Supplementary Material

Novel N-phosphorylated iminophosphoranes based on 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide

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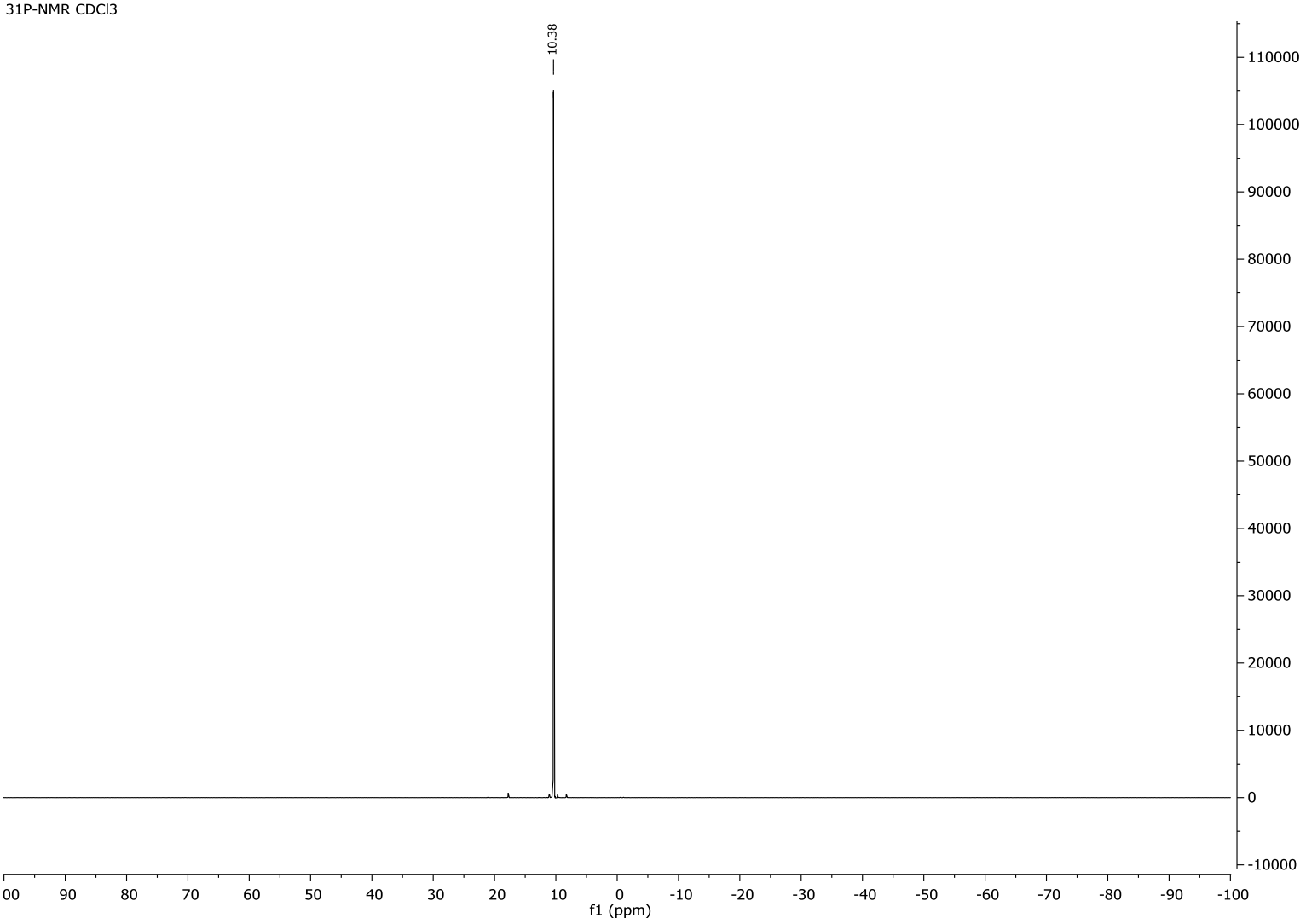
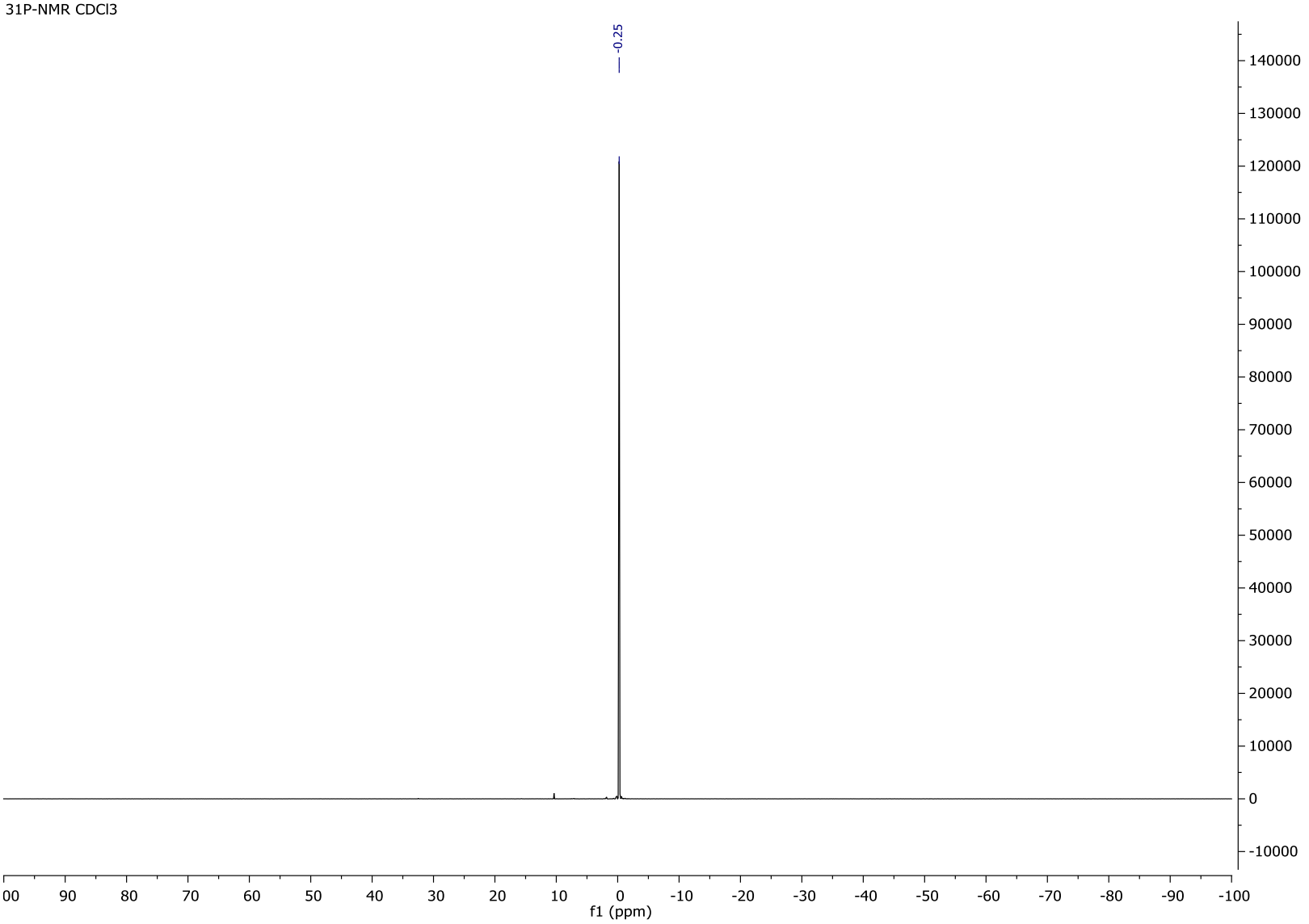
1. ^{31}P-NMR spectra

