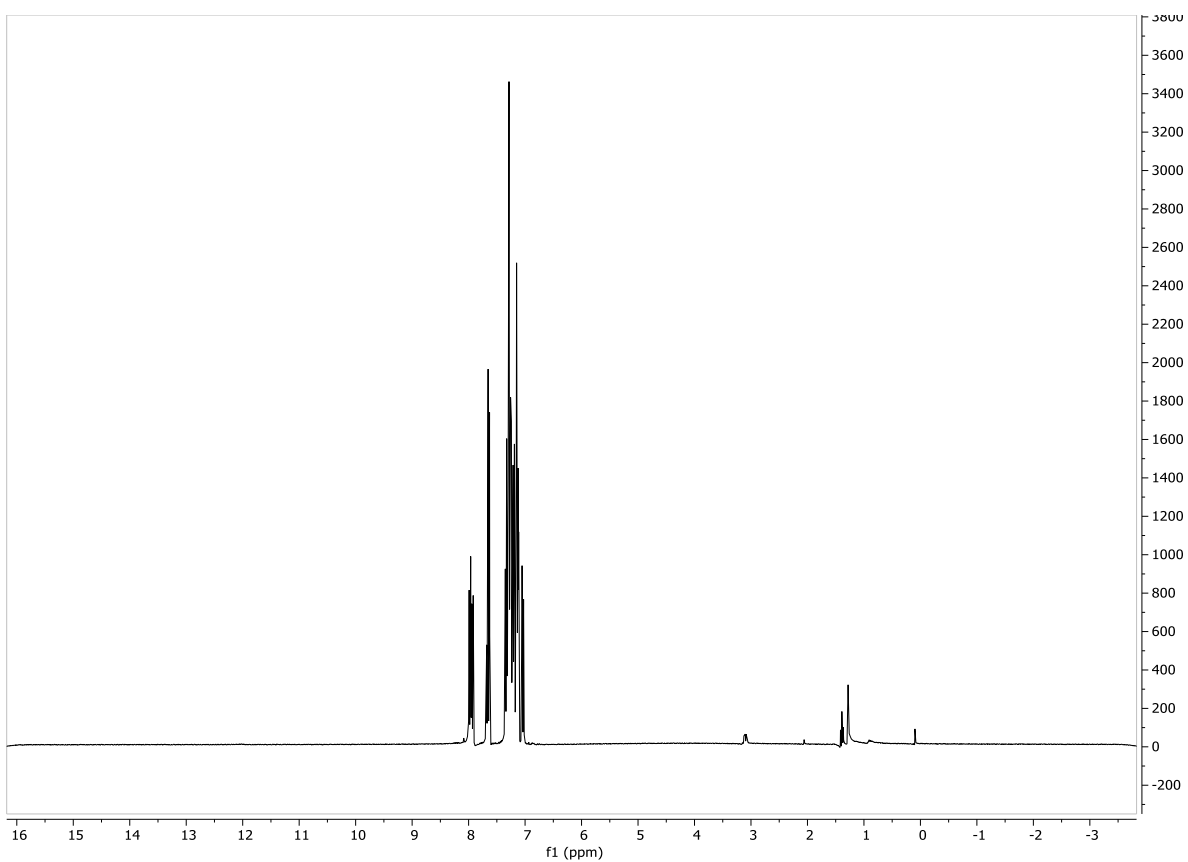
Nuclear magnetic resonance spectra of DPP-NH-DOPO

³¹P-NMR



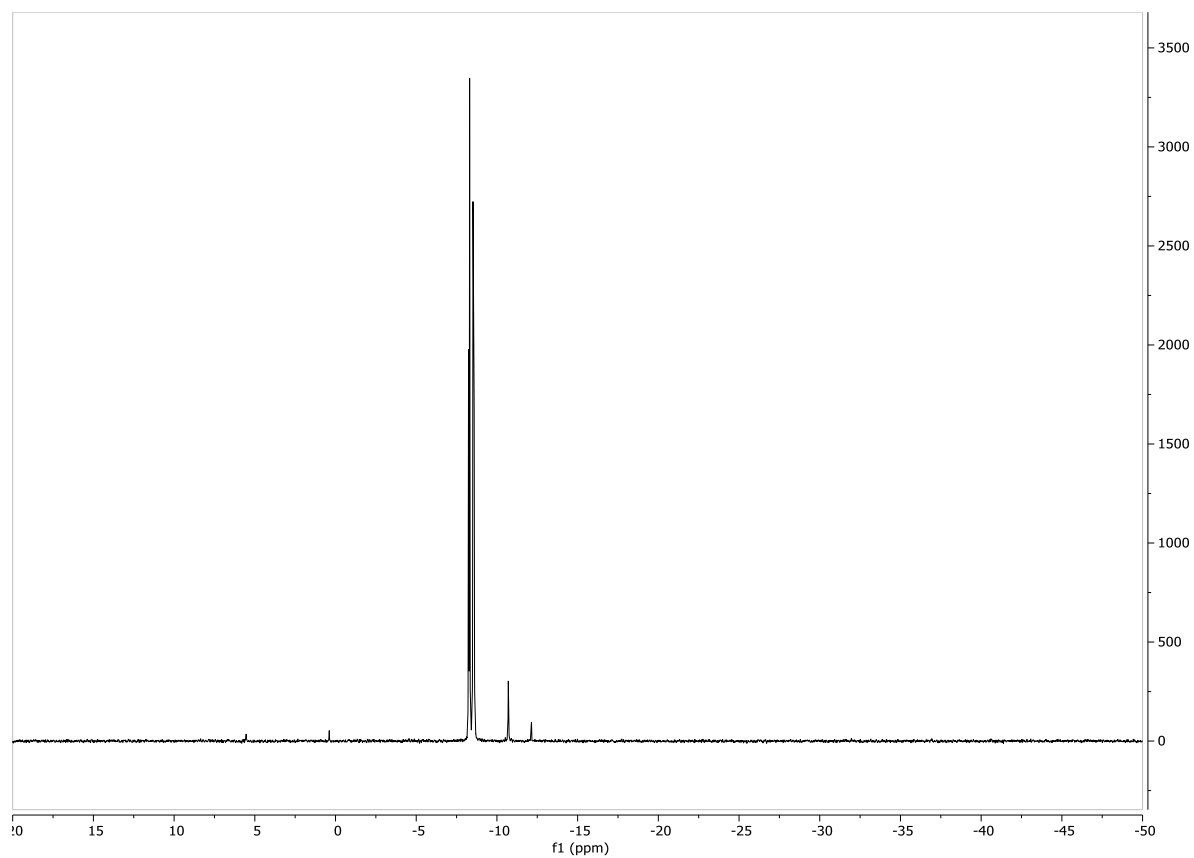
