Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Metal-free S_N^H cross-coupling of pyridines with phosphine chalcogenides: polarization/deprotonation/oxidation effect of electron-deficient acetylenes

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1. Quantum chemical calculations

Computational details

The structural parameters of the studied systems were optimized using the density functional theory (DFT) at the B3LYP[1,2] level of theory with the 6-31+G* basis set. The vibrational corrections to enthalpies and Gibbs free energies were calculated at the same level of theory (B3LYP/6-31+G*) at a standard temperature 298.15 K.

Further, the energies at the stationary points were refined by using the double-hybrid functional B2PLYP[3] in combination with the extended 6-311+G**. Such a combined B2PLYP/6-311+G**//B3LYP/6-31+G* method provides accuracy comparable to CCSD(T)/6-311+G**//CCSD/6-31G* and CBS-Q//B3 approaches.[4] For all structures solvation energy in MeCN was computed additionally by the polarizable dielectric model using the IEFPCM model.[5,6]

To estimate free energy in the solution we have used approach, which based upon results by Wertz.[7] Being applied to MeCN solution this approach suggests that the entropy in MeCN solution S_{sol} can be obtain from S_{harm}, the entropy found in the harmonic approximation for ideal gas, as

$$S_{sol} = 0.71S_{harm} - 2.68 \text{ cal}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}.$$

All calculations were carried out using the GAUSSIAN 09 program package.[8]

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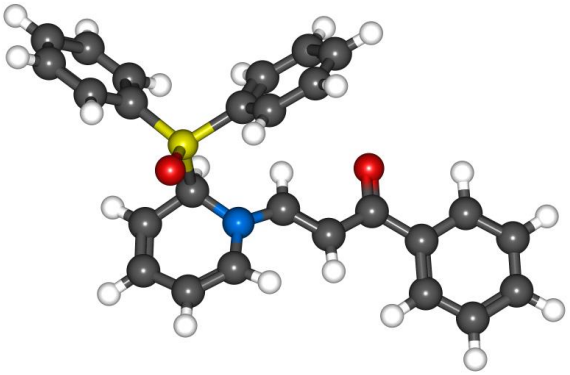
[2] C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.
[3] M. Page, C. Doubleday and J. W. McIver, *J. Chem. Phys.*, 1990, **935**, 5634–5642.
[4] S. Grimme, *J. Chem. Phys.*, 2006, **124**, 034108.
[5] N. M. Vitkovskaya, V. B. Orel, V. B. Kobychev, A. S. Bobkov, D. Z. Absalyamov and B. A. Trofimov, *Int. J. Quantum Chem.*, 2020, **120**, e26158.
[6] J. Tomasi, B. Mennucci and E. Cancès, *J. Mol. Struct. THEOCHEM*, 1999, **464**, 211–226.
[7] D. H. Wertz, *J. Am. Chem. Soc.*, 1980, **102**, 5316–5322.
[8] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc.: Wallingford, CT, 2010.

Total energies, enthalpies and Gibbs free energies (a.u.) calculated in the frame of B2PLYP/6-311+G//B3LYP/6-31+G*, Cartesian coordinates (Å) of stationary points**

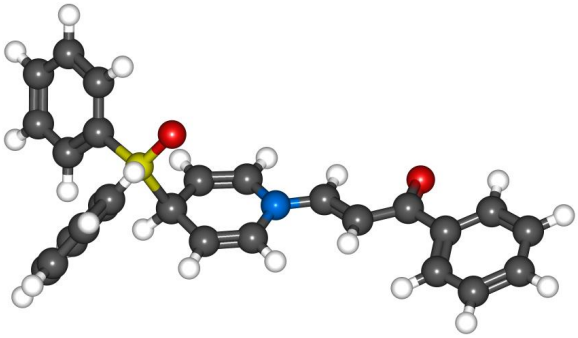
Cartesian coordinates			
C	1.6615300	3.6844080	0.1576780
C	1.9923680	2.6431610	-0.6291160
C	0.5630340	3.5648440	1.1026280
H	2.7958030	2.7012920	-1.3569660
H	0.4034230	4.3175310	1.8666010
C	1.2889560	1.3198700	-0.4635470
C	-0.2807660	2.5165670	1.0060370
H	1.2083850	0.8089060	-1.4279640
H	-1.1529080	2.3921460	1.6369650
N	-0.0789370	1.5166880	0.0436080
H	2.1937840	4.6284380	0.0771190
C	-1.1054390	0.7571460	-0.4538380
H	-0.8016320	-0.0000630	-1.1702820
C	-2.4325450	0.8345680	-0.1620980
H	-2.8246880	1.5715590	0.5264760
C	-3.3444720	-0.1167050	-0.8049520
O	-2.9369690	-1.0195660	-1.5479410
C	-4.8231000	0.0058020	-0.5416780
C	-5.4234280	1.1585390	-0.0087950
C	-5.6400510	-1.0888770	-0.8717160
C	-6.8049570	1.2137560	0.1912170
C	-7.0168250	-1.0398420	-0.6604650
C	-7.6045440	0.1132630	-0.1280950
H	-4.8248410	2.0317130	0.2315620
H	-5.1698760	-1.9706270	-1.2955640
H	-7.2557430	2.1173310	0.5940020
H	-7.6341160	-1.8985460	-0.9128210
H	-8.6789510	0.1547000	0.0332140
P	2.3209800	0.1735470	0.6741090
O	2.6346640	0.7574050	2.0254340
C	3.8385600	-0.1382740	-0.3106030
C	3.8457550	-0.5065890	-1.6660860
C	5.0597010	0.0303520	0.3600880
C	5.0539210	-0.7121790	-2.3357240
C	6.2670940	-0.1787100	-0.3111480
C	6.2662970	-0.5510080	-1.6578970
H	2.9166870	-0.6357250	-2.2154300
H	5.0480350	0.3312460	1.4038870
H	5.0476060	-0.9975060	-3.3845900
H	7.2075820	-0.0476730	0.2179100
H	7.2058990	-0.7122350	-2.1801920
C	1.3717400	-1.3859920	0.8167150
C	0.9975470	-2.1886440	-0.2724040
C	0.9945570	-1.7664470	2.1139810
C	0.2537280	-3.3516730	-0.0681780
C	0.2537140	-2.9333480	2.3158680
C	-0.1187830	-3.7250370	1.2265460
H	1.2791080	-1.9190770	-1.2866580
H	1.2905010	-1.1416110	2.9516810
H	-0.0430100	-3.9582610	-0.9192530
H	-0.0339300	-3.2213830	3.3238090
H	-0.7023550	-4.6285770	1.3831560



1,2-dihydropyridine **4a**

	a.u.
E(B2PLYP)	-1549.719467
E(B2PLYP)+*ZPE*	-1549.306036
E(B2PLYP)+H_{corr}	-1549.27898
E(B2PLYP)+G_{corr}	-1549.367004

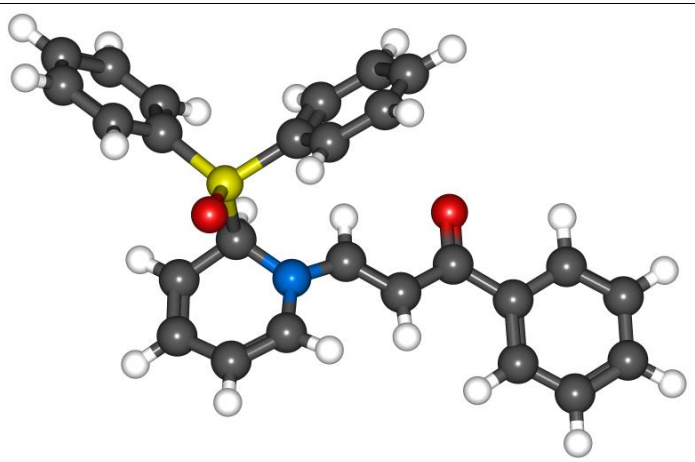
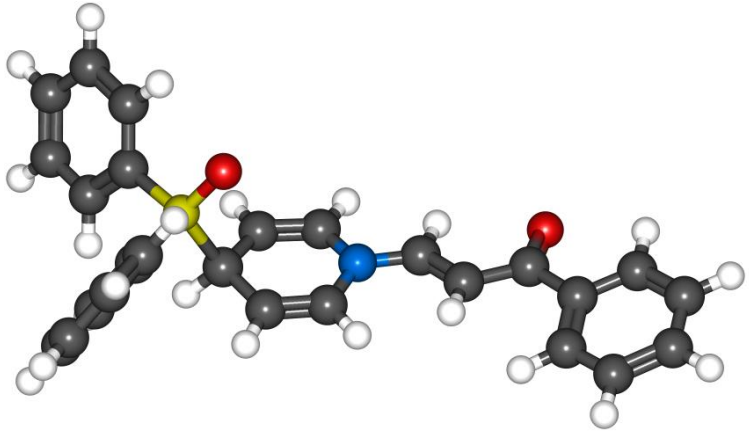
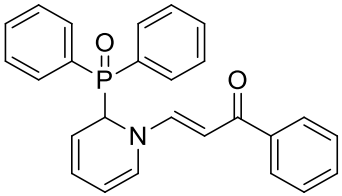
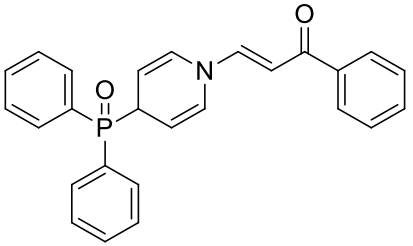
Cartesian coordinates			
C	1.5334590	-0.2762750	-1.1193280
C	0.9870680	-1.6799390	-1.1037280
C	0.4057930	0.7167600	-1.2126910
H	1.6757380	-2.5124790	-1.2050910
H	0.6417370	1.7570170	-1.4143380
C	-0.3144870	-1.9456090	-0.9295070
C	-0.8793190	0.3787340	-1.0339870
H	-0.6984770	-2.9587600	-0.8841700
H	-1.6749500	1.1092370	-1.0917390
N	-1.2950110	-0.9445620	-0.8134370
H	2.2258830	-0.1419990	-1.9655050
C	-2.5985580	-1.2912950	-0.5505190
H	-2.7675120	-2.3631190	-0.4906850
C	-3.6687520	-0.4776030	-0.3576050
H	-3.5767380	0.6006670	-0.3521450
C	-4.9757240	-1.0932440	-0.0909080
O	-5.1161970	-2.3195500	-0.0126240
C	-6.1723900	-0.2004790	0.1100000
C	-6.1971570	1.1588300	-0.2433640
C	-7.3299710	-0.7746560	0.6626550
C	-7.3488350	1.9246710	-0.0468990
C	-8.4758040	-0.0089610	0.8696160
C	-8.4891790	1.3446920	0.5146750
H	-5.3290170	1.6286990	-0.6948730
H	-7.3060010	-1.8281640	0.9225800
H	-7.3547510	2.9730620	-0.3344730
H	-9.3604220	-0.4660990	1.3060020
H	-9.3835960	1.9424030	0.6722000
P	2.5727890	0.0486390	0.4290720
O	1.8093660	-0.0618430	1.7214580
C	3.2708800	1.7296780	0.1932900
C	3.9663060	2.1395890	-0.9557640
C	3.0640120	2.6478760	1.2338880
C	4.4536070	3.4441580	-1.0584320
C	3.5541190	3.9525940	1.1298780
C	4.2490300	4.3521850	-0.0144440
H	4.1386030	1.4496060	-1.7777410
H	2.5179020	2.3266500	2.1163460
H	4.9923880	3.7508130	-1.9513930
H	3.3913210	4.6557350	1.9427400
H	4.6299330	5.3671290	-0.0952110
C	3.9498680	-1.1606090	0.3434500
C	4.7271380	-1.3932110	-0.8028560
C	4.2073340	-1.9002580	1.5077190
C	5.7506200	-2.3430030	-0.7814750
C	5.2335390	-2.8486250	1.5276990
C	6.0064110	-3.0706850	0.3851320
H	4.5436670	-0.8419960	-1.7215740
H	3.5924620	-1.7267700	2.3863120
H	6.3460250	-2.5153560	-1.6744940
H	5.4259240	-3.4152520	2.4351680
H	6.8037170	-3.8094210	0.4004370



1,4-dihydropyridine **5a**

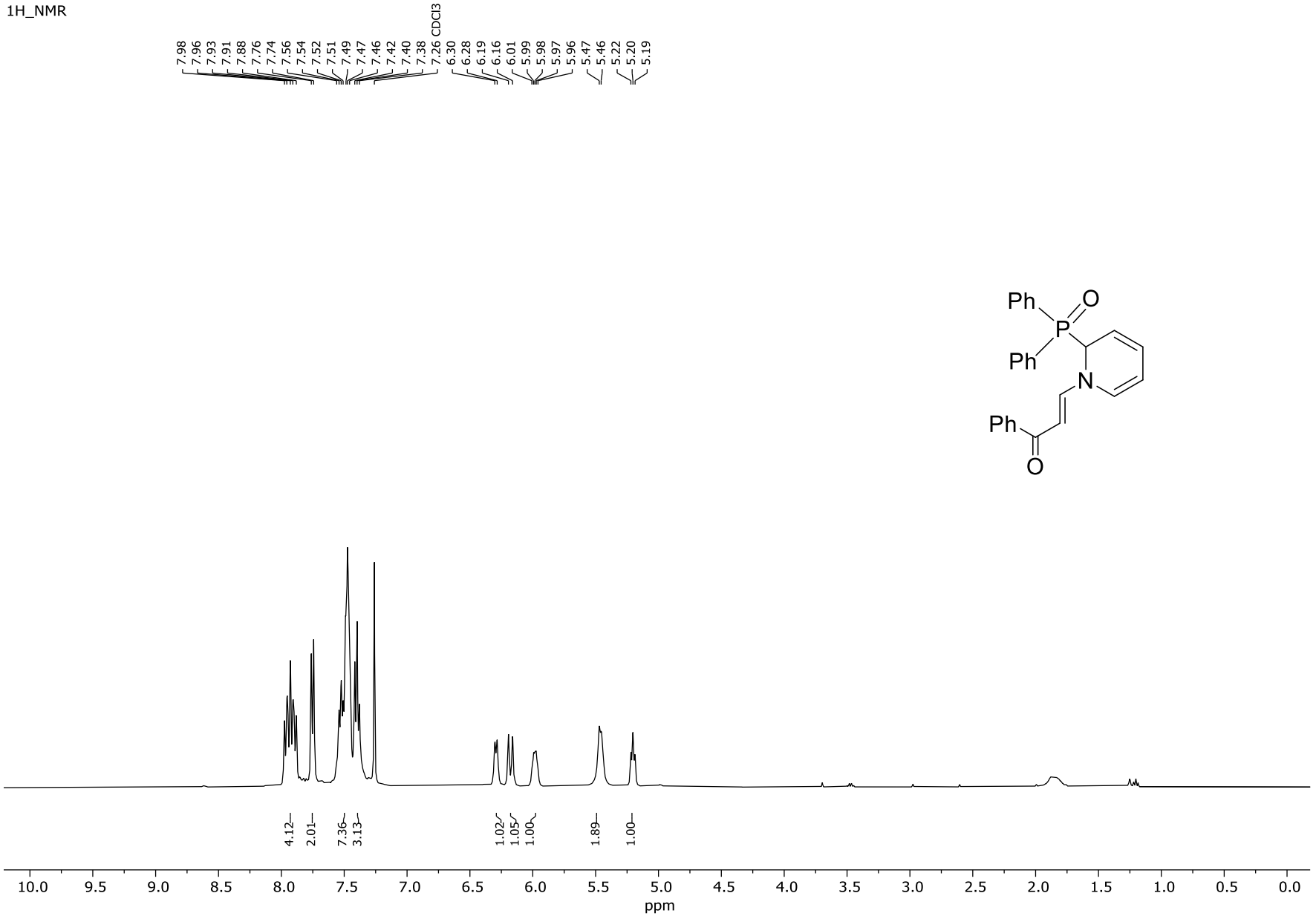
	a.u.
E(B2PLYP)	-1549.725277
E(B2PLYP)+*ZPE*	-1549.311495
E(B2PLYP)+H_{corr}	-1549.284454
E(B2PLYP)+G_{corr}	-1549.374603