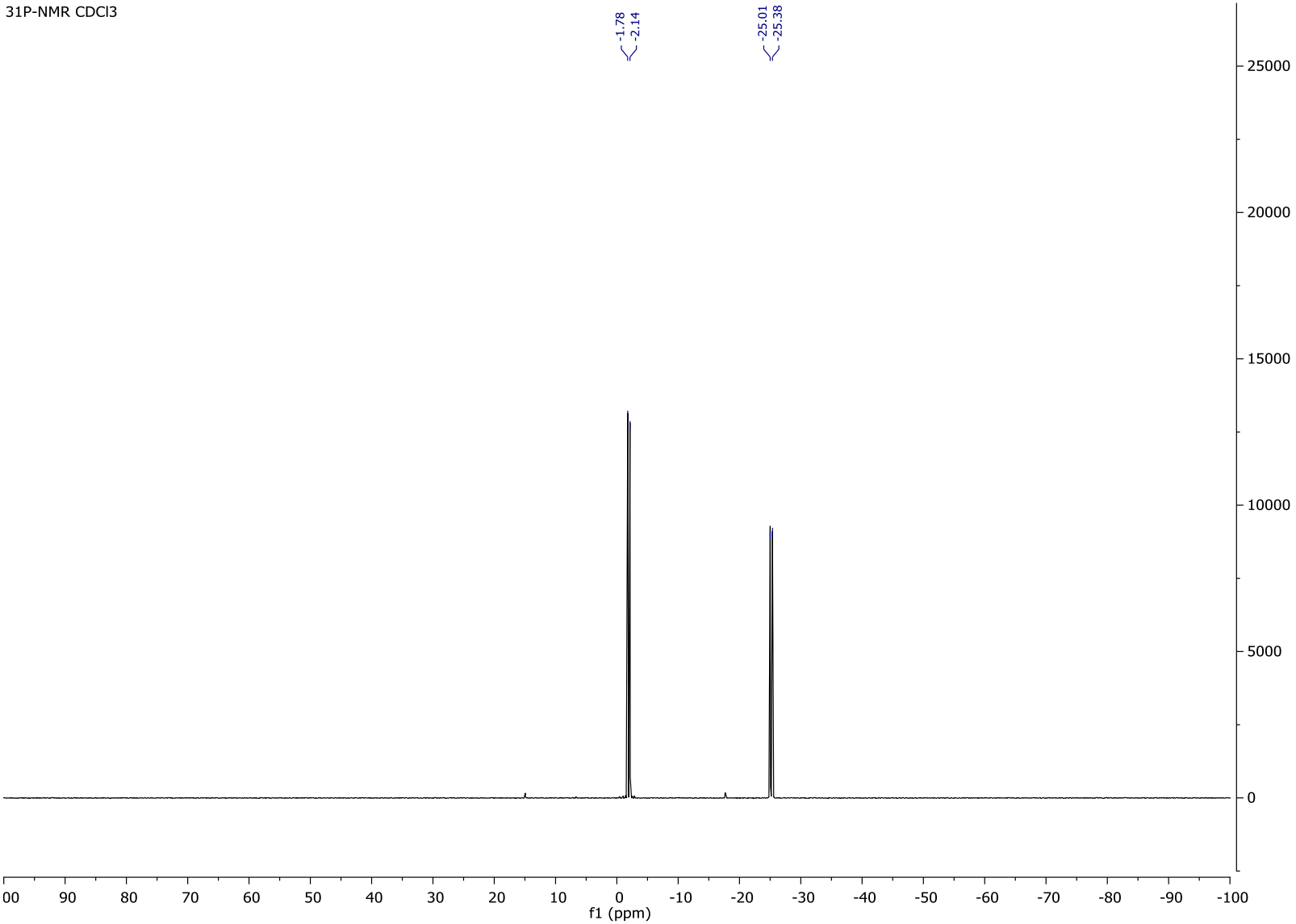
6-Azidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-oxid (DOPO-N_3)



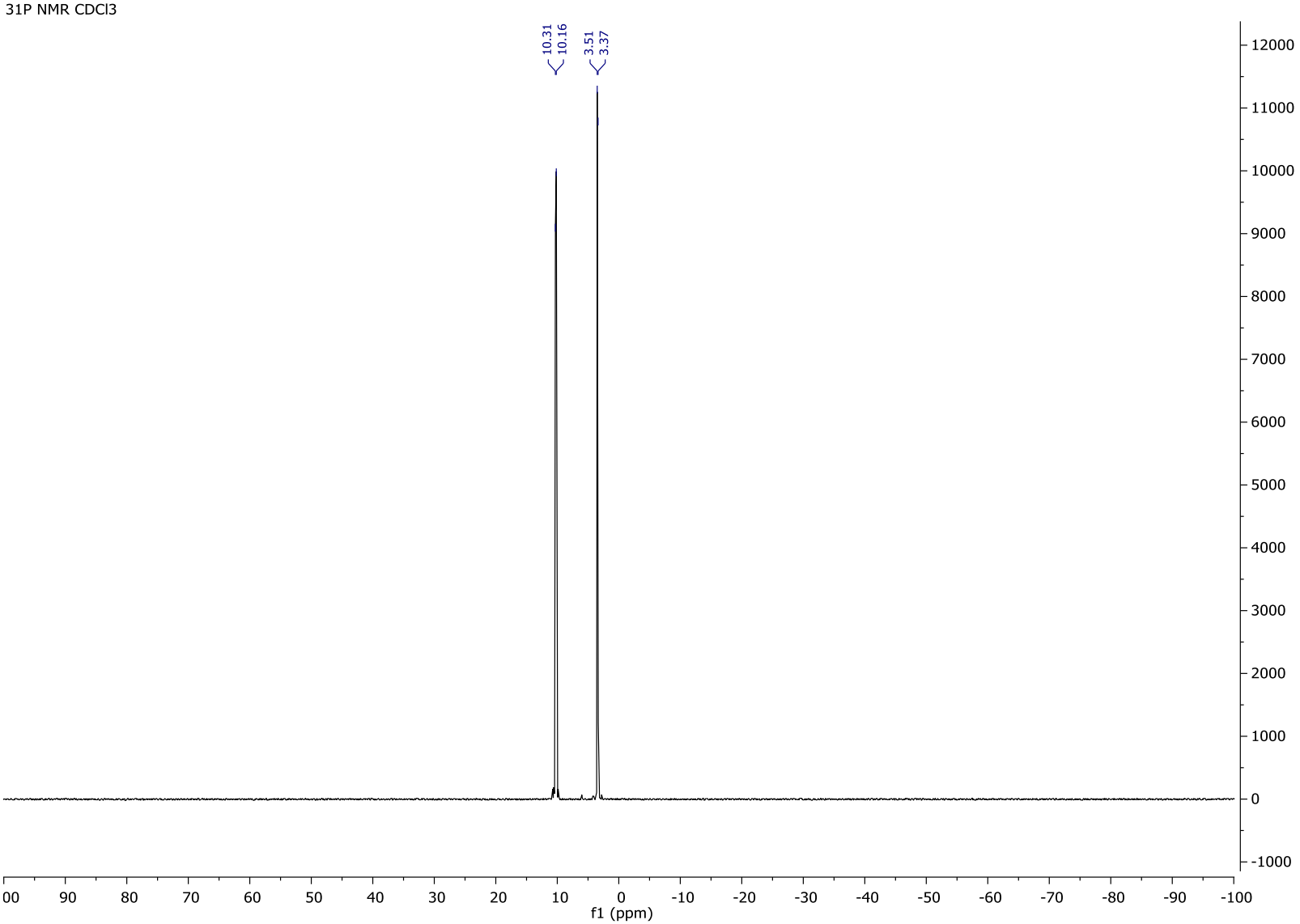
Trimethyl (6-oxidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-yl)phosphorimidate (DOPO-N=P(OMe)$_3$)