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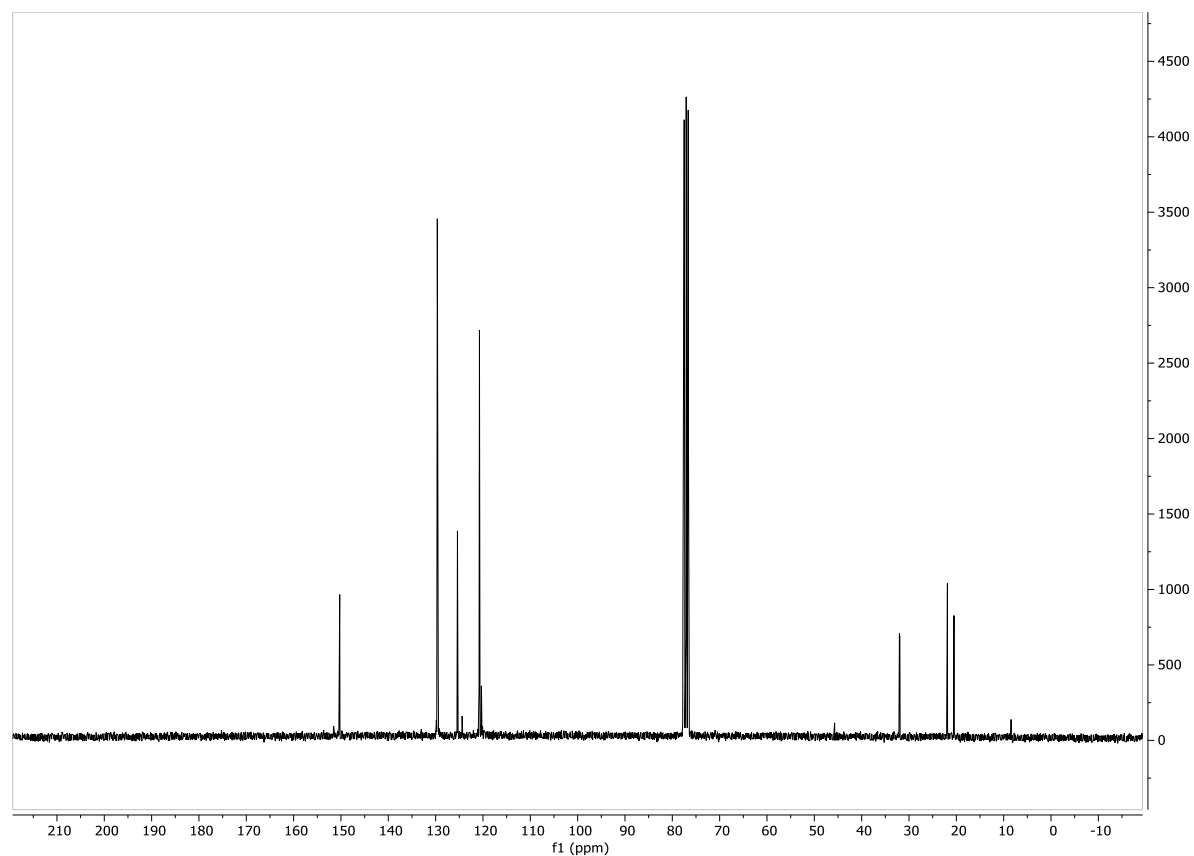