B2PLYP/6-311+G**//B3LYP/6-31+G* + IEF PCM (B3LYP/6-31+G*, Acetonitrile)

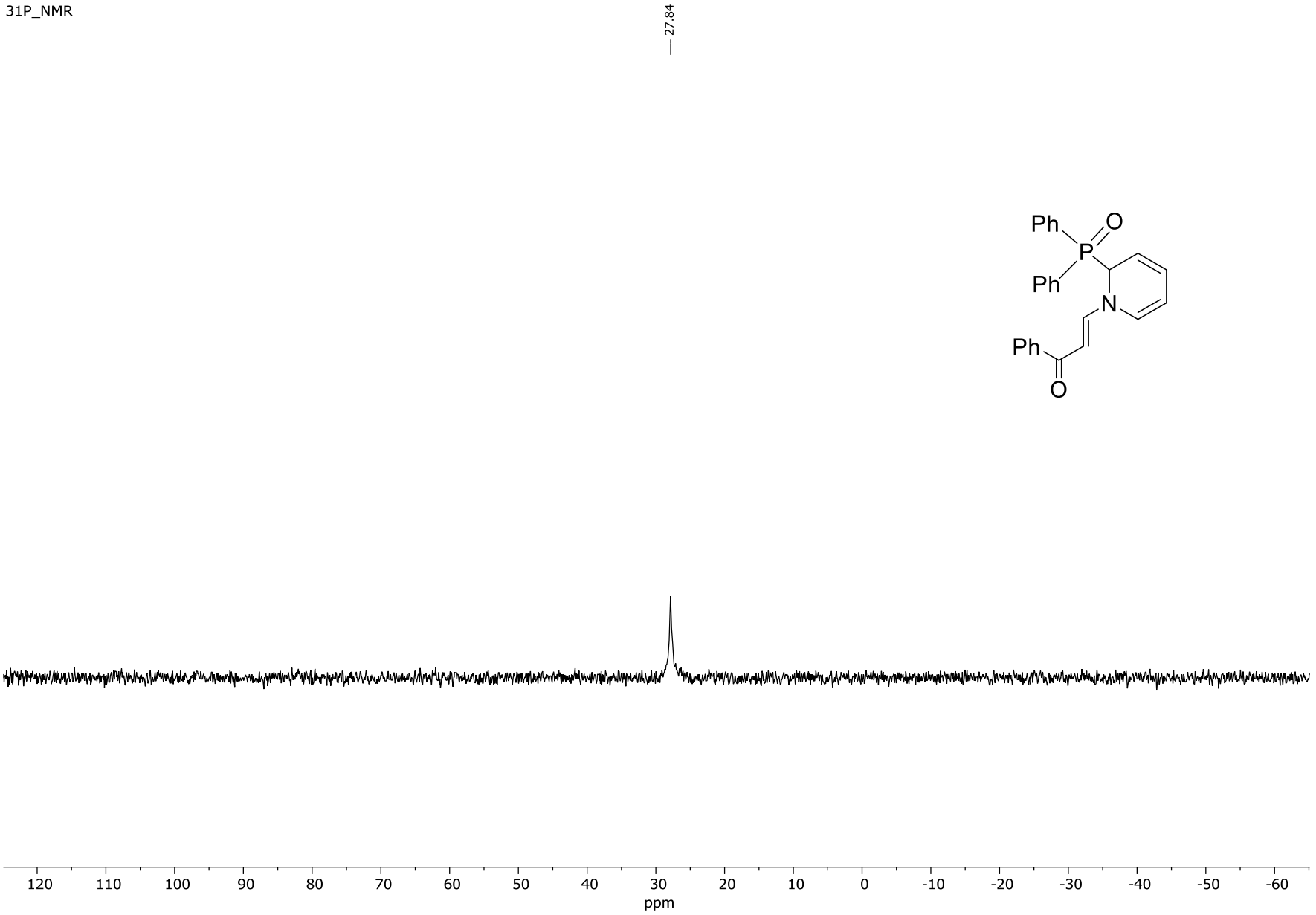
		
		
	(2*E*)-3-[2-(diphenylphosphoryl)pyridin-1(2*H*)-yl]-1-phenylprop-2-en-1-one	(2*E*)-3-[4-(diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one
	GAS	**Acetonitrile**	**GAS**	**Acetonitrile**
Δ*H*, kcal/mol	0.0	0.0	–3.4	–4.0
Δ*G*, kcal/mol	0.0	0.0	–4.8	–5.0
Ratio, %	0%		**100%**	

2. NMR Spectra

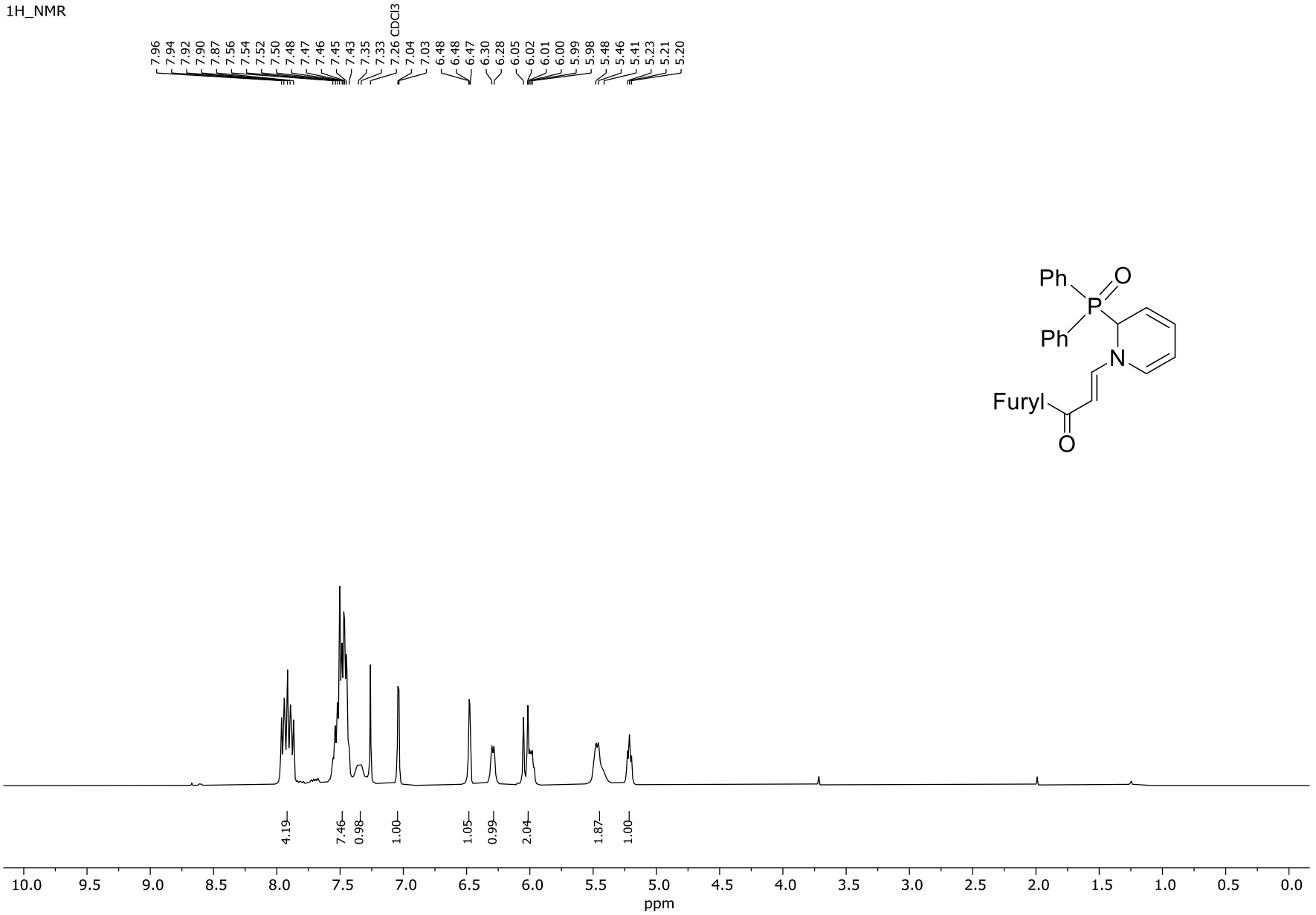
(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl]-1-phenylprop-2-en-1-one (4a)



(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl]-1-phenylprop-2-en-1-one (4a)



(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (4b)