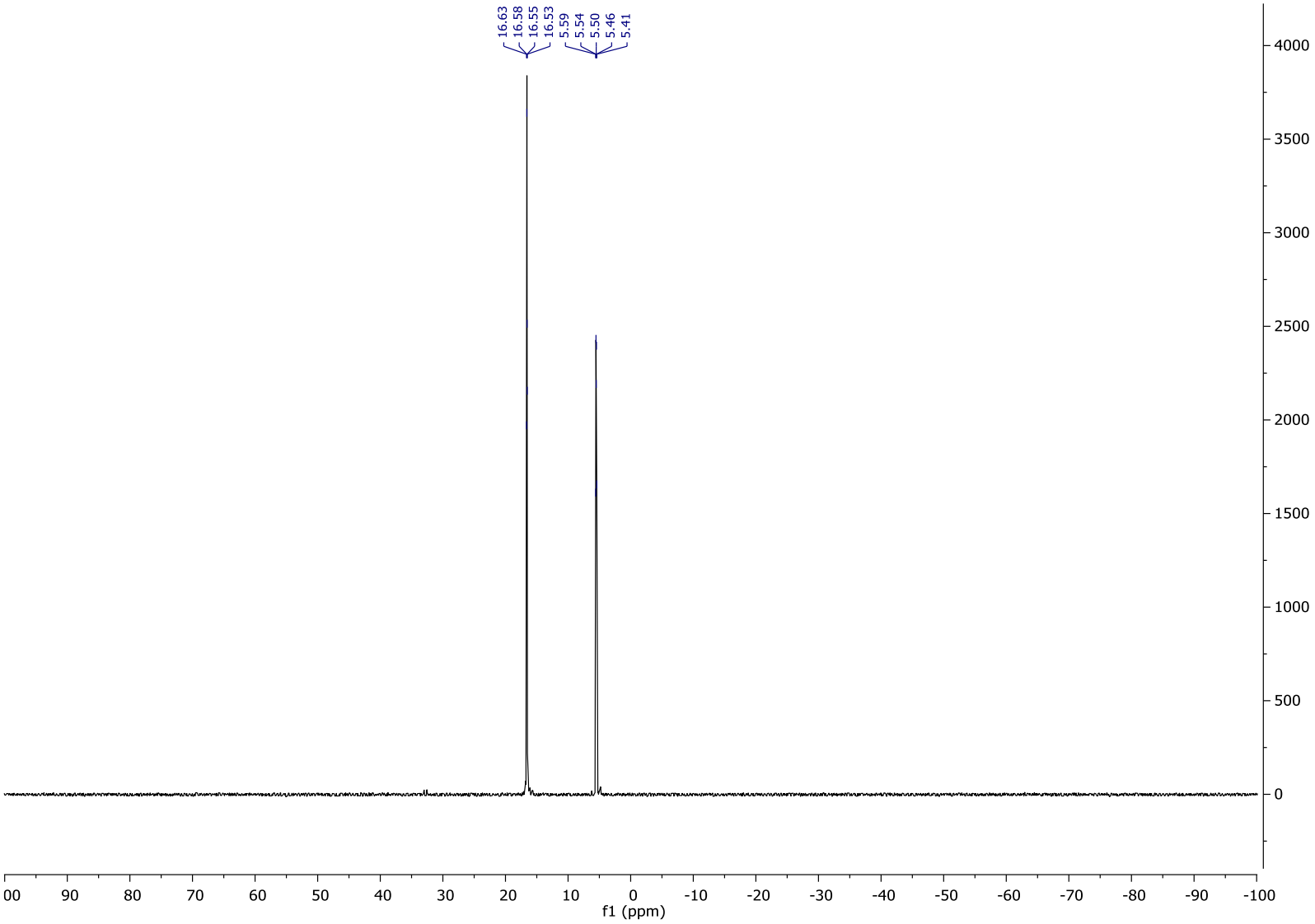
Triphenyl (6-oxidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-yl)phosphorimidate (DOPO-N=P(OPh)$_3$)



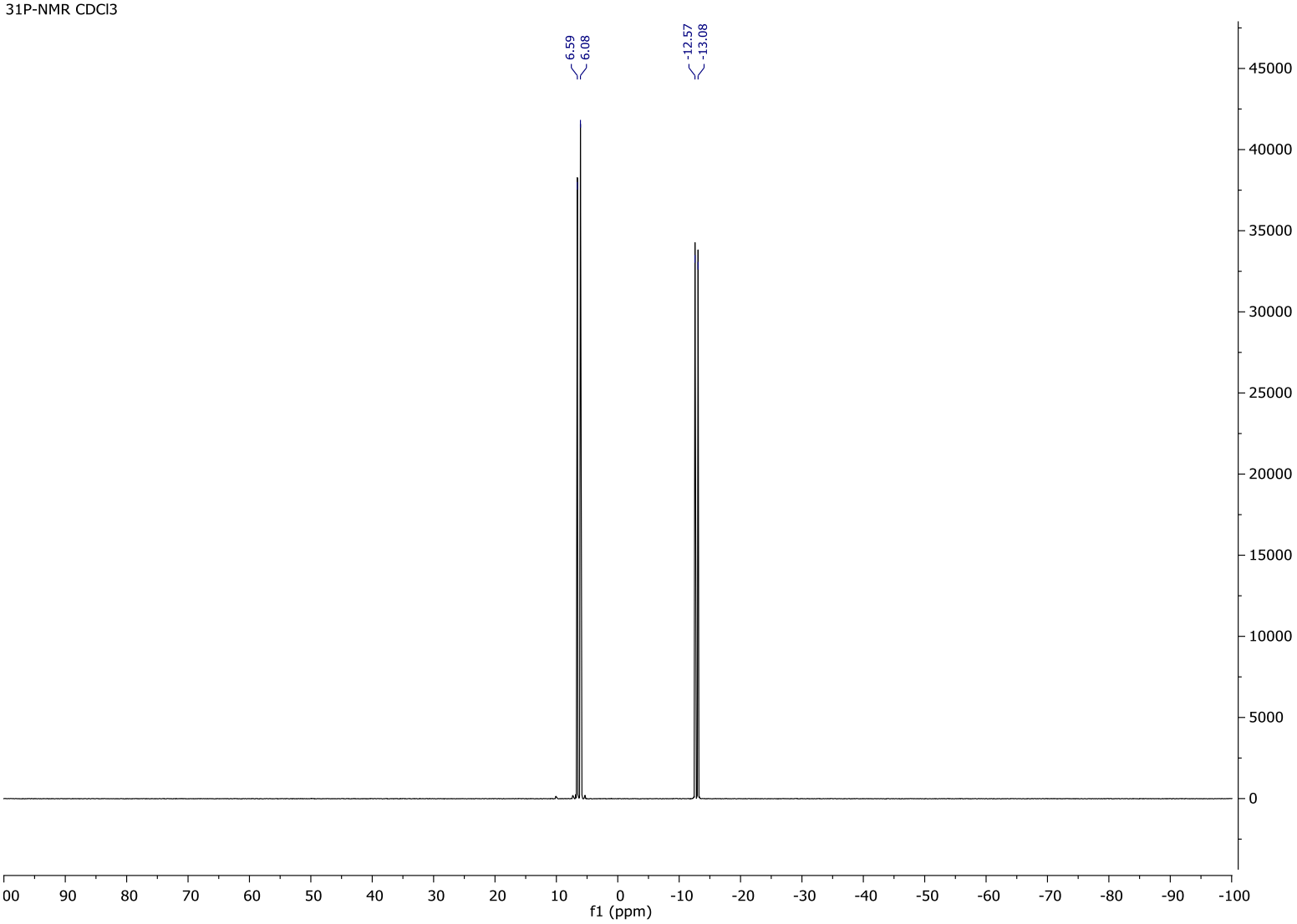
6-((Triphenyl-λ^5-phosphanylidene)amino)dibenzo[*c*,*e*][1,2]oxaphosphinine 6-oxide (DOPO-N=P(Ph)$_3$)