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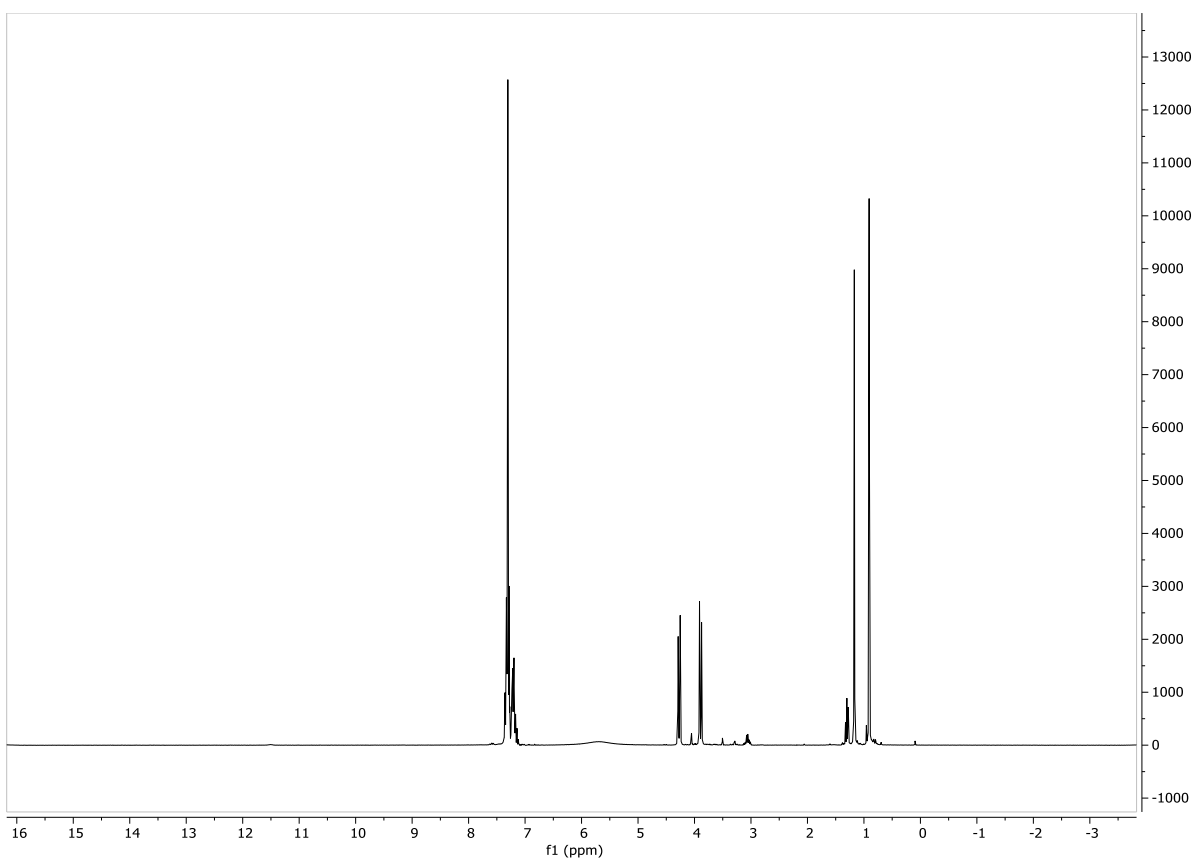
Nuclear magnetic resonance spectra of DPP-NH-DDPO

³¹P-NMR