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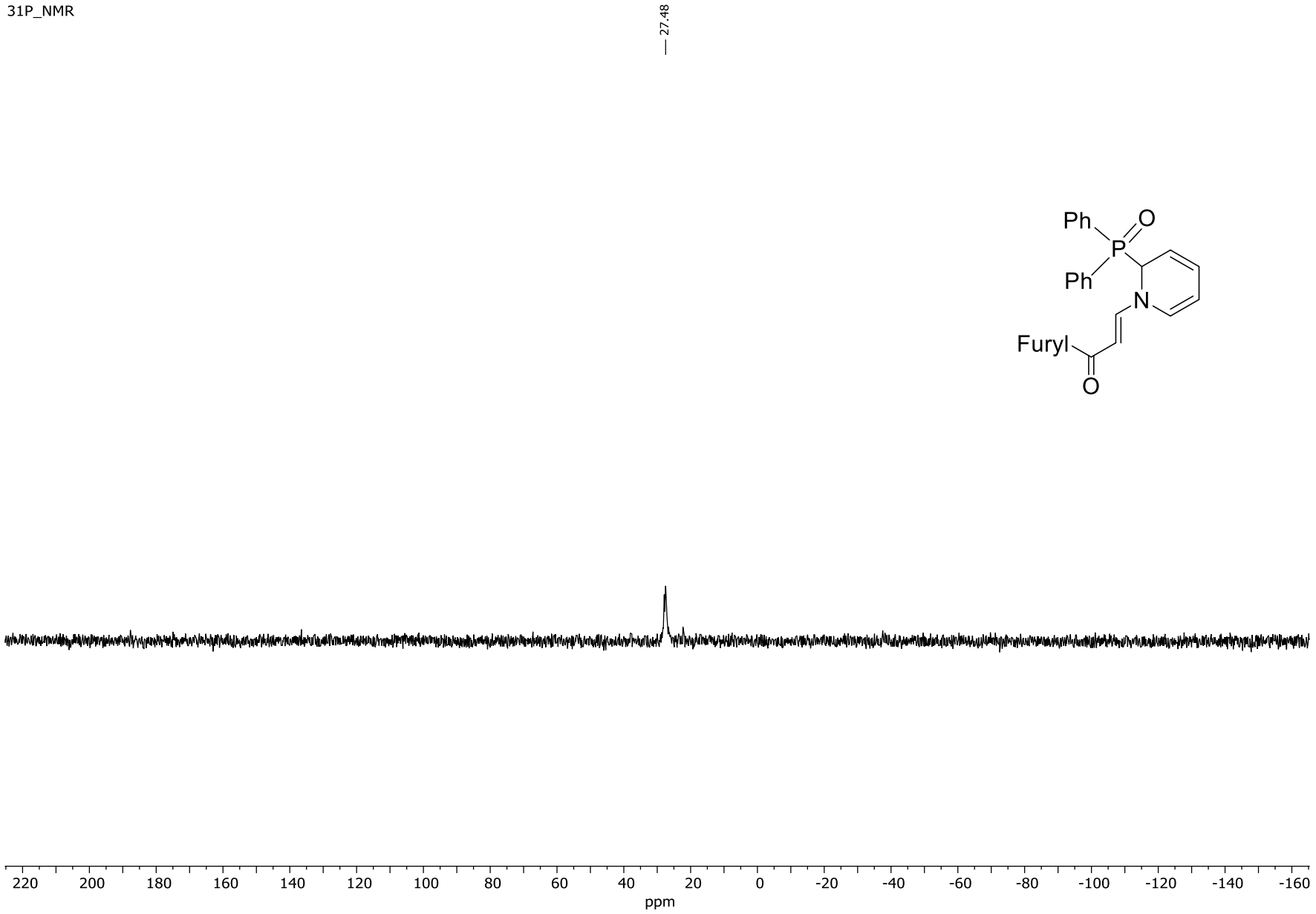
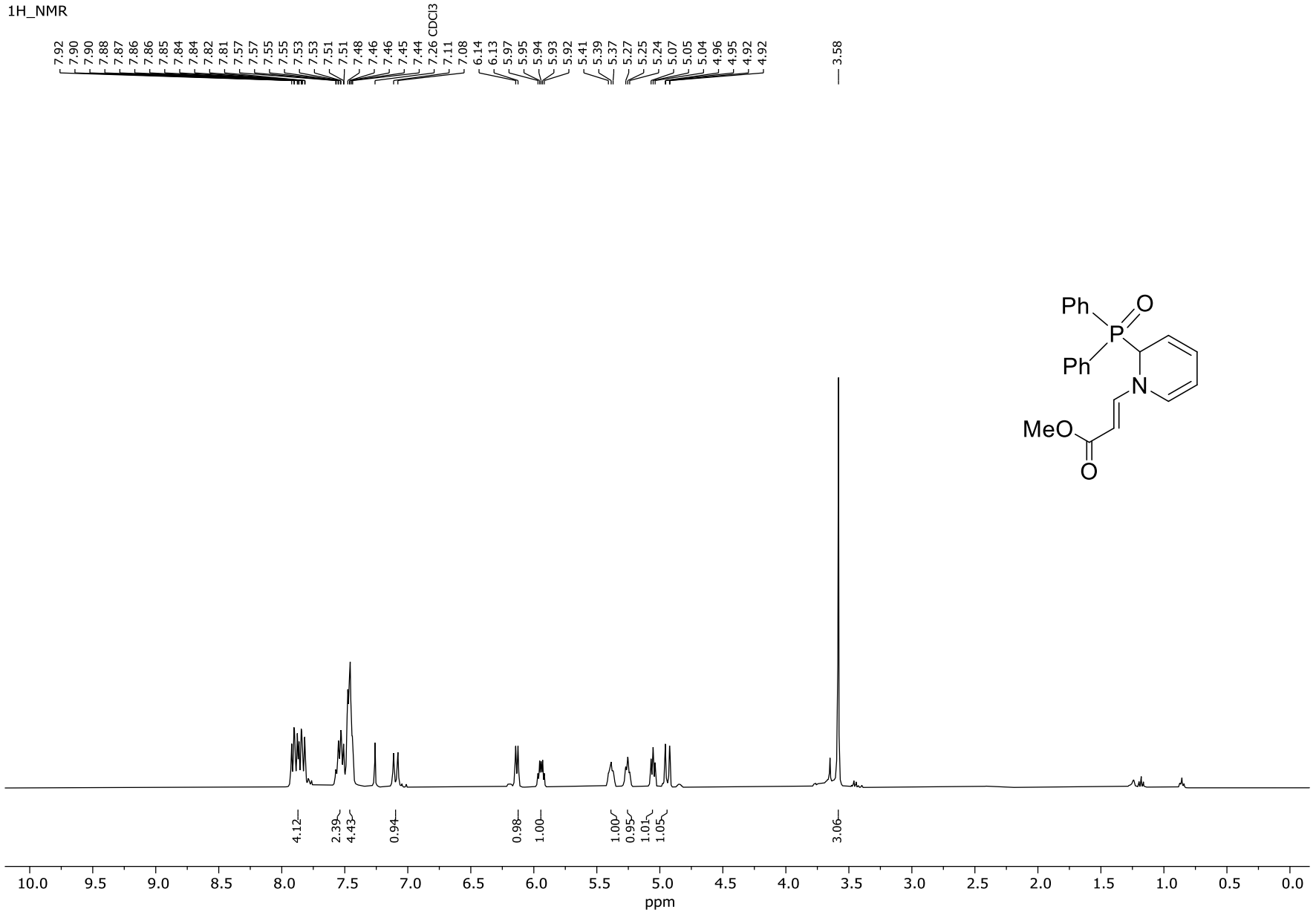
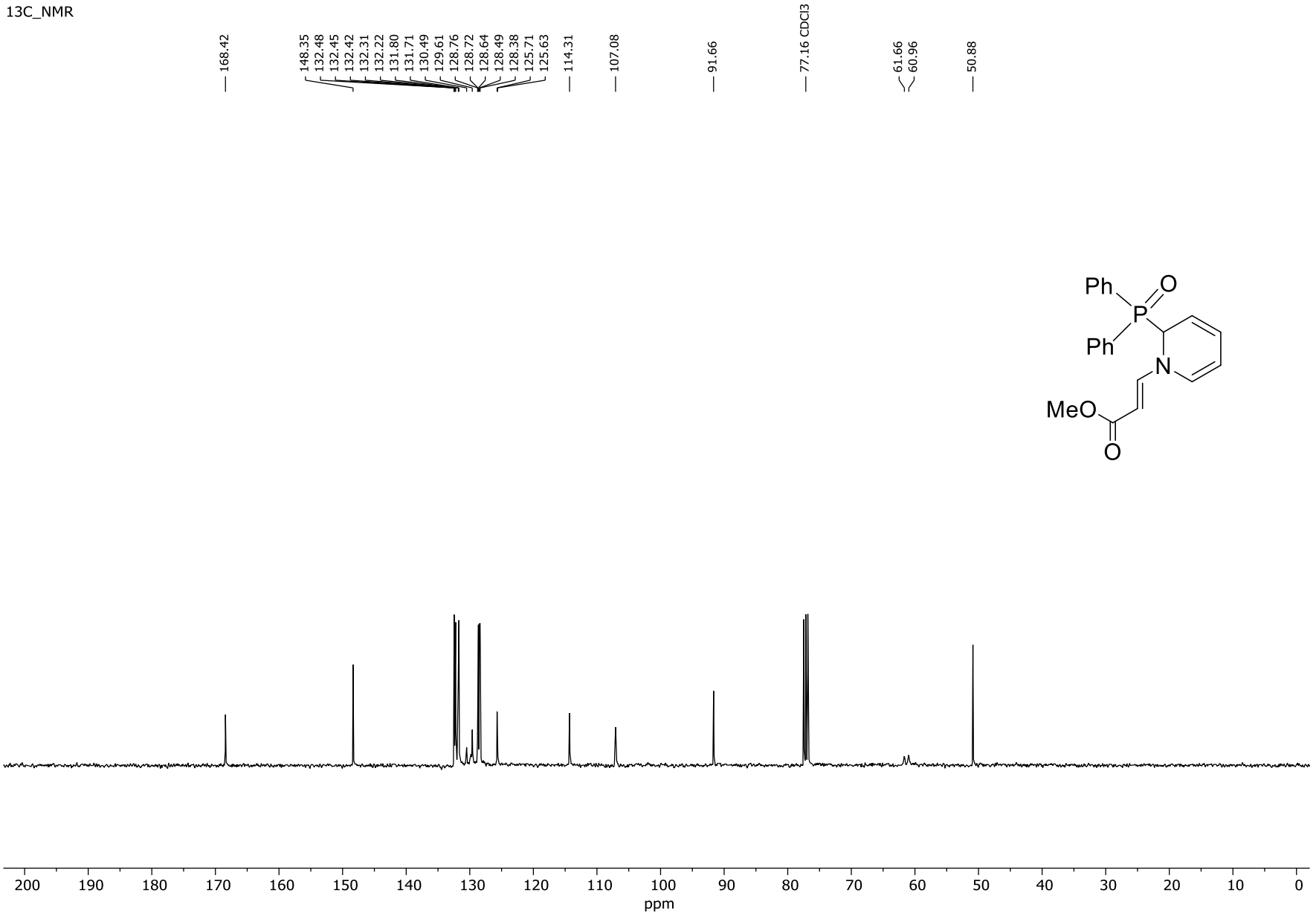


Methyl (2*E*)-3-[2-(diphenylphosphoryl)pyridin-1(2*H*)-yl]prop-2-enoate (4c)



Methyl (2*E*)-3-[2-(diphenylphosphoryl)pyridin-1(2*H*)-yl]prop-2-enoate (4c)



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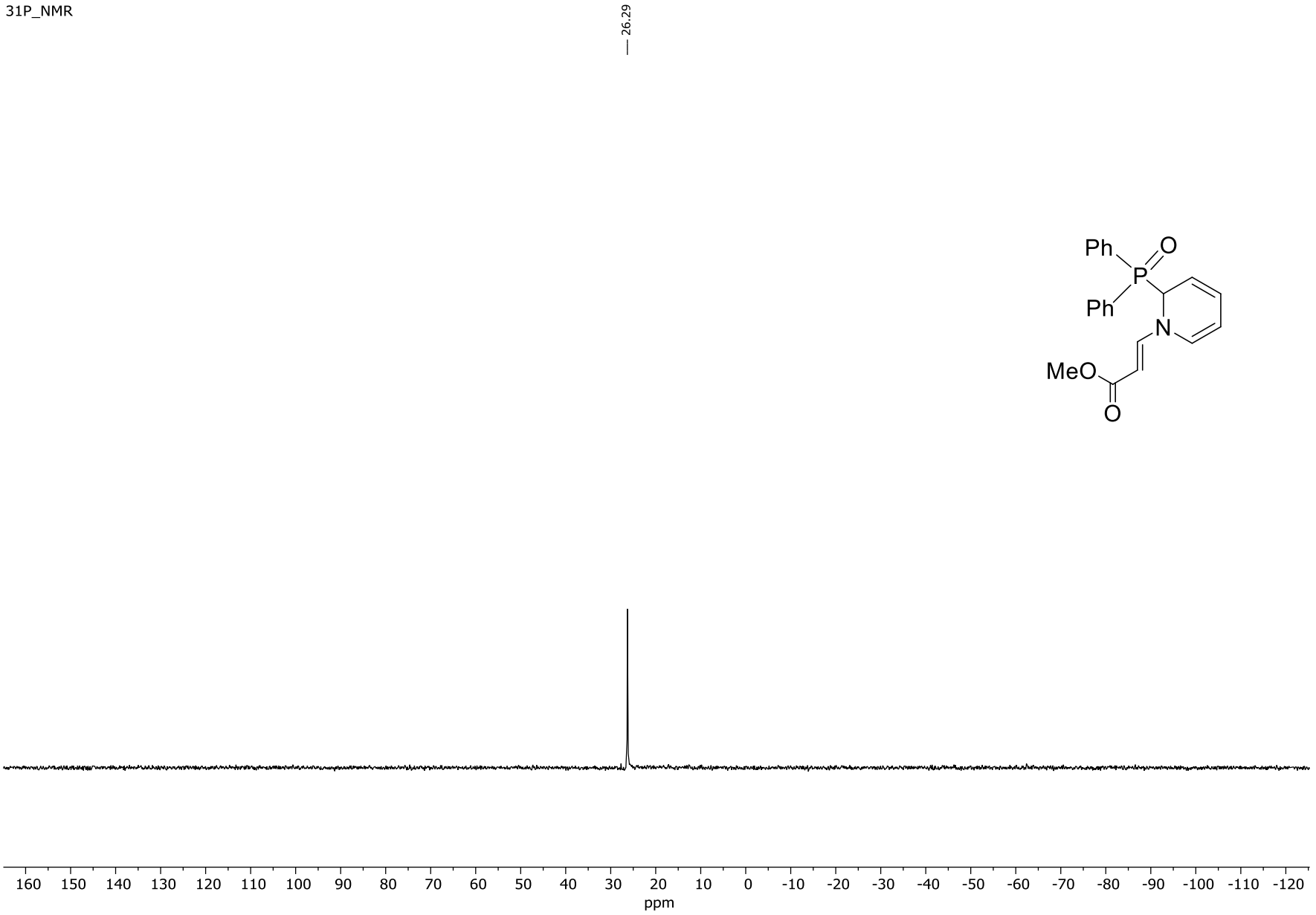

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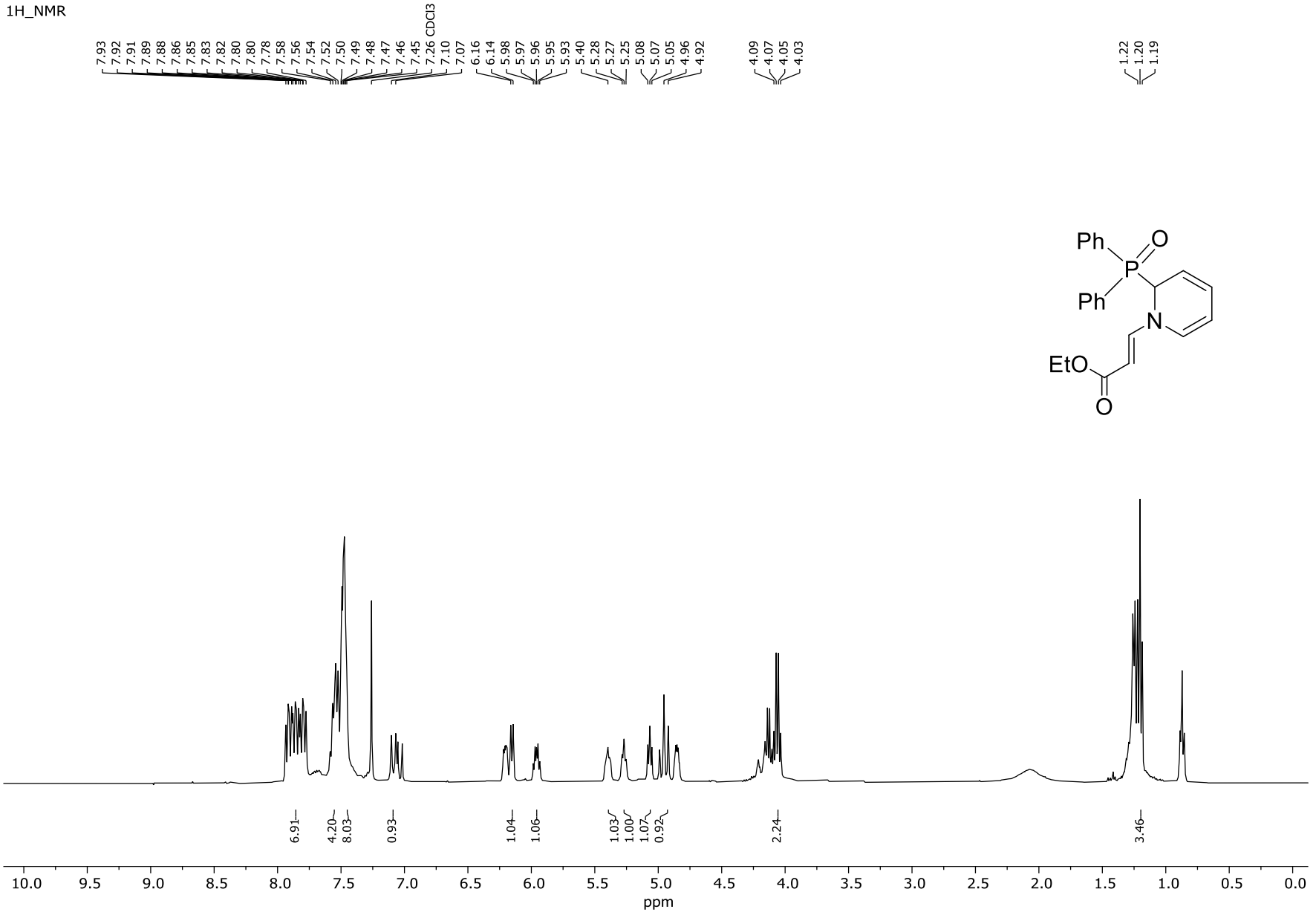
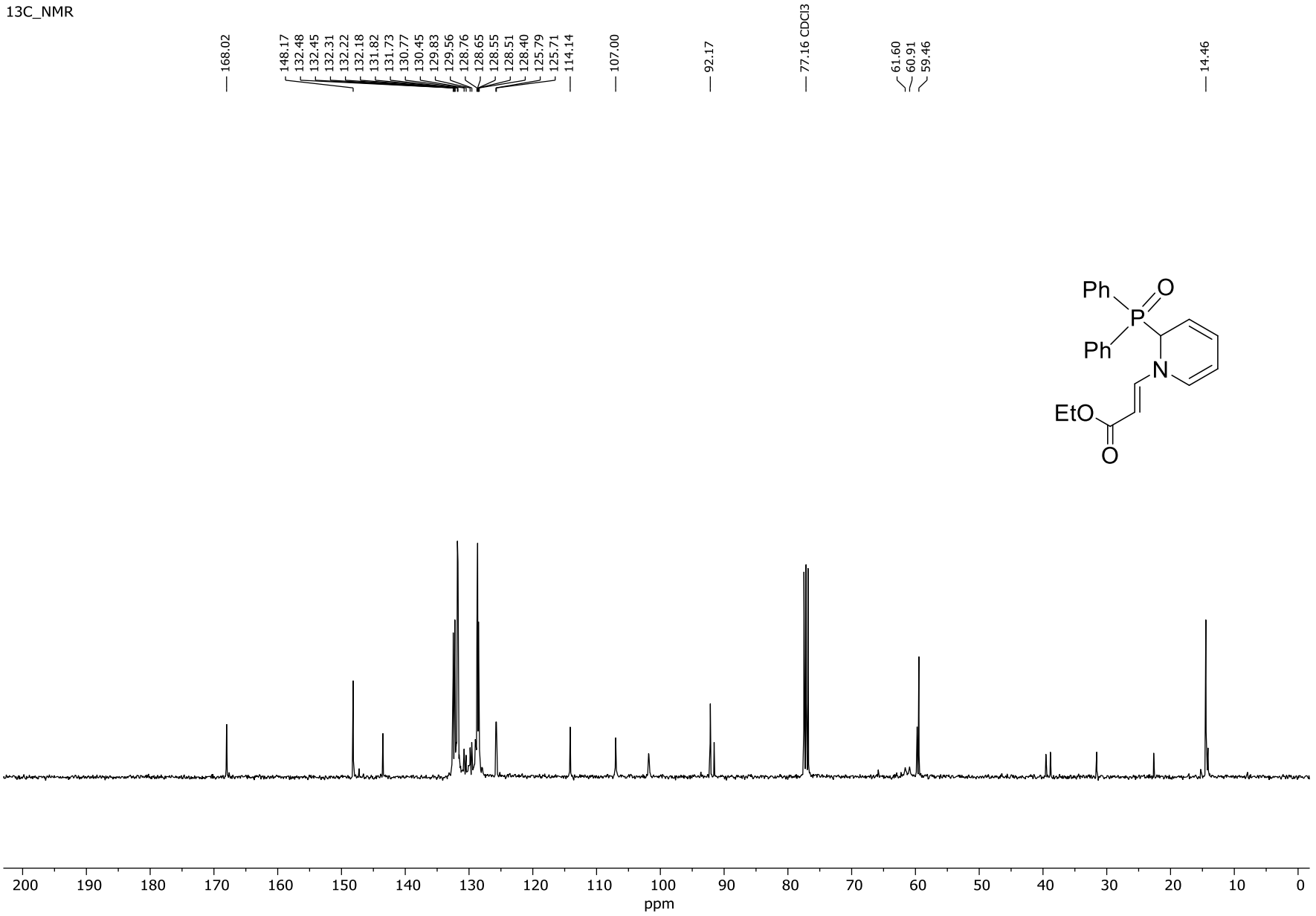