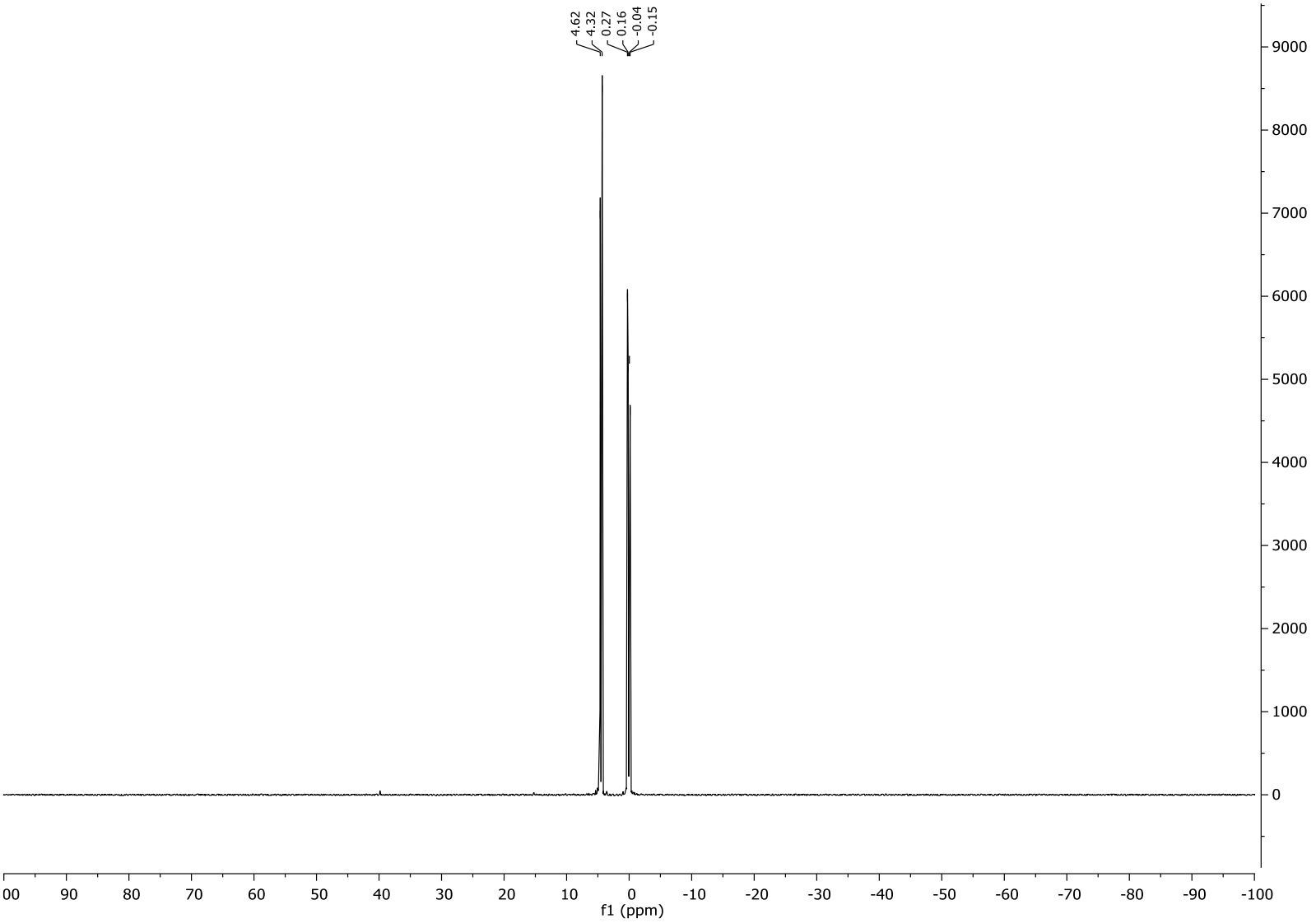
6,6'-((Ethane-1,2-diylbis(diphenyl-λ^5-phosphanylylidene))bis(azanylylidene))bis(dibenzo[*c,e*][1,2]oxaphosphinine 6-oxide) ([DOPO-N=P(Ph)$_2$CH$_2$]$_2$)