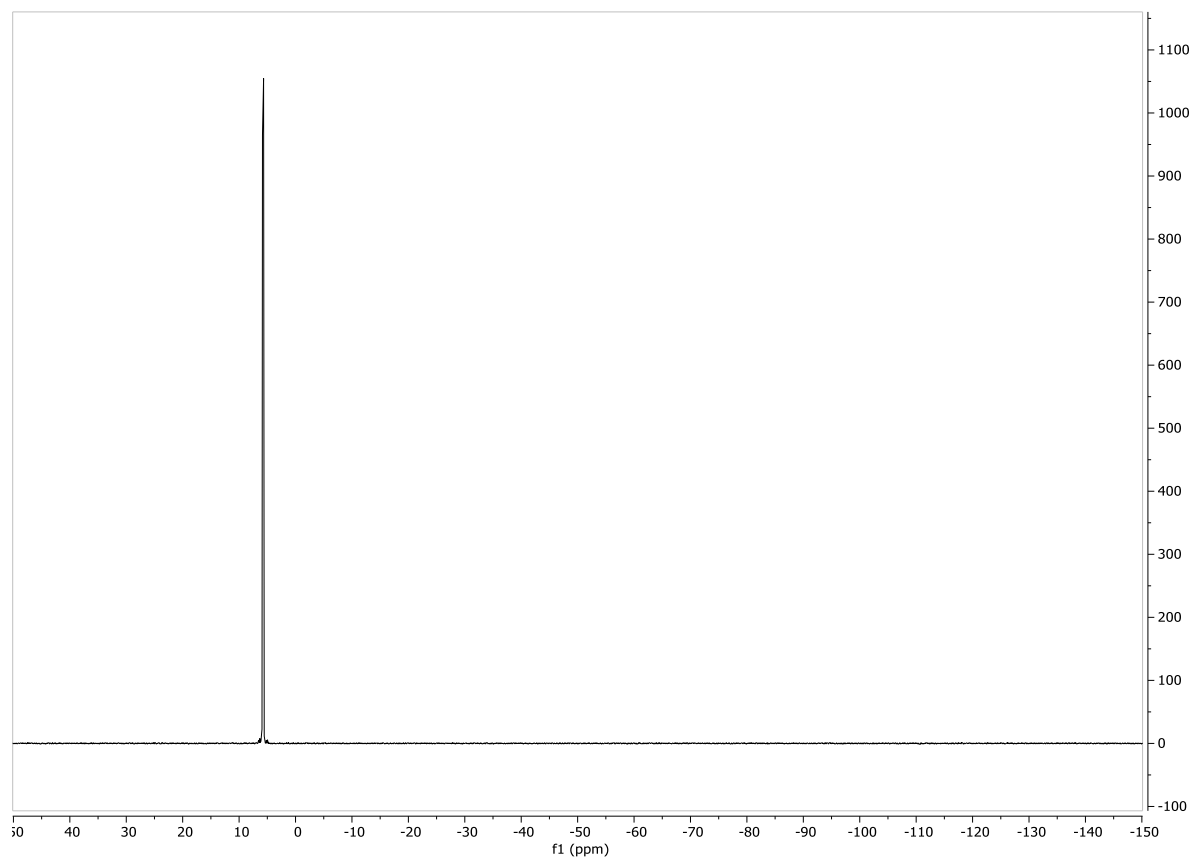
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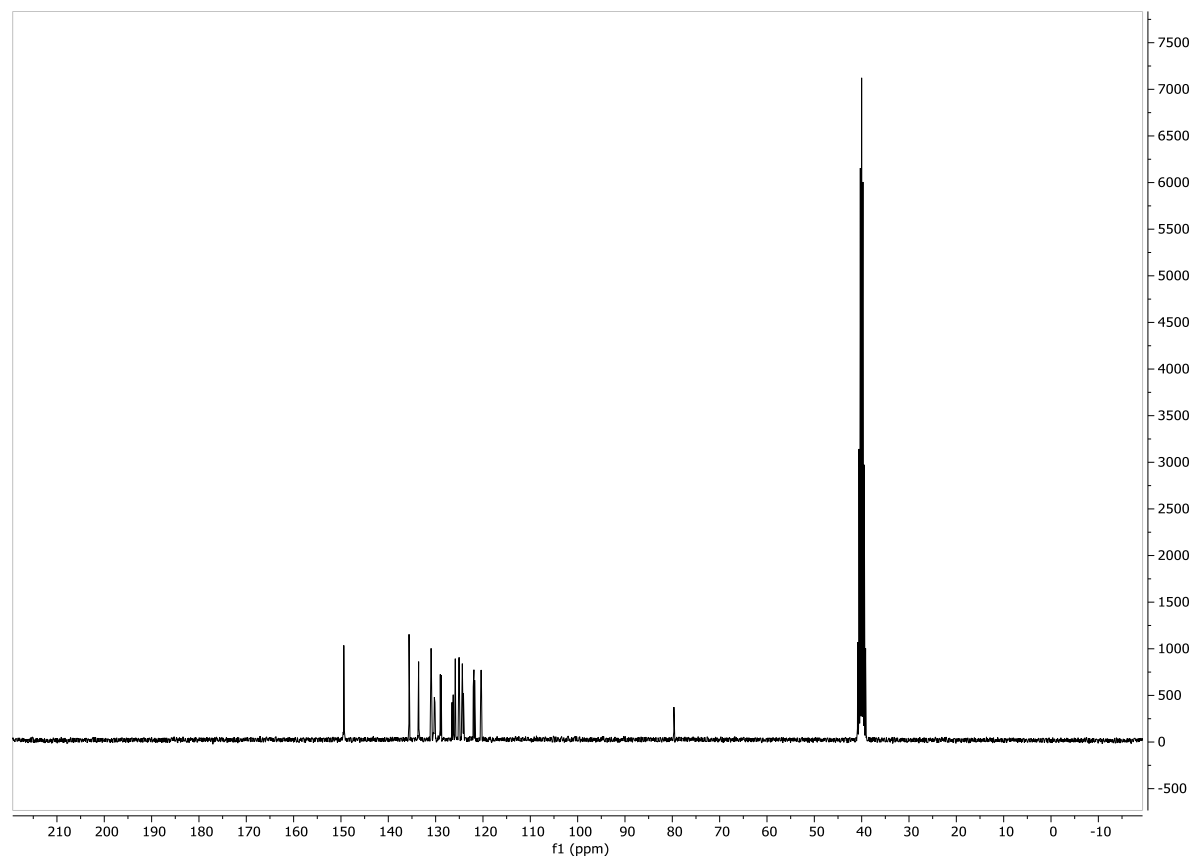