Ethyl (2*E*)-3-[2-(diphenylphosphoryl)pyridin-1(2*H*)-yl]prop-2-enoate (4d)



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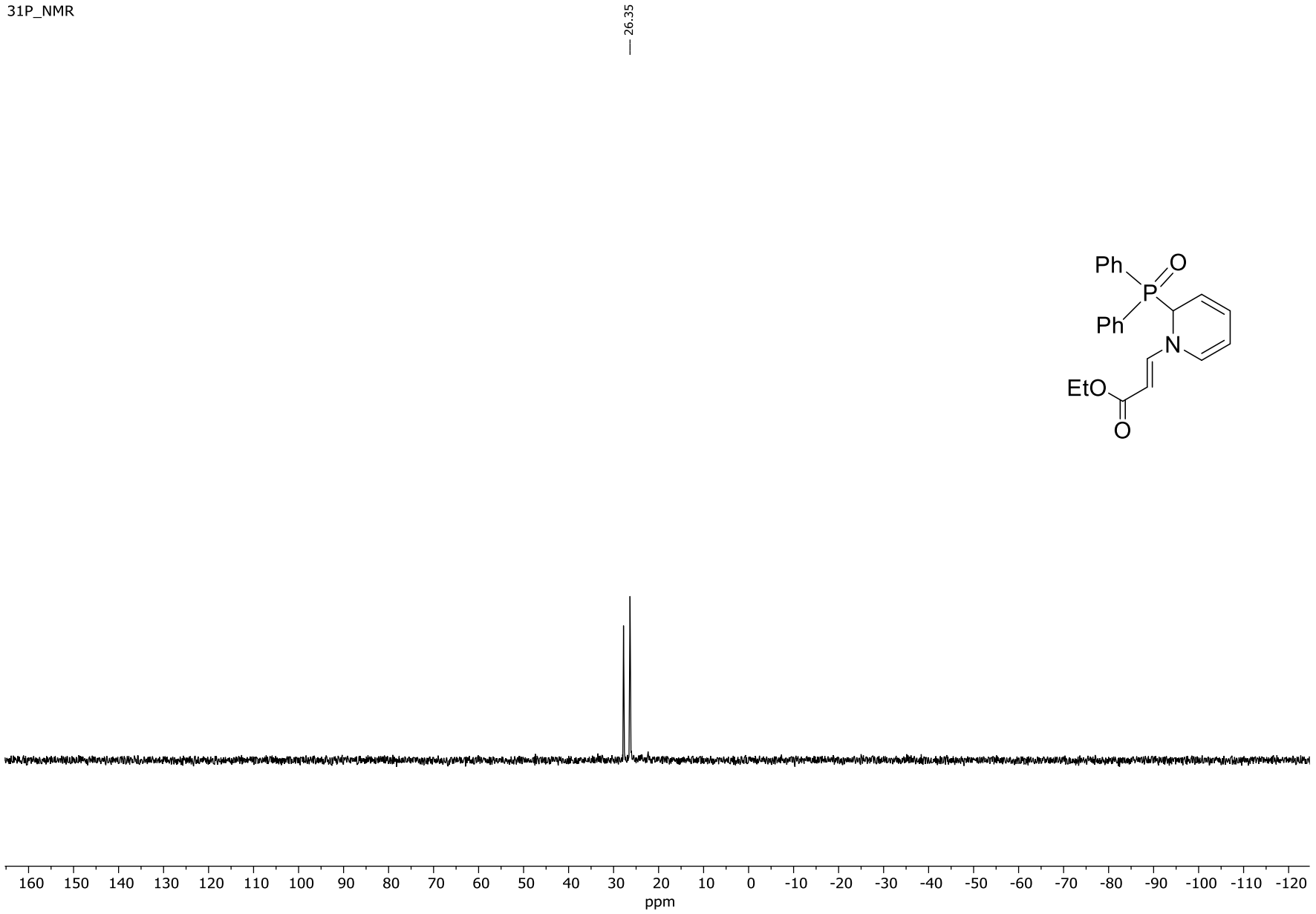
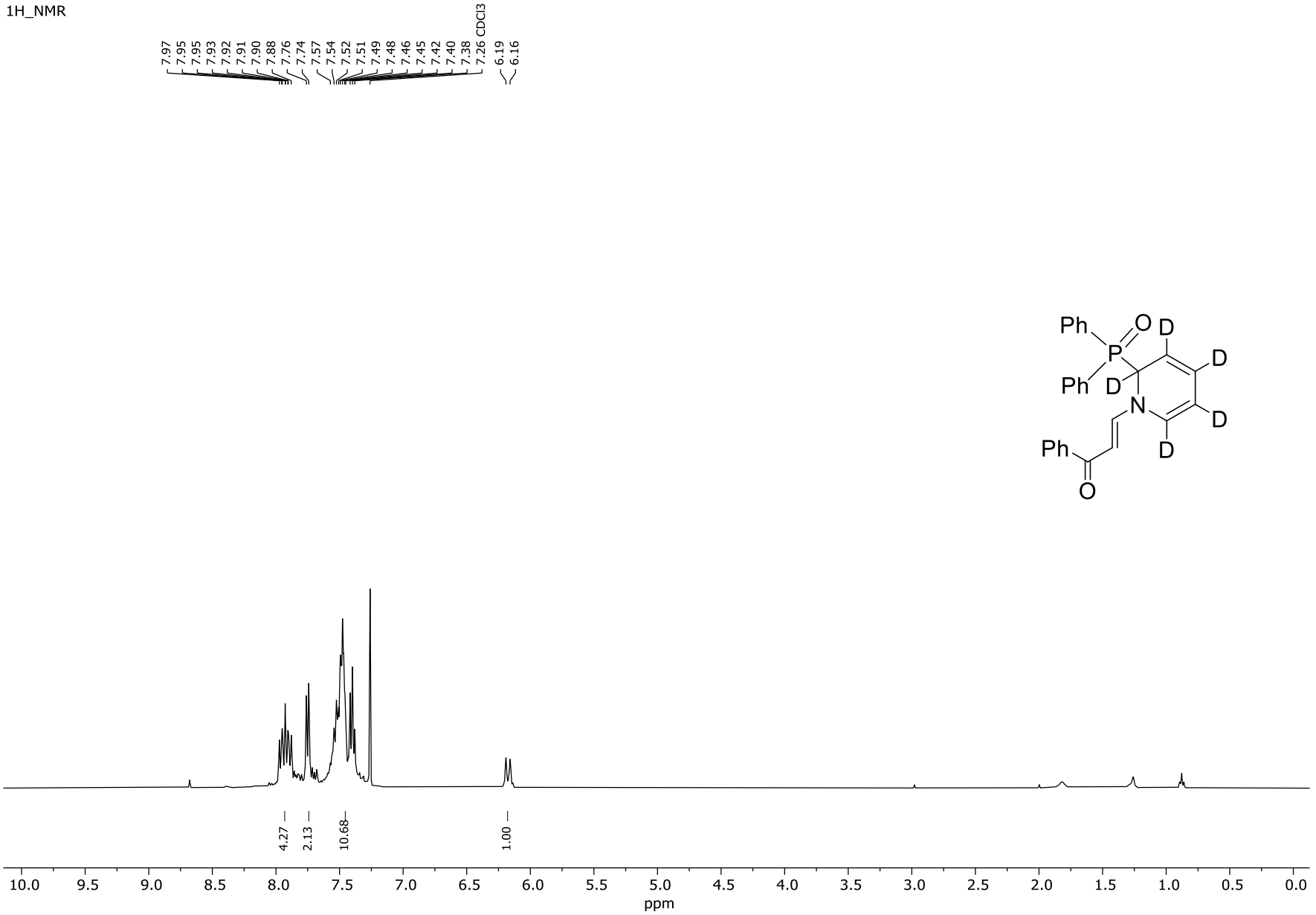


(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (4e)



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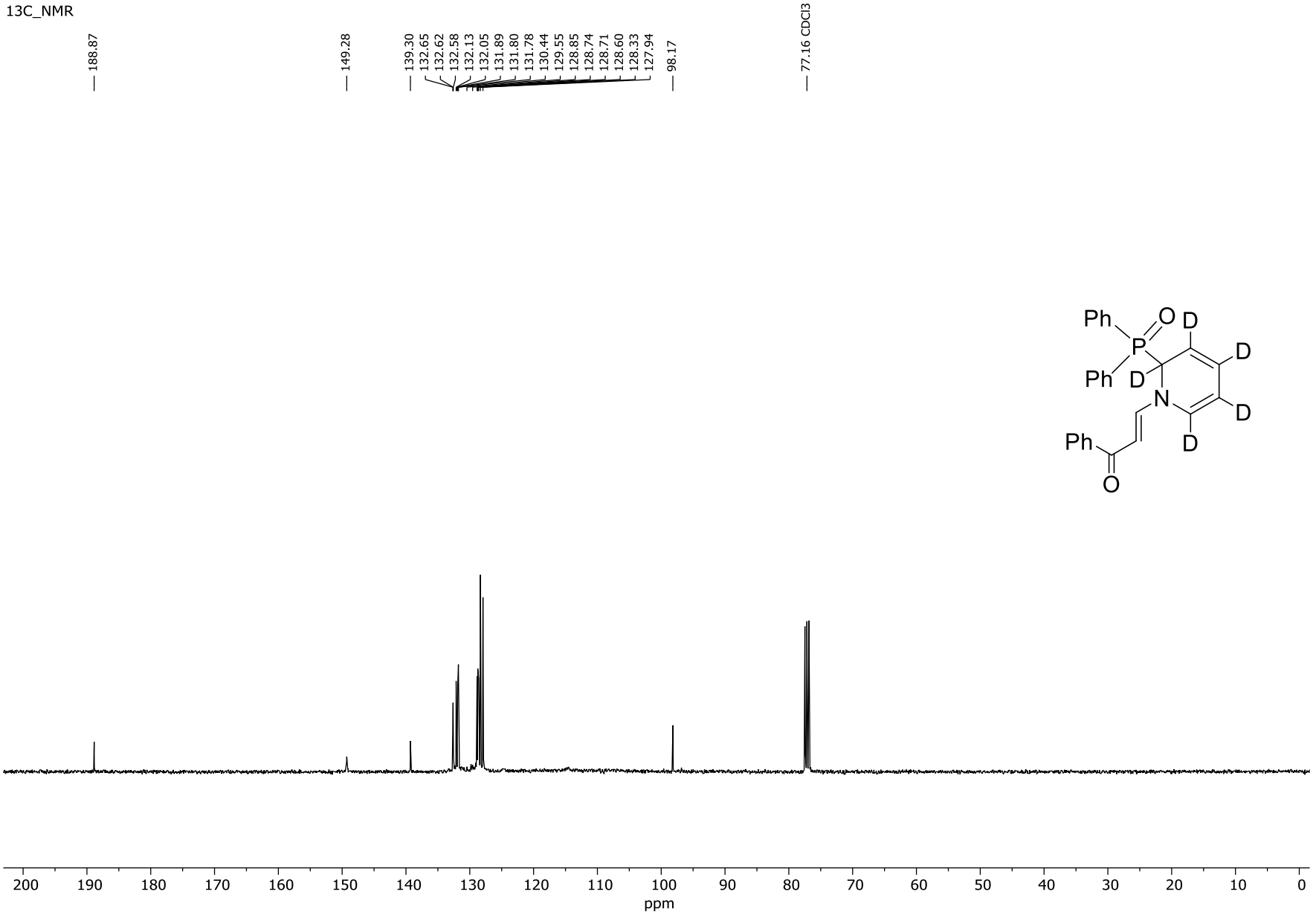