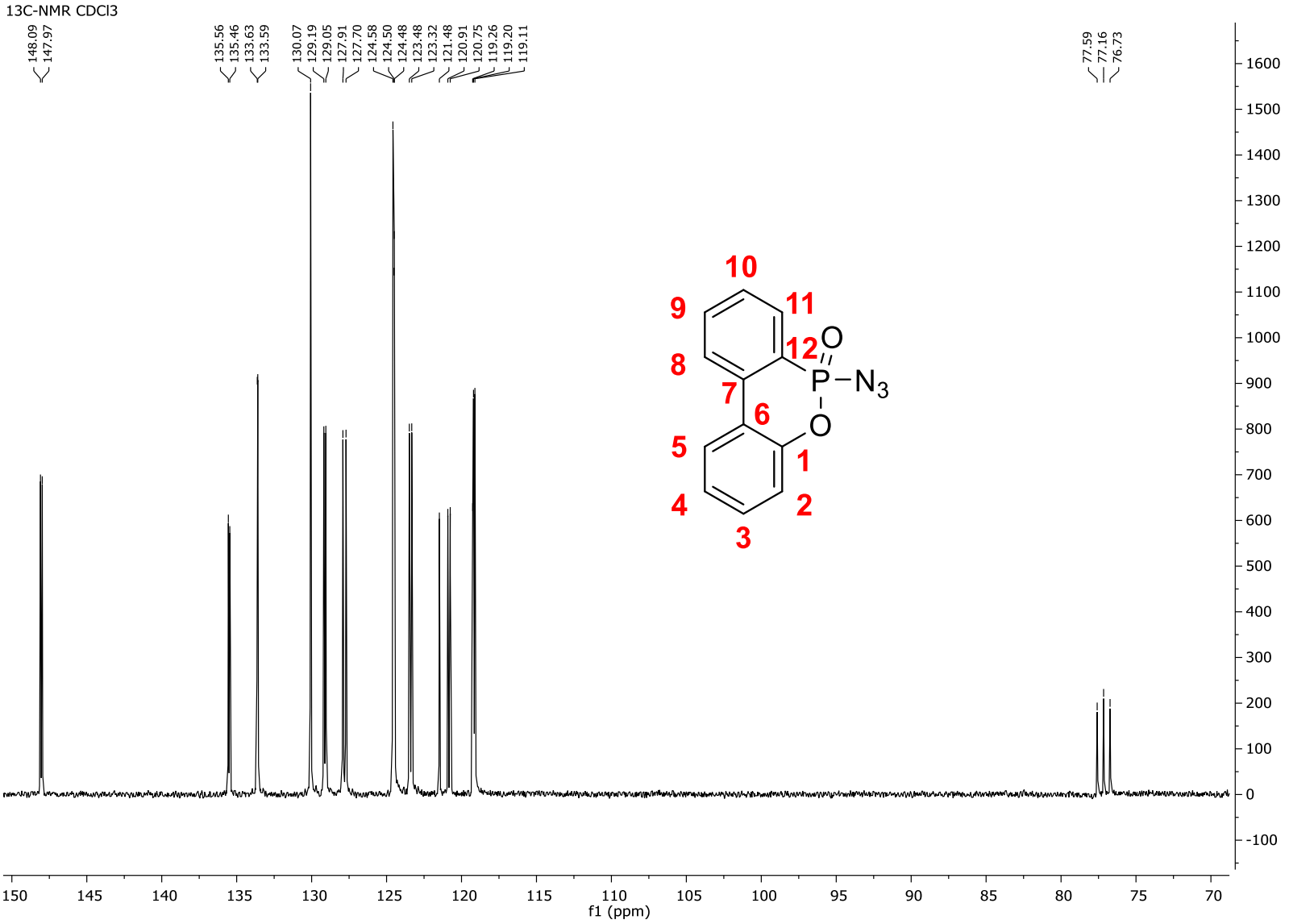
Diphenyl (6-ethoxy-6*H*-6λ^5-dibenzo[*c*,*e*][1,2]oxaphosphinin-6-ylidene)phosphoramidate ((PhO)$_2$(O)P-N=DOP-OEt)



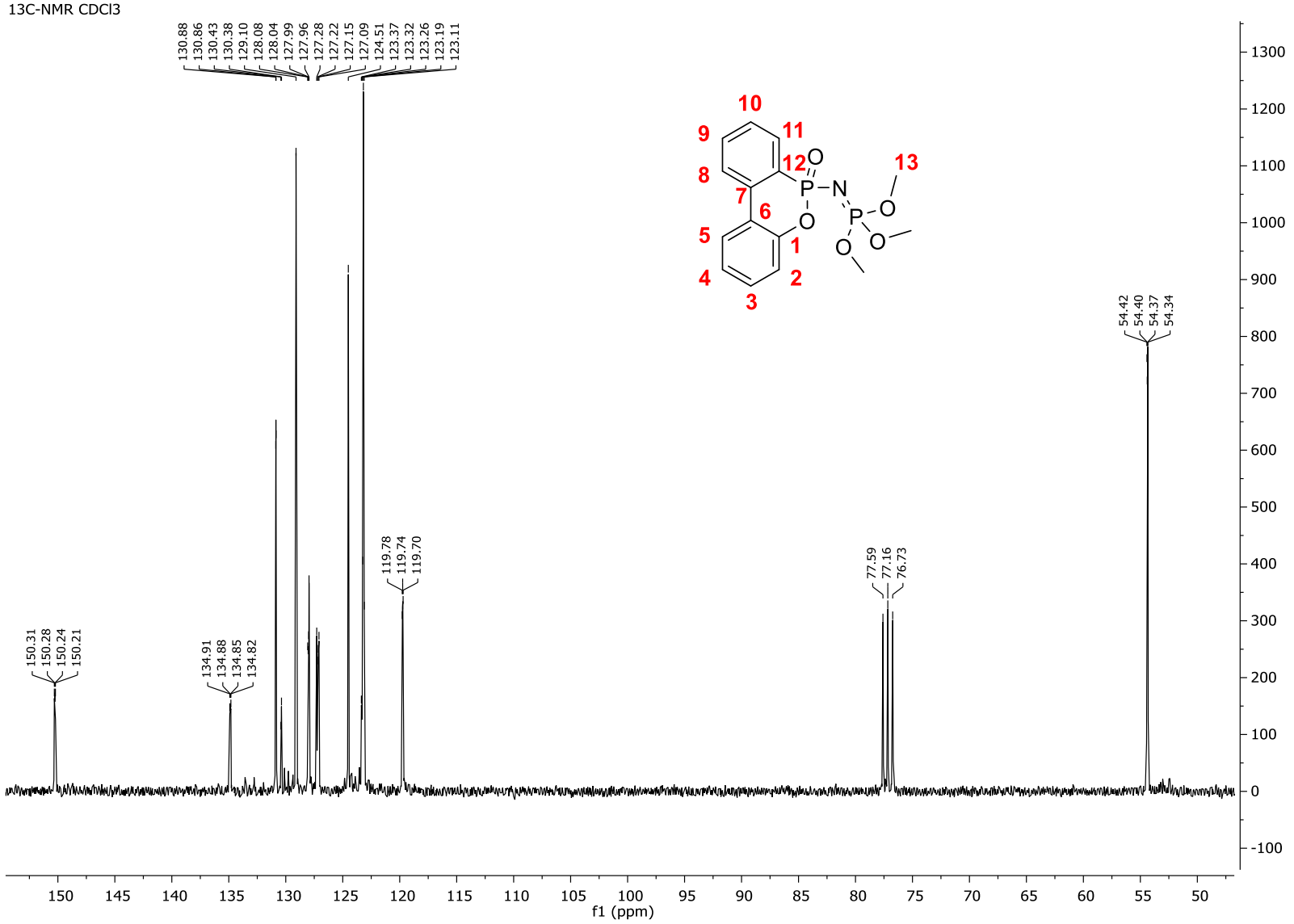
6-((6-ethoxy-6H-6λ^5-dibenzo[c,e][1,2]oxaphosphinin-6-ylidene)amino)dibenzo[c,e][1,2]oxaphosphinine 6-oxide (DOPO-N=DOP-OEt)