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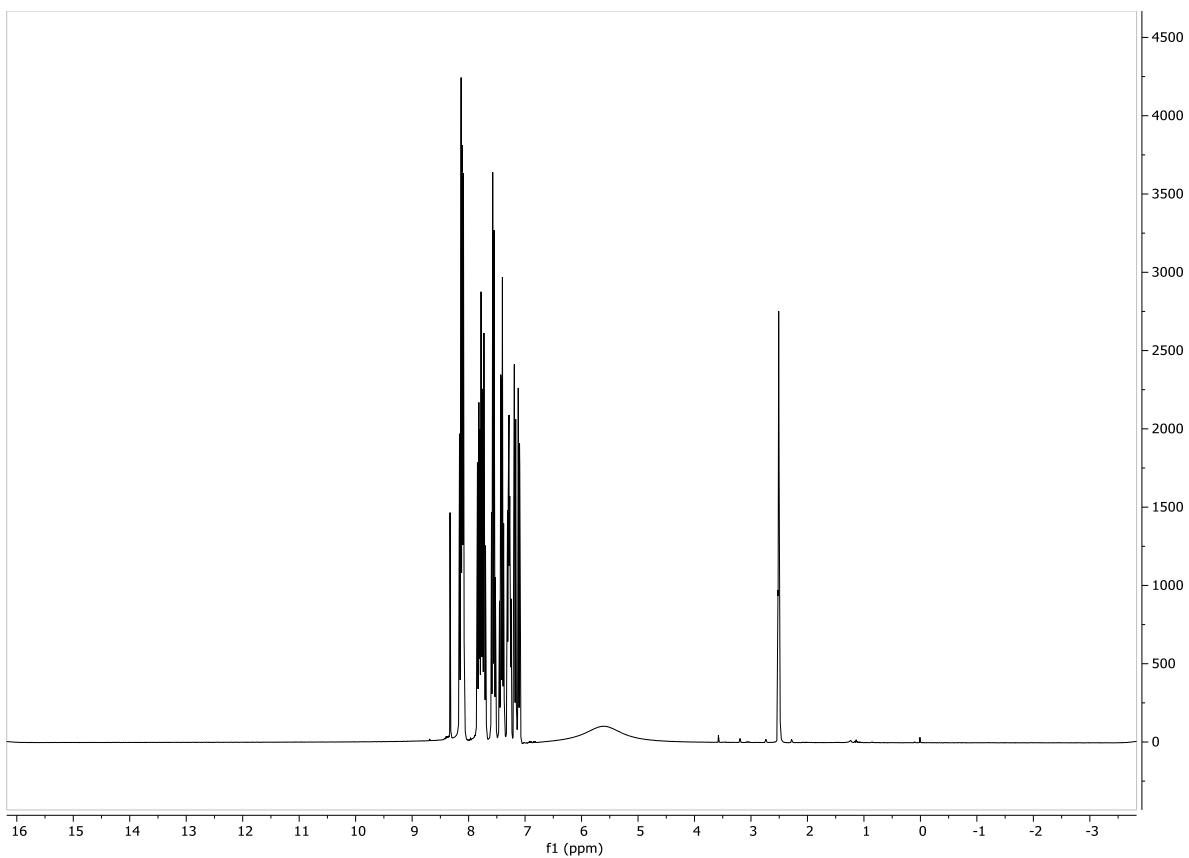
Nuclear magnetic resonance