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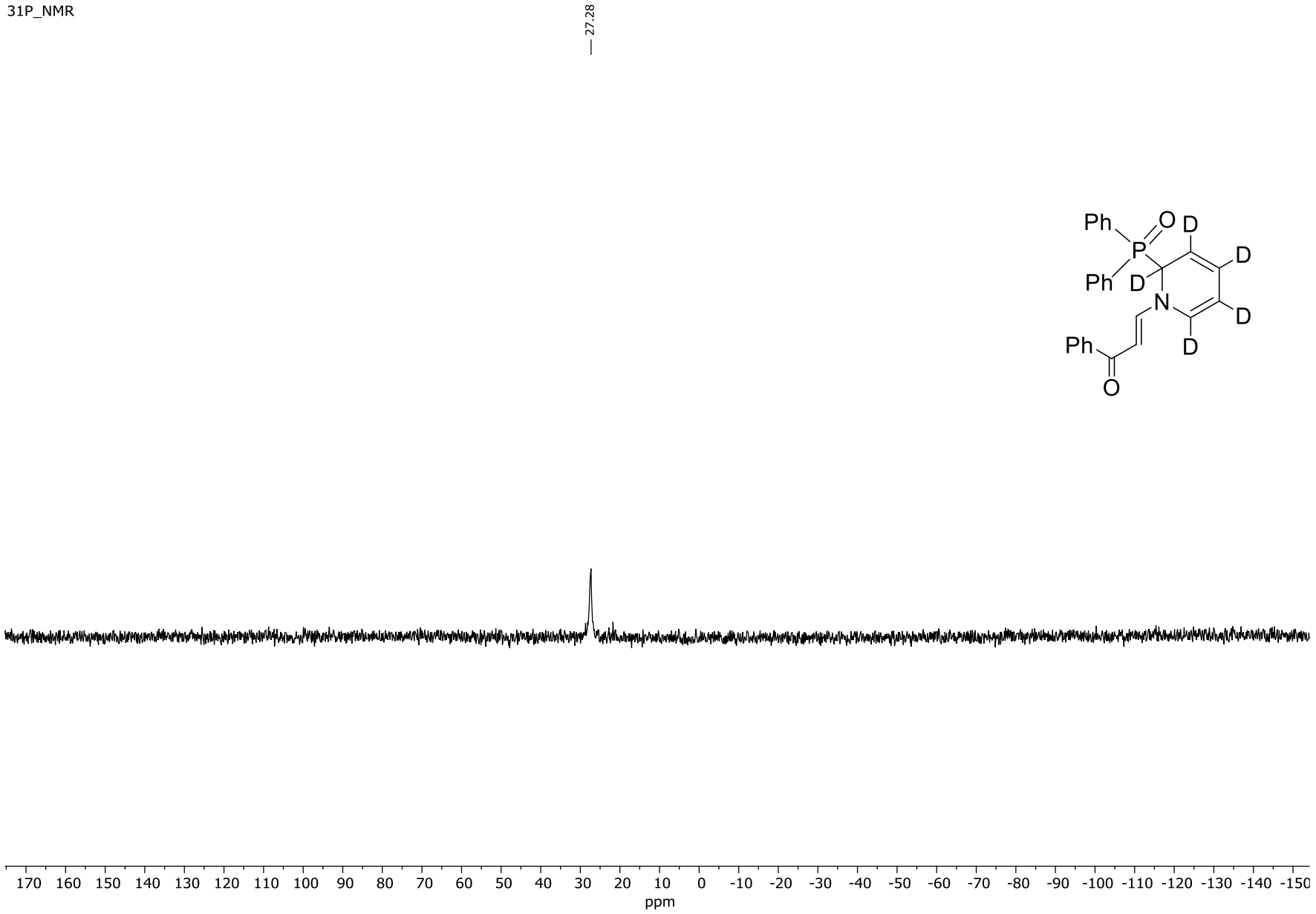
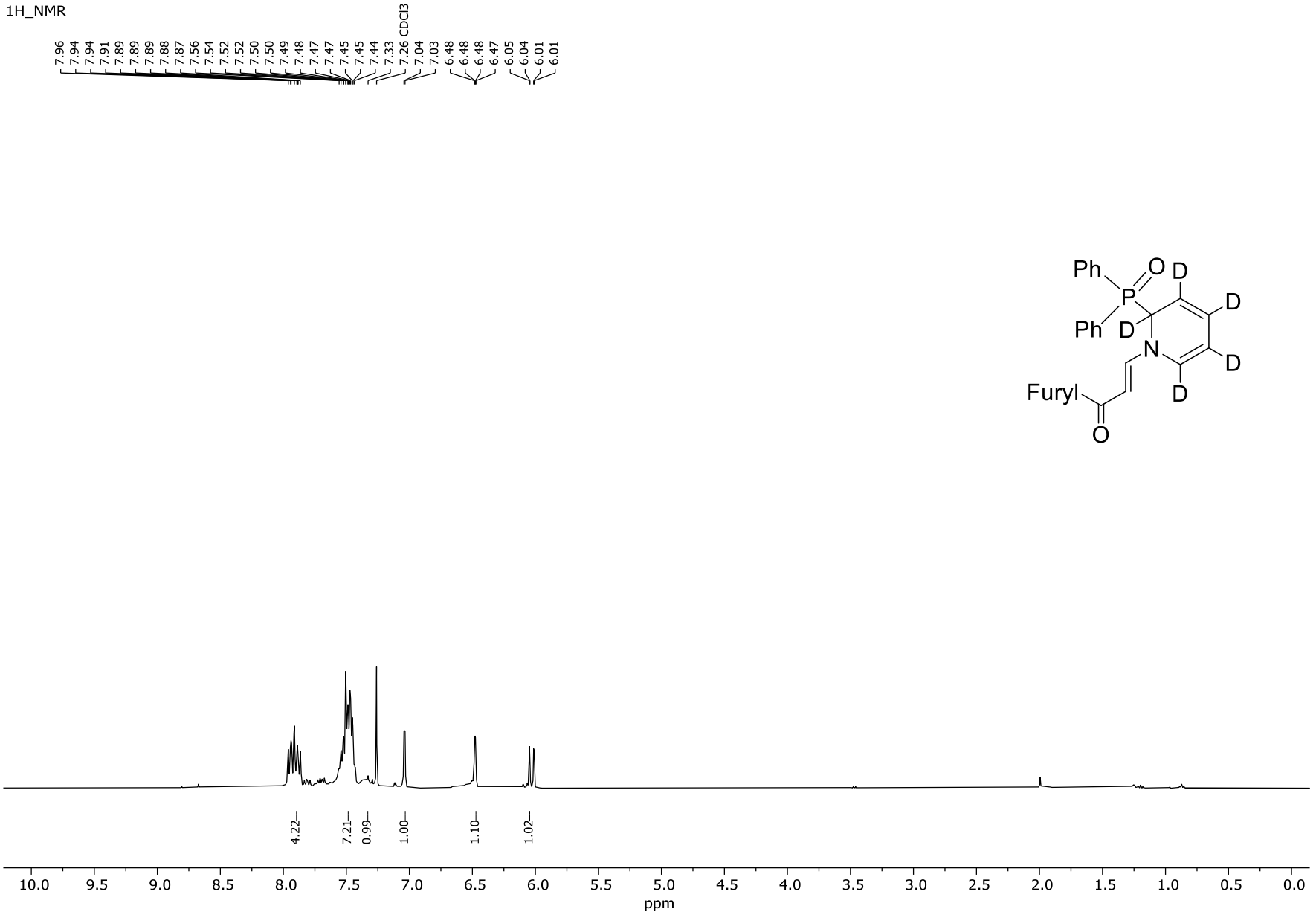
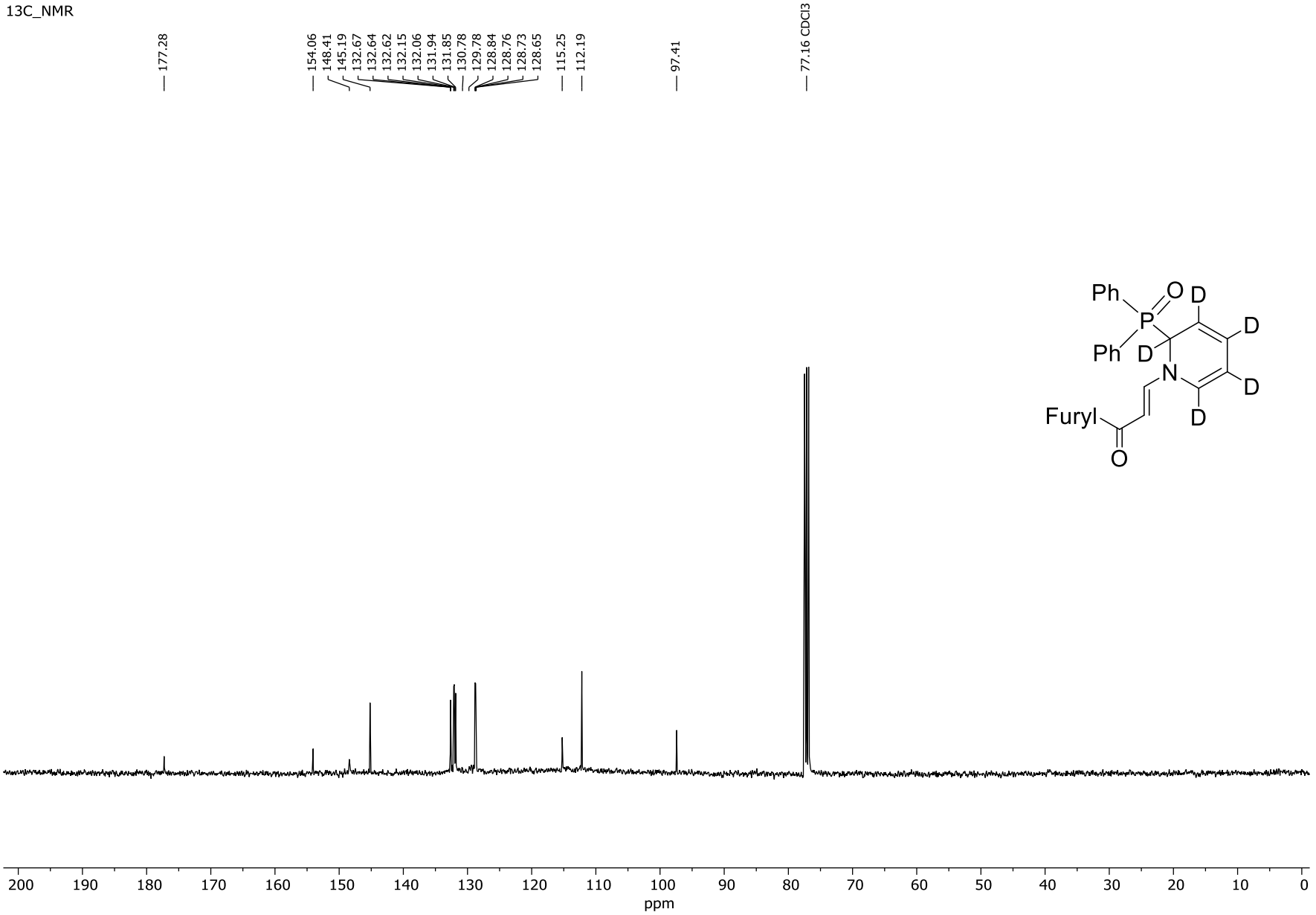


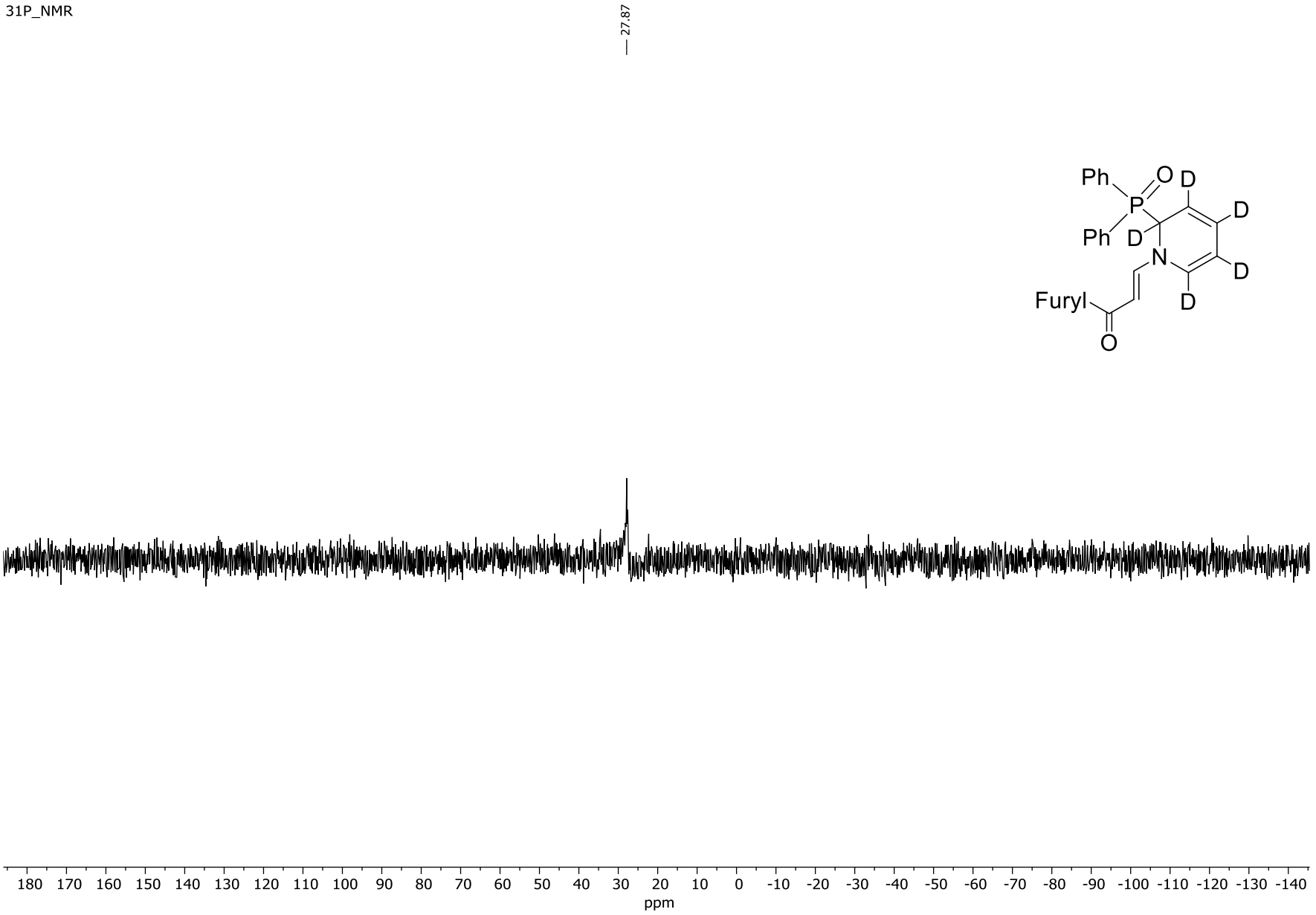
(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (4f)



(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (4f)



(2*E*)-3-[2-(Diphenylphosphoryl)pyridin-1(2*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (4f)