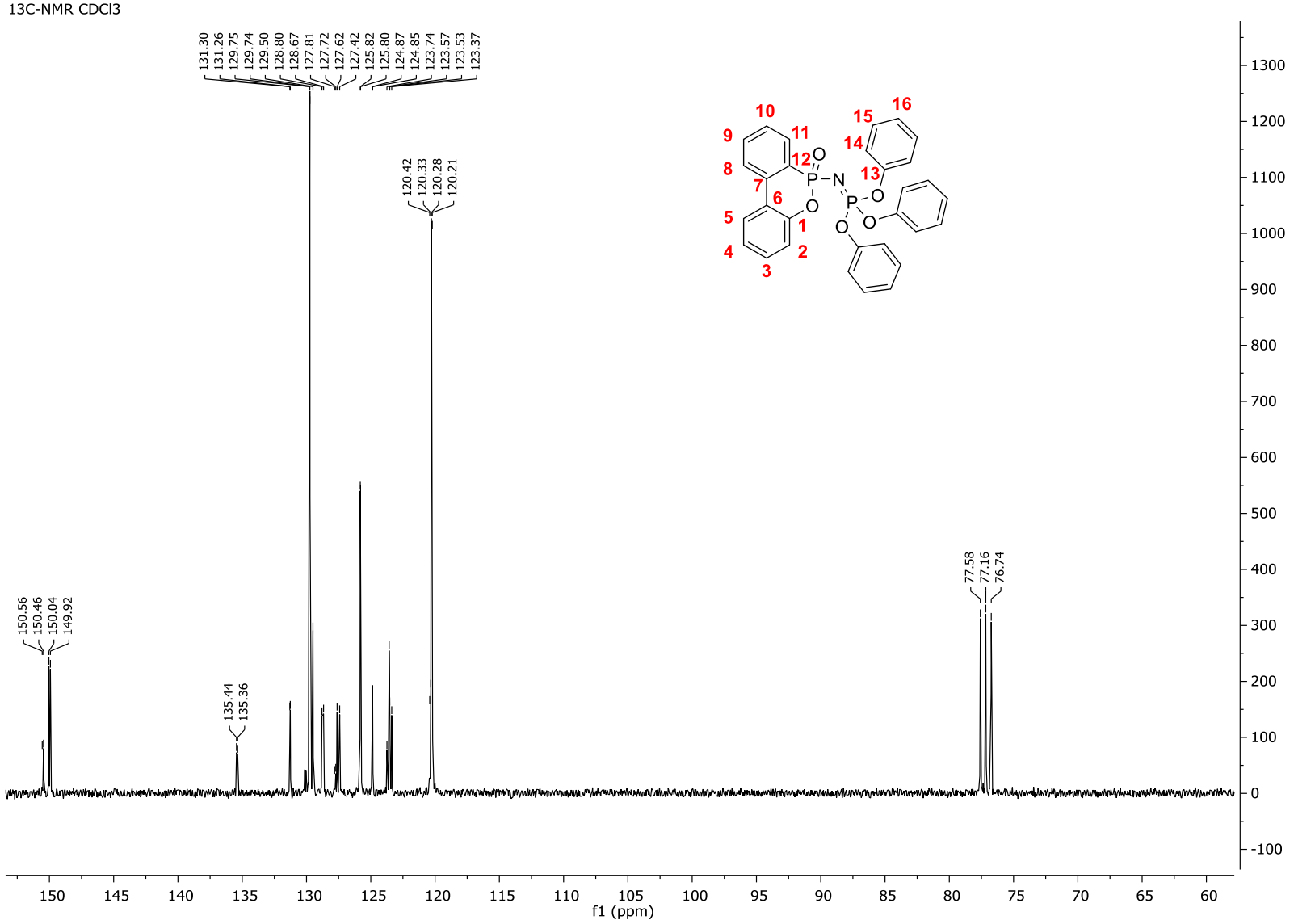
6-Azidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-oxid (DOPO-N_3)



Trimethyl (6-oxidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-yl)phosphorimidate (DOPO-N=P(OMe)$_3$)

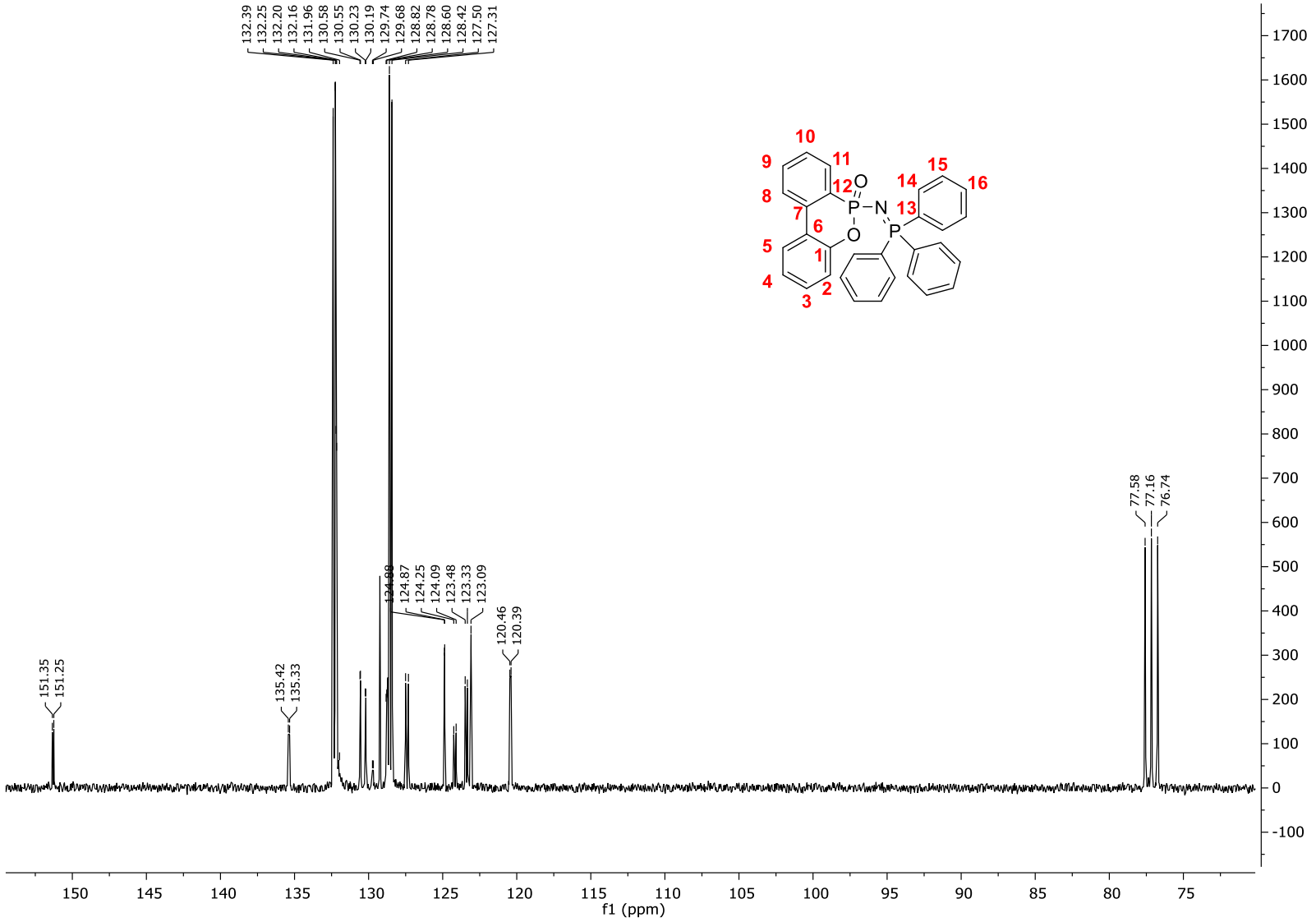


Triphenyl (6-oxidodibenzo[*c*,*e*][1,2]oxaphosphinin-6-yl)phosphorimidate (DOPO-N=P(OPh)$_3$)