spectra of DOPO-NH-DOPO

³¹P-NMR



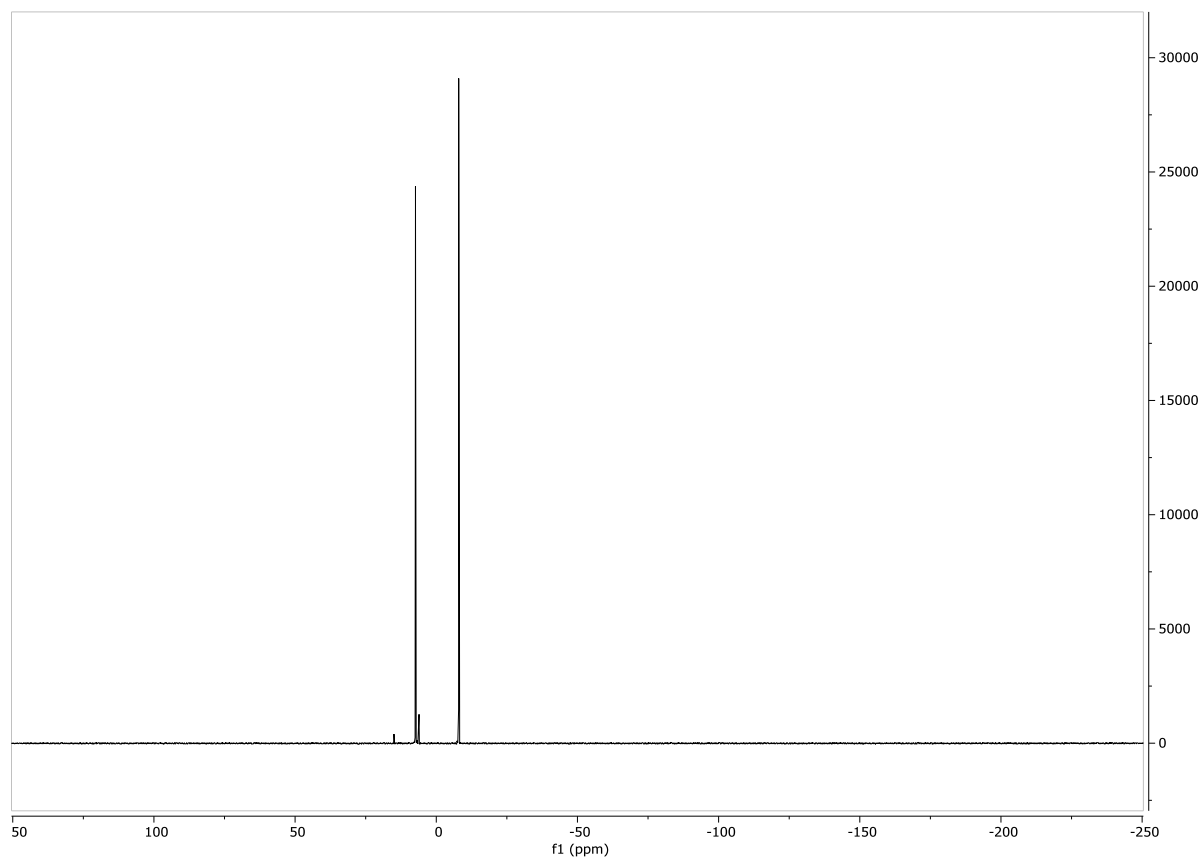
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