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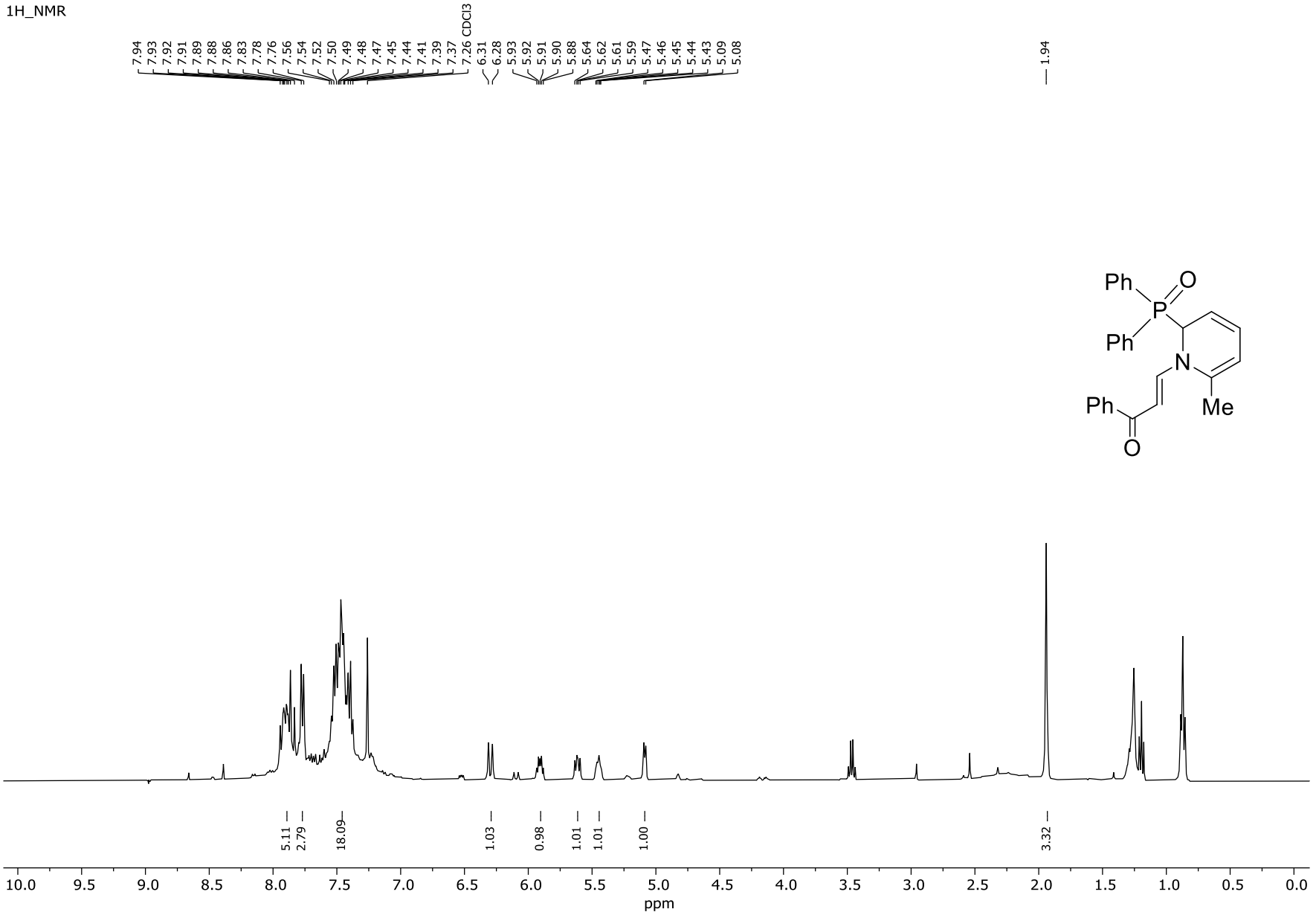
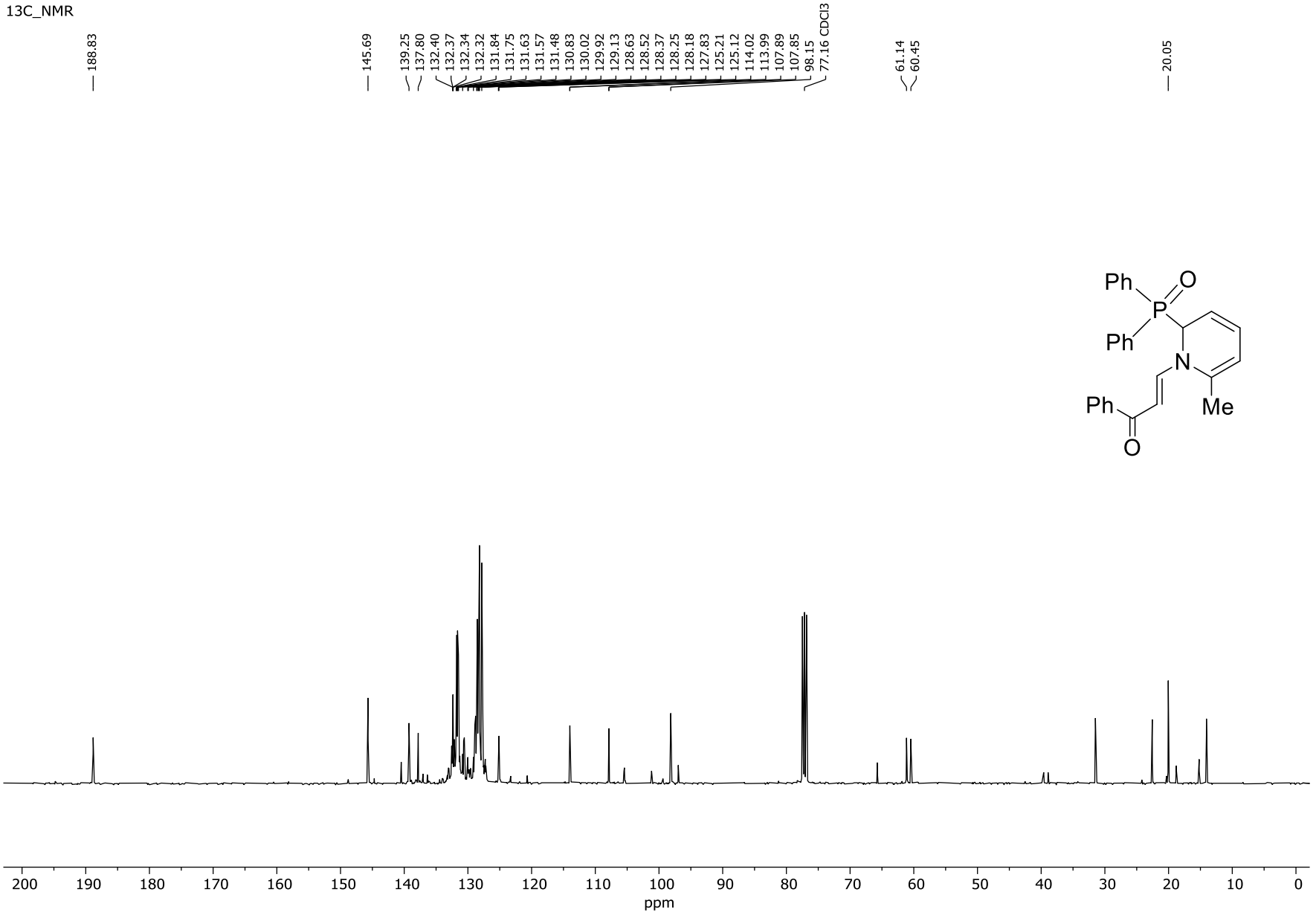


(2*E*)-3-[2-(Diphenylphosphoryl)-6-methylpyridin-1(2*H*)-yl]-1-phenylprop-2-en-1-one (4g)



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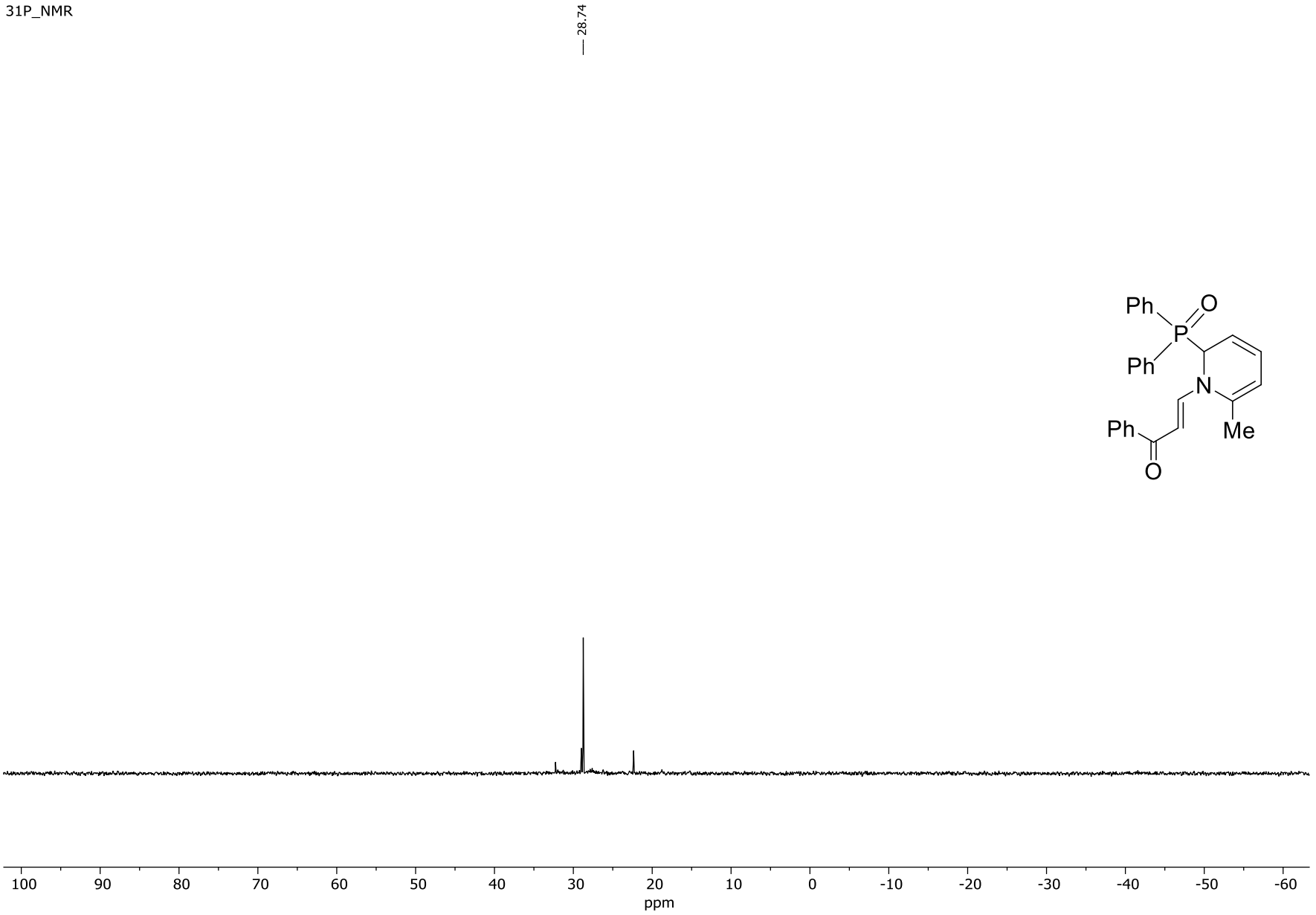

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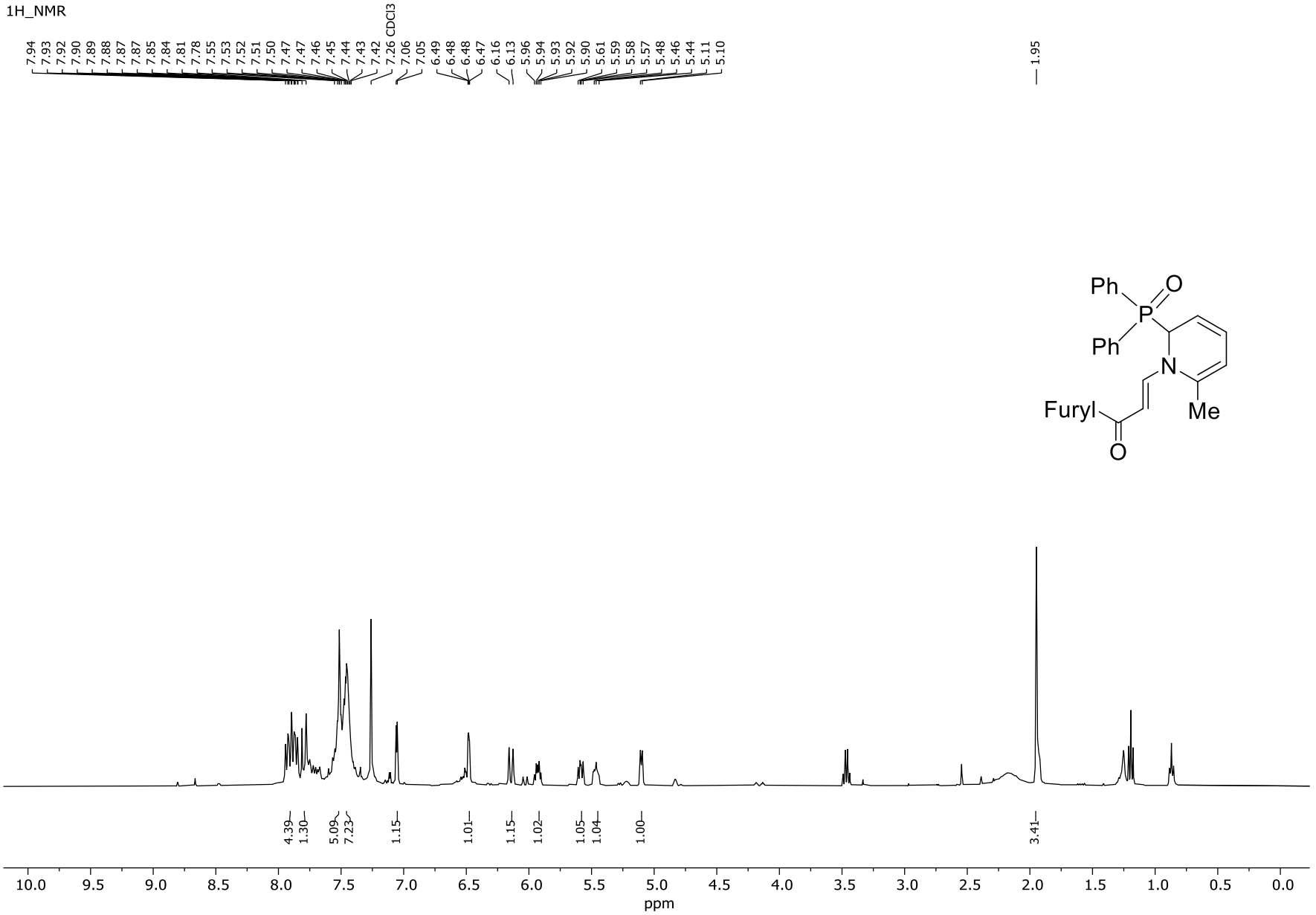