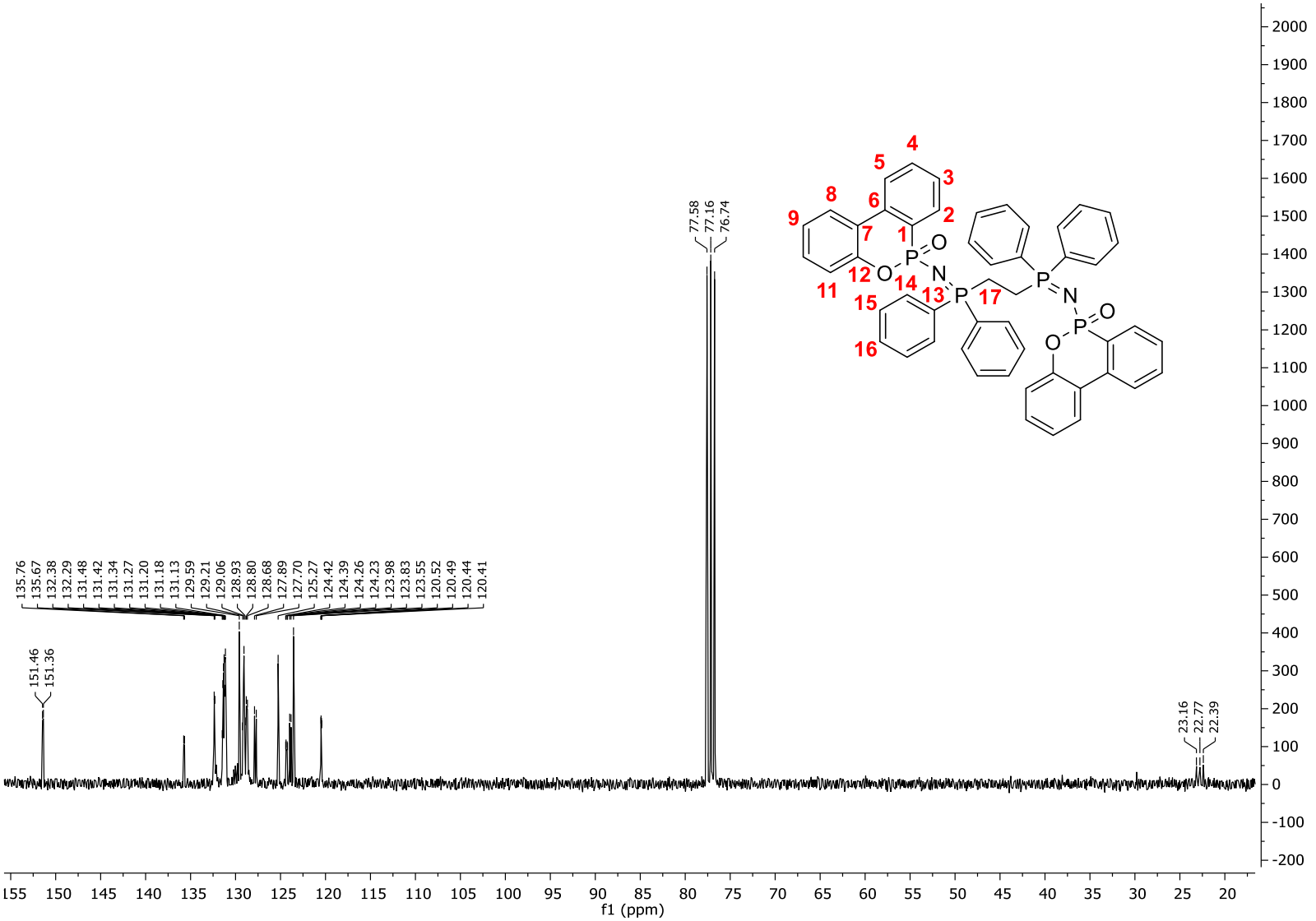
6-((Triphenyl-λ^5-phosphanylidene)amino)dibenzo[*c*,*e*][1,2]oxaphosphinine 6-oxide (DOPO-N=P(Ph)$_3$)

13C-NMR CDCl3

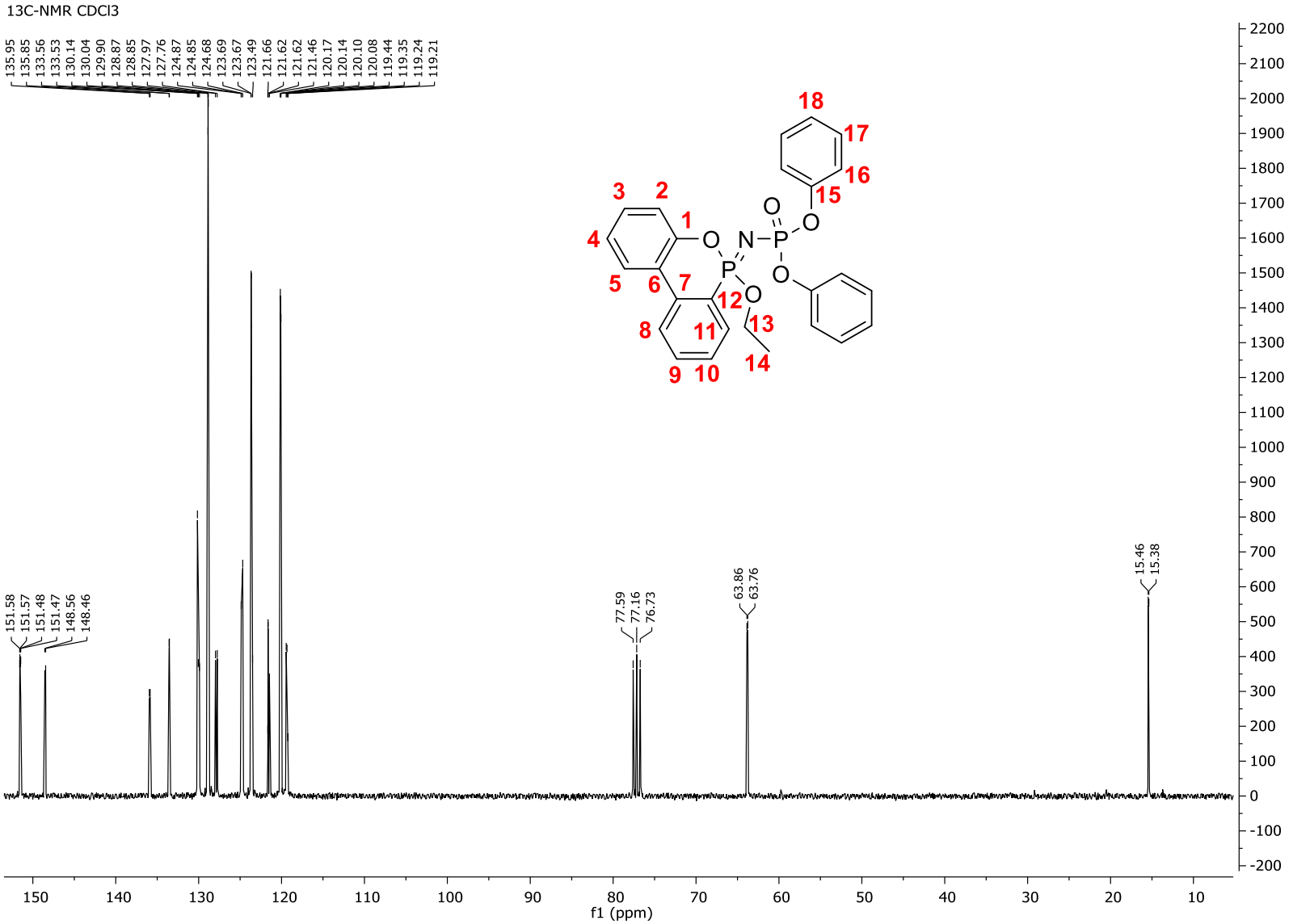


6,6'-((Ethane-1,2-diylbis(diphenyl-λ^5-phosphanylylidene))bis(azanylylidene))bis(dibenzo[c,e][1,2]oxaphosphinine 6-oxide) ([DOPO-N=P(Ph)$_2$CH$_2$]$_2$)