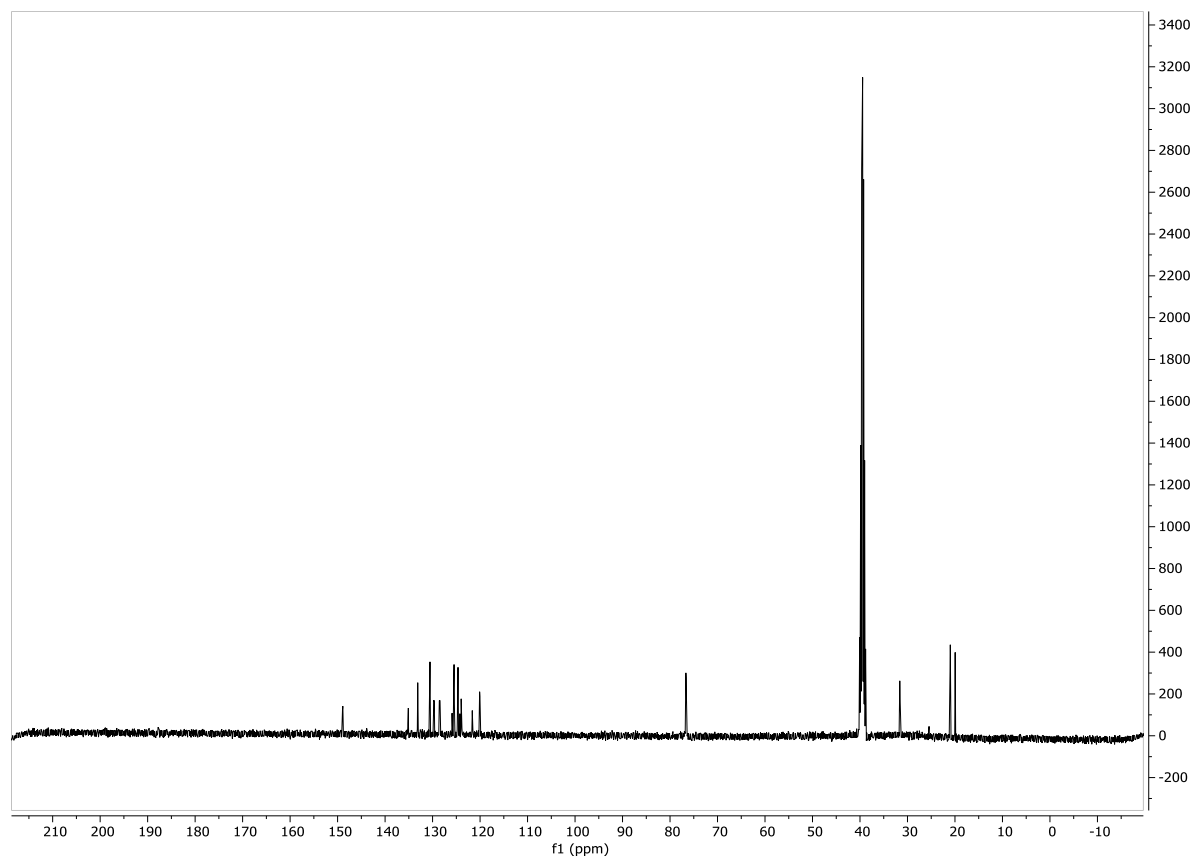
^1H -NMR

Nuclear magnetic resonance spectra of DOPO-NH-DDPO

³¹P-NMR



¹³C-NMR



^1H -NMR