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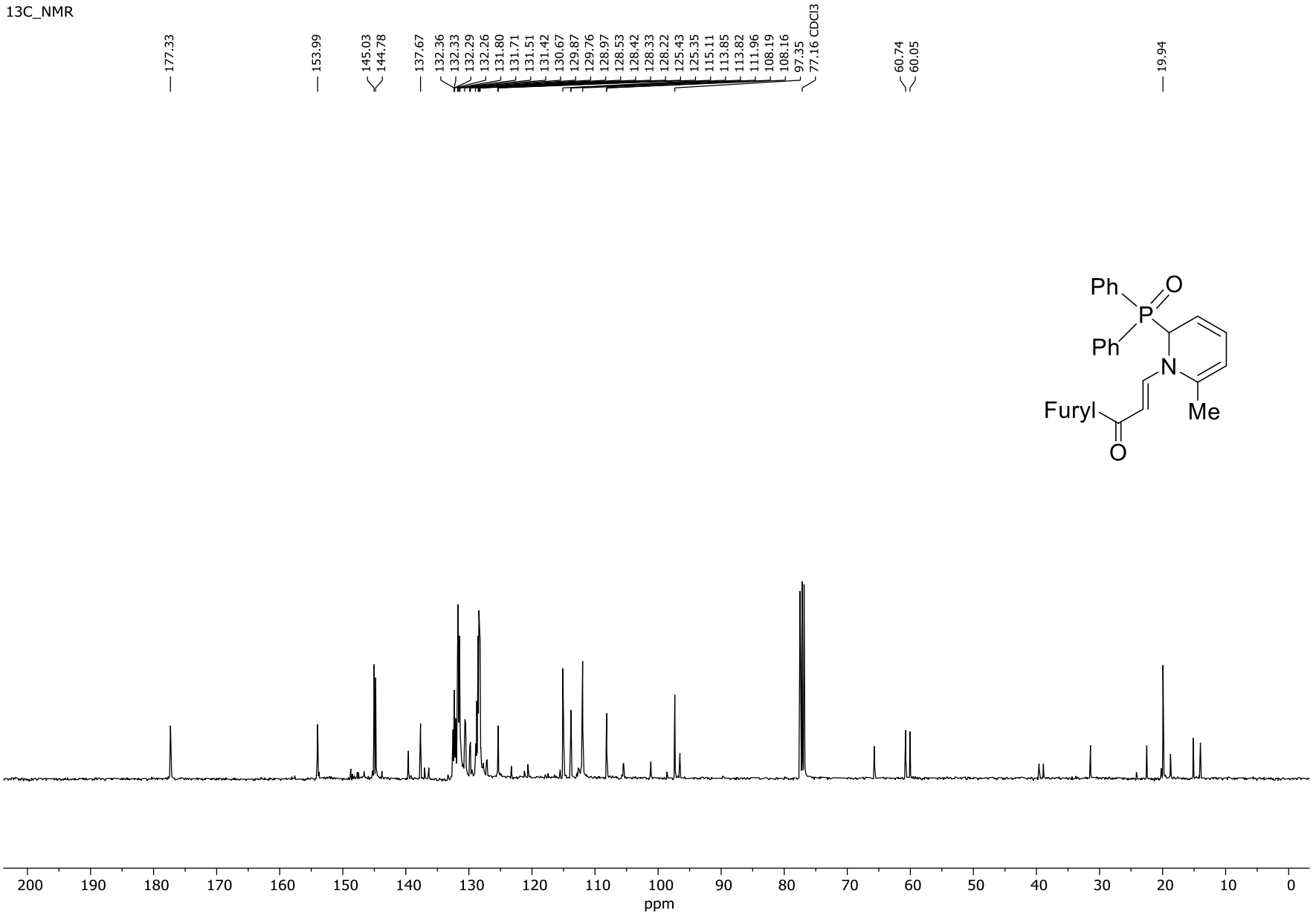

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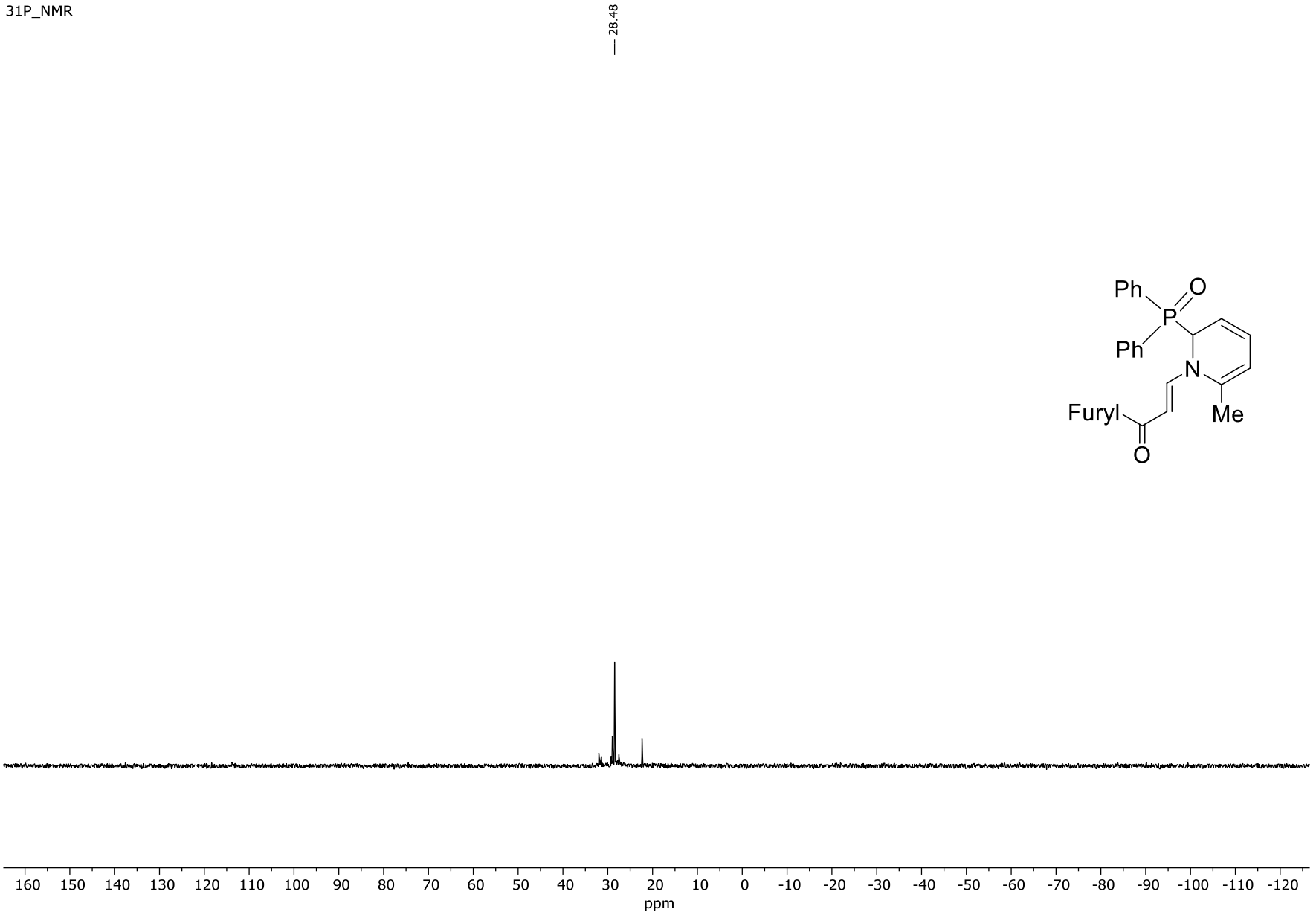

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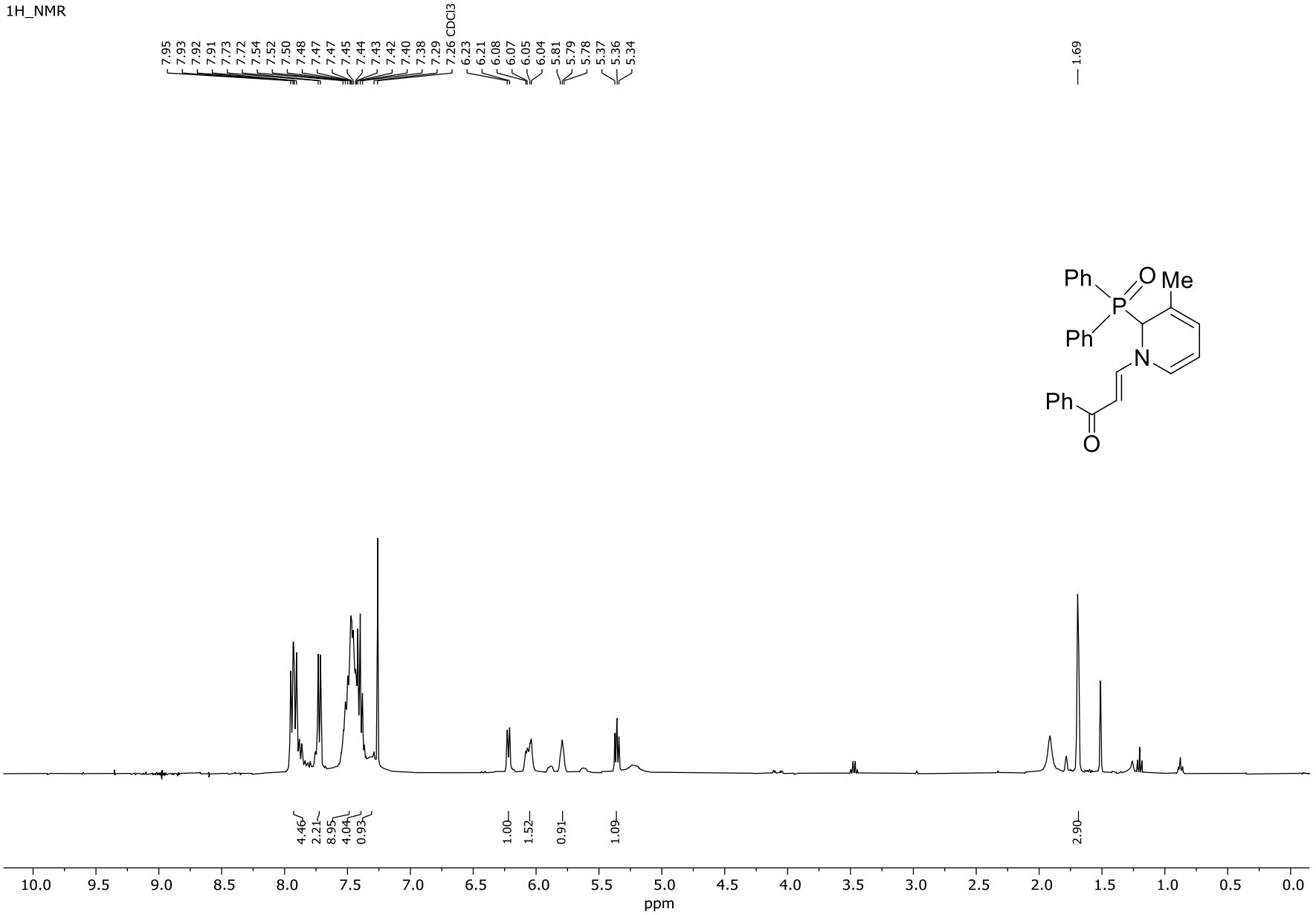

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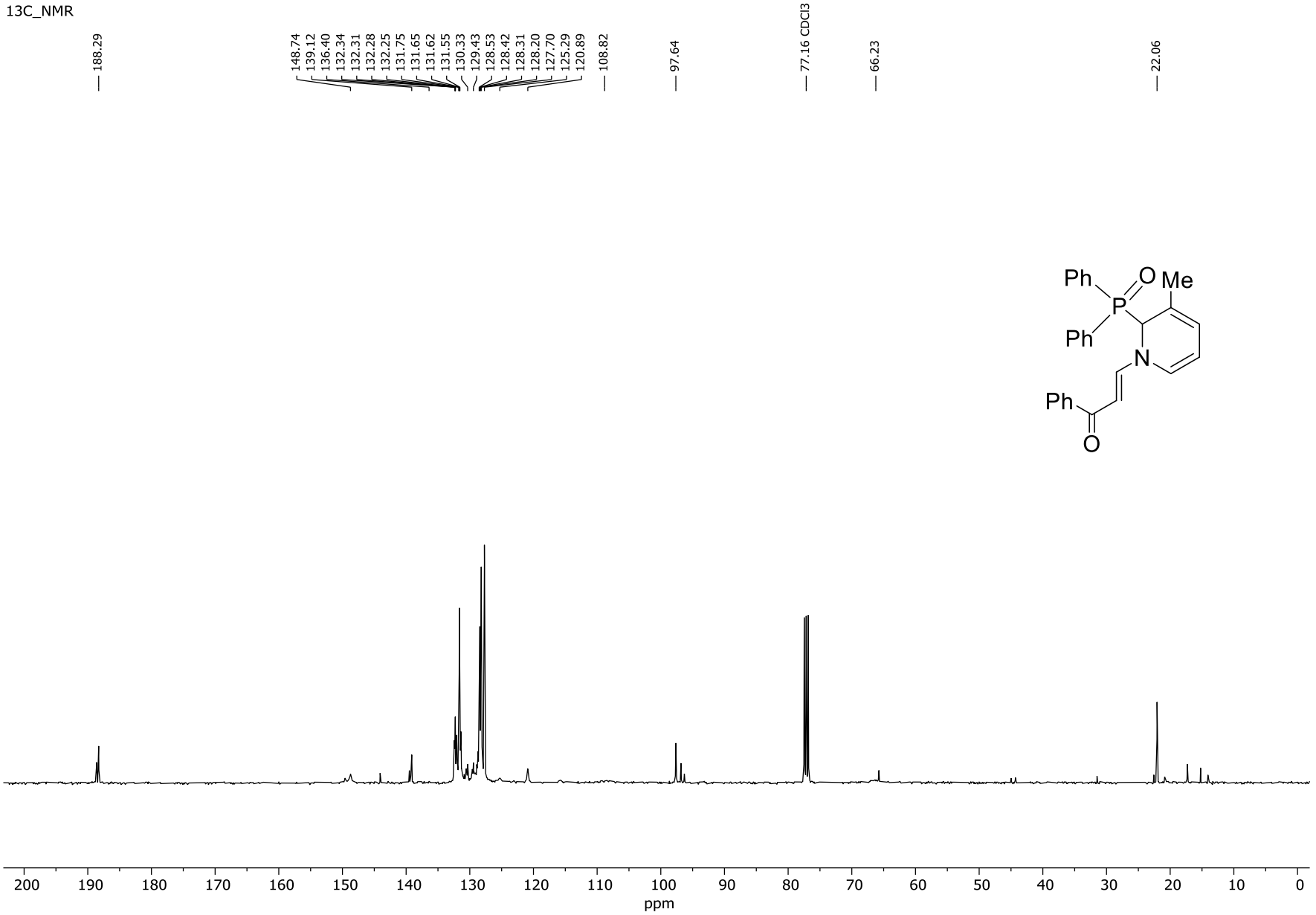

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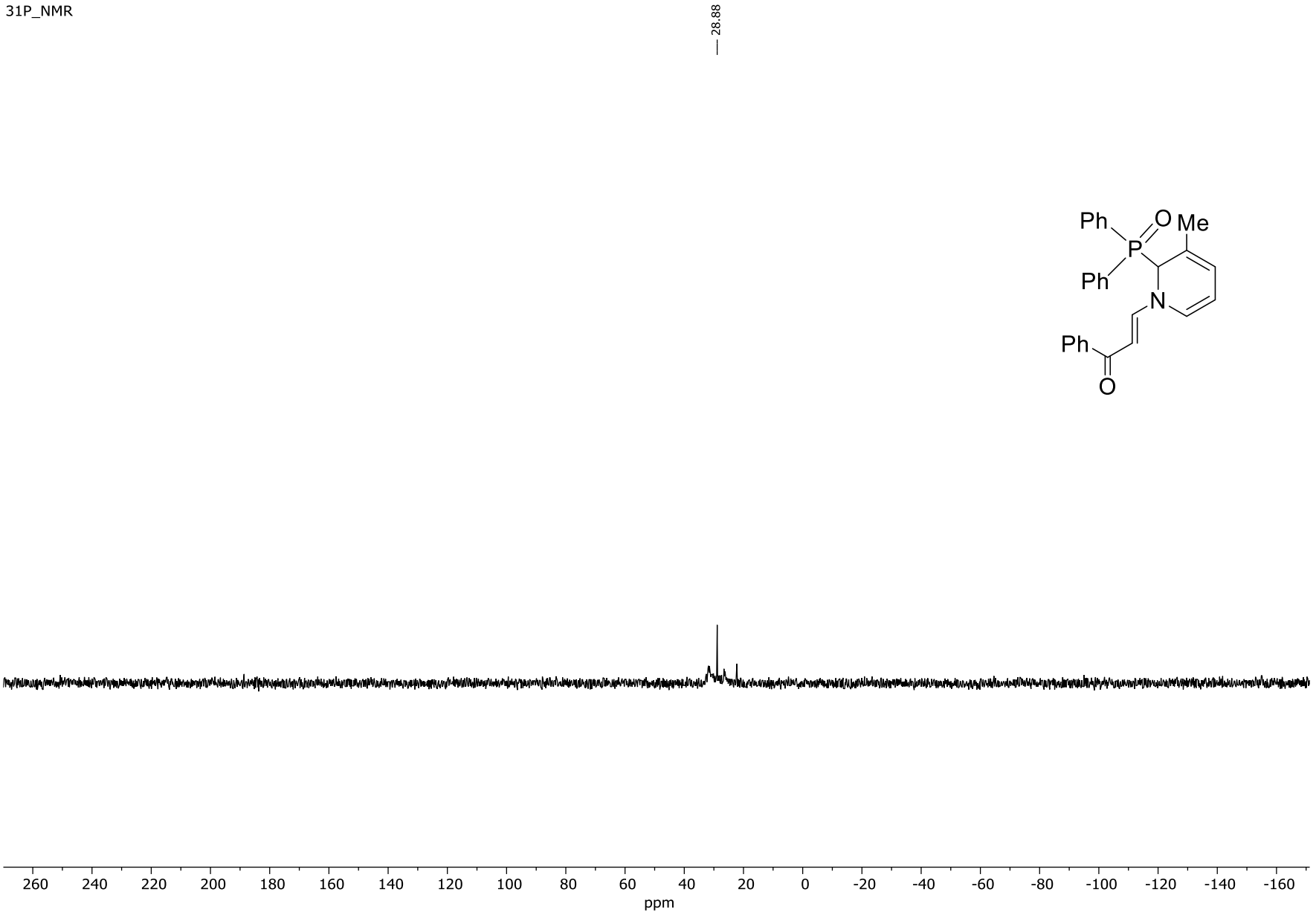
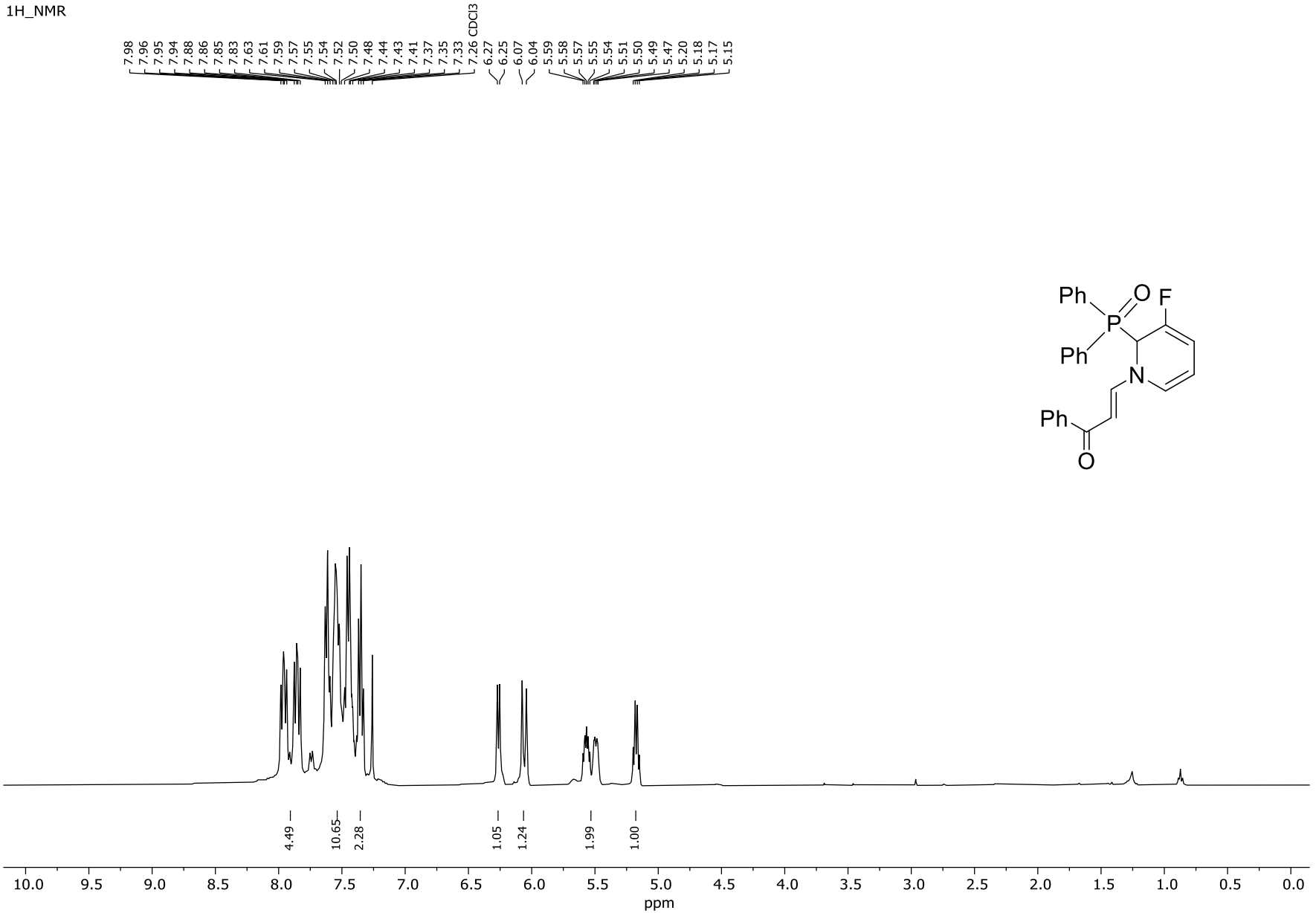


(2*E*)-3-[2-(Diphenylphosphoryl)-3-fluoropyridin-1(2*H*)-yl]-1-phenylprop-2-en-1-one (4j)



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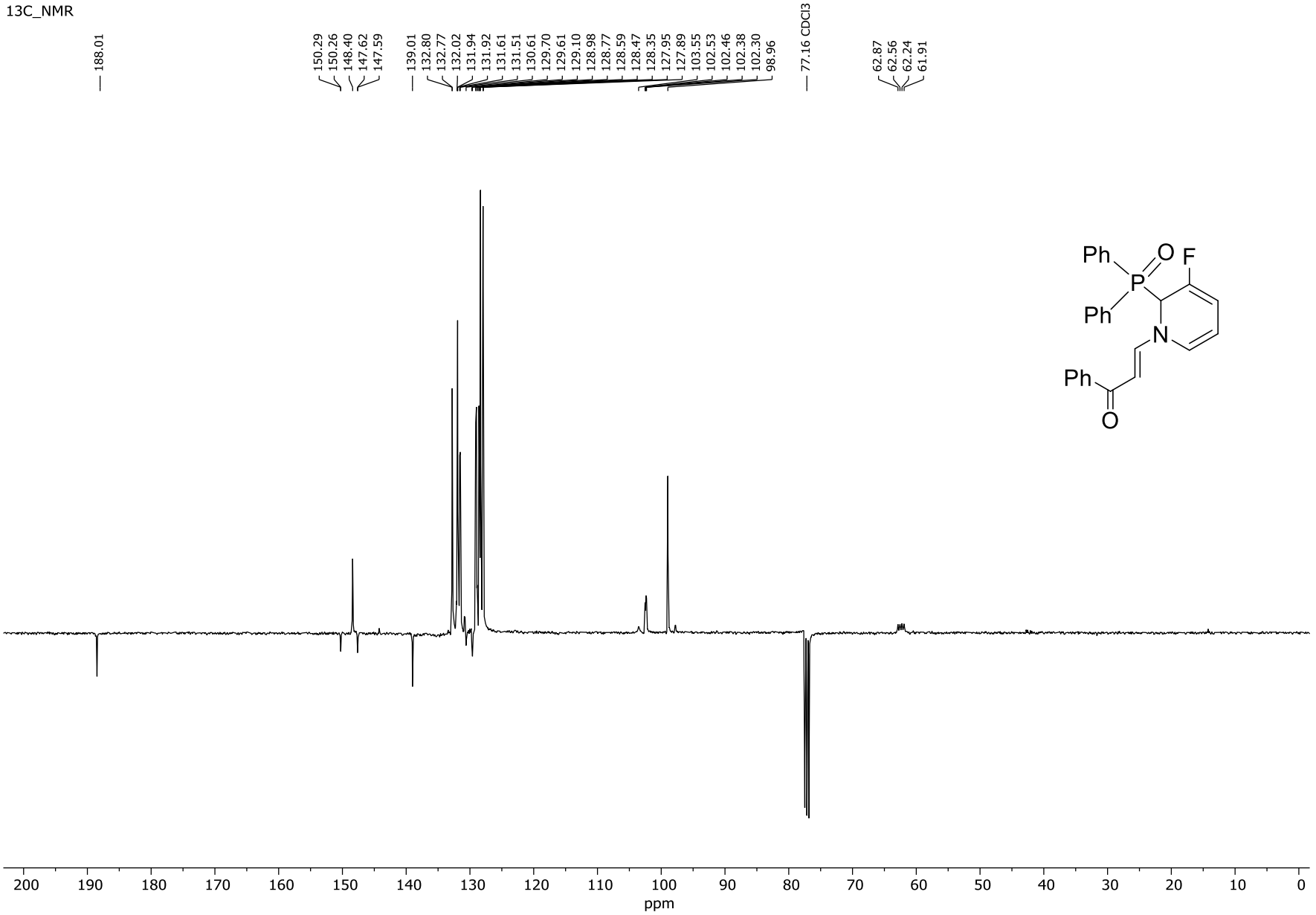

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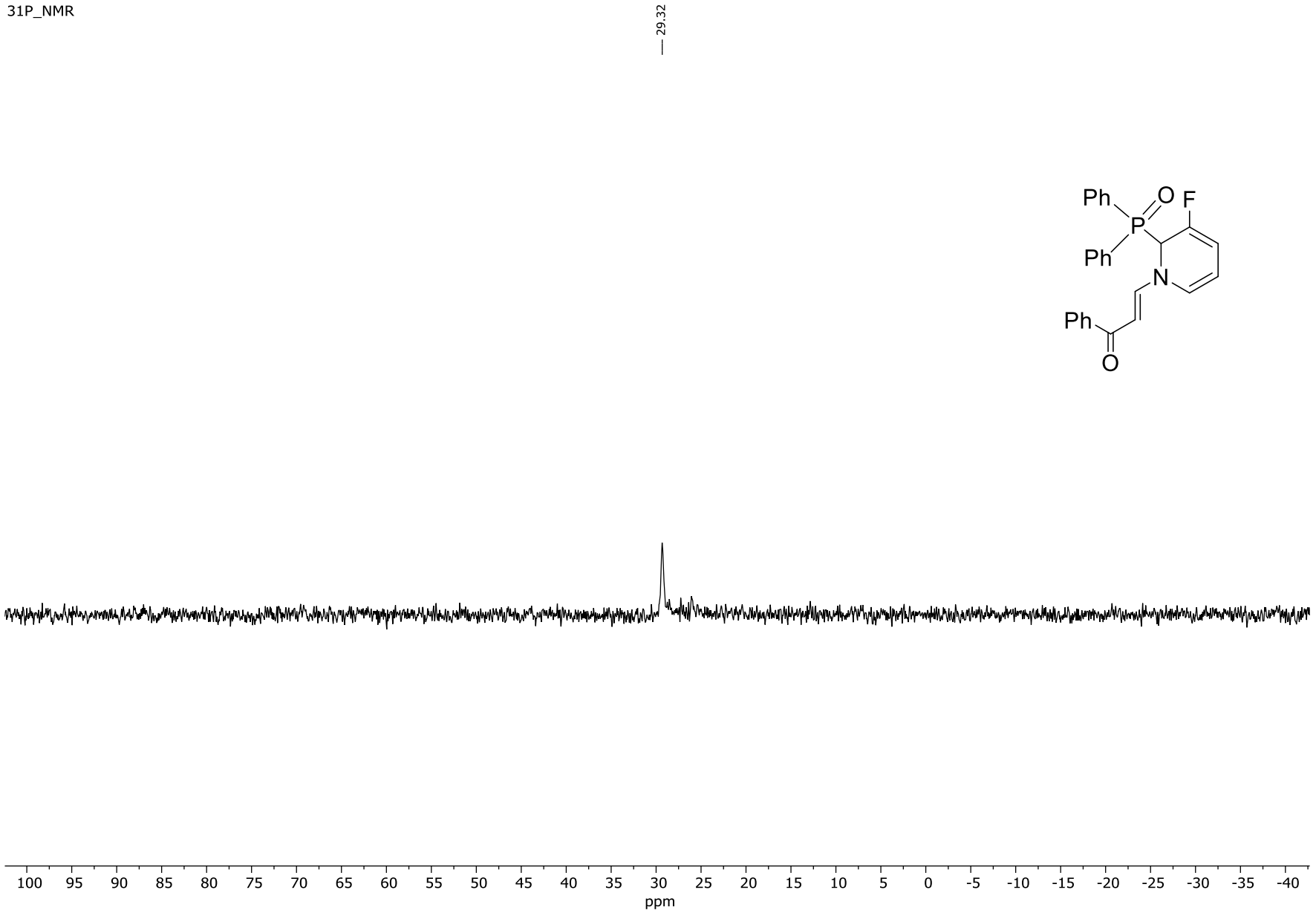

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