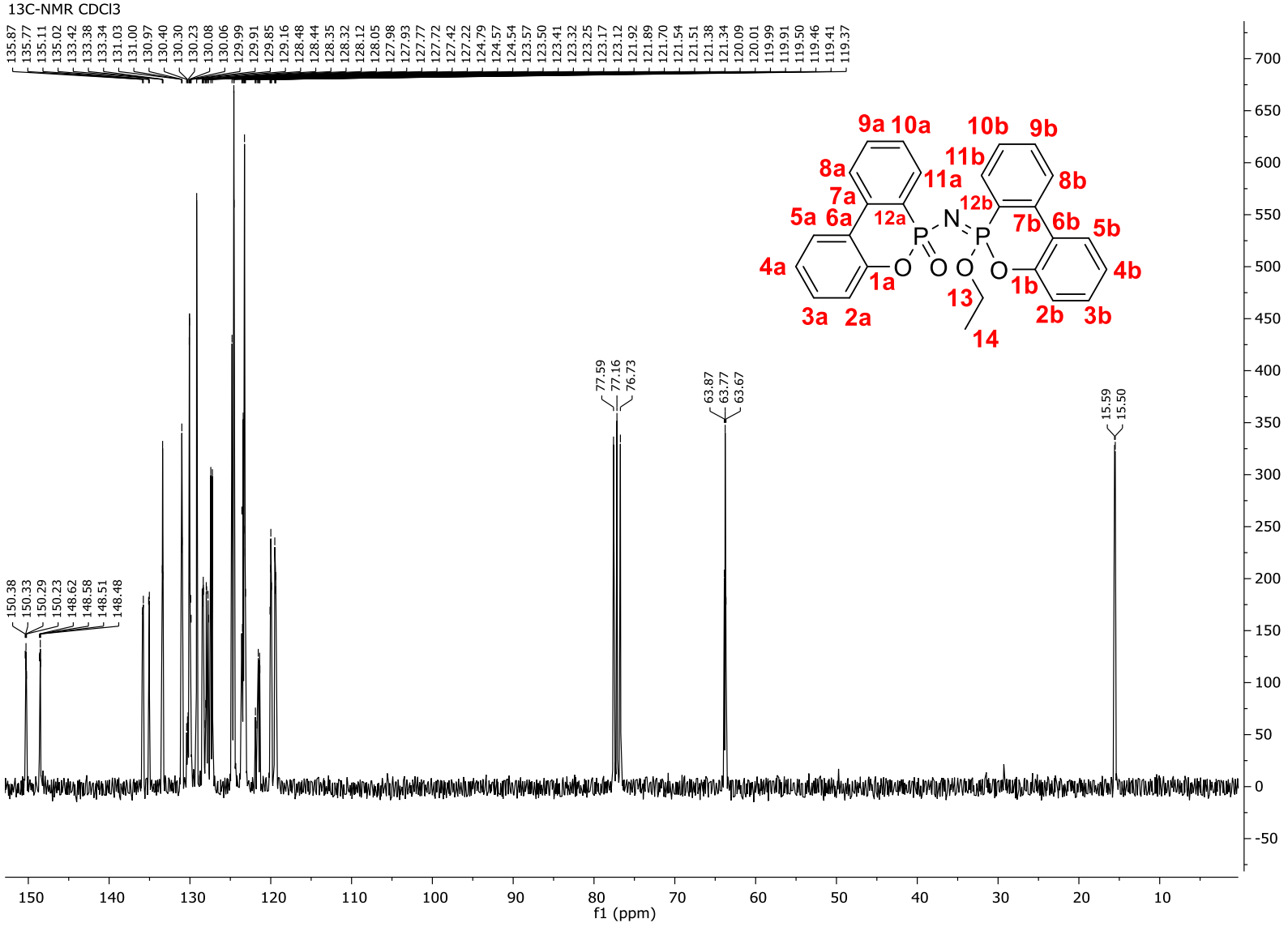
13C-NMR CDCl3



Diphenyl (6-ethoxy-6*H*-6λ^5-dibenzo[*c*,*e*][1,2]oxaphosphinin-6-ylidene)phosphoramidate ((PhO)$_2$(O)P-N=DOP-OEt)



dibenzo[c,e][1,2]oxaphosphinin-6-ylidene)amino)dibenzo[c,e][1,2]oxaphosphinine 6-oxide (DOPO-N=DOP-OEt)



2. Crystallographic data

Table 1. Crystallographic data and structure refinement details of DOPO-N=P(OPh)$_3$, DOPO-N=P(Ph)$_3$ and [DOPO-N=P(Ph)$_2$CH$_2$]$_2$·2C$_3$H$_7$OH.

Compound	**DOPO-N=P(OPh)$_3$**	**DOPO-N=P(Ph)$_3$**	**[DOPO-N=P(Ph)$_2$CH$_2$]$_2$**·2C$_3$H$_7$OH
Empirical formula	$C_{30}H_{23}NO_5P_2$	$C_{30}H_{23}NO_2P_2$	$C_{56}H_{56}N_2O_6P_4$
Formula weight	539.43	491.43	976.90
Crystal system	monoclinic	triclinic	orthorhombic
Space group	*P*2$_1$/*n*	*P*$\bar{1}$	*Pbca*
a/Å	14.748(3)	8.9017(5)	9.3639(4)
b/Å	9.0863(8)	10.4666(6)	20.6288(14)
c/Å	19.621(3)	14.0434(8)	25.7559(14)
α/°	90	88.854(5)	90
β/°	102.174(12)	85.112(4)	90
γ/°	90	67.020(4)	90
Volume/Å^3	2570.3(6)	1200.09(12)	4975.2(5)
Z	4	2	4
ρ_{calc}/g·cm^{-3}	1.394	1.360	1.304
μ/mm^{-1}	0.212	0.211	0.205
F(000)	1120.0	512.0	2056.0
Crystal size/mm^3	0.37 × 0.26 × 0.24	0.35 × 0.28 × 0.21	0.38 × 0.12 × 0.11
2Θ range for data collection/°	4.25–52.0	4.99–51.3	5.032–51.992
Reflections collected	13946	9159	16406
Independent reflections	5082 [R_{int} = 0.0495]	4459 [R_{int} = 0.0170]	4881 [R_{int} = 0.0883]
Ind. refl. with [I≥2σ (I)]	3975	4079	2520
Data/restraints/parameters	5082/0/331	4459/0/316	4881/0/310
Goodness-of-fit on F^2	1.151	1.035	0.894
Final R indexes [I≥2σ (I)]	R_1 = 0.0874, wR_2 = 0.2711	R_1 = 0.0540, wR_2 = 0.1259	R_1 = 0.0673, wR_2 = 0.1639
Final R indexes [all data]	R_1 = 0.1054, wR_2 = 0.2798	R_1 = 0.0578, wR_2 = 0.1281	R_1 = 0.1355, wR_2 = 0.1875
Largest diff. peak/hole / e·Å^{-3}	0.99/–1.16	1.79/–0.91	0.87/–0.62
CCDC number	1569140	1569141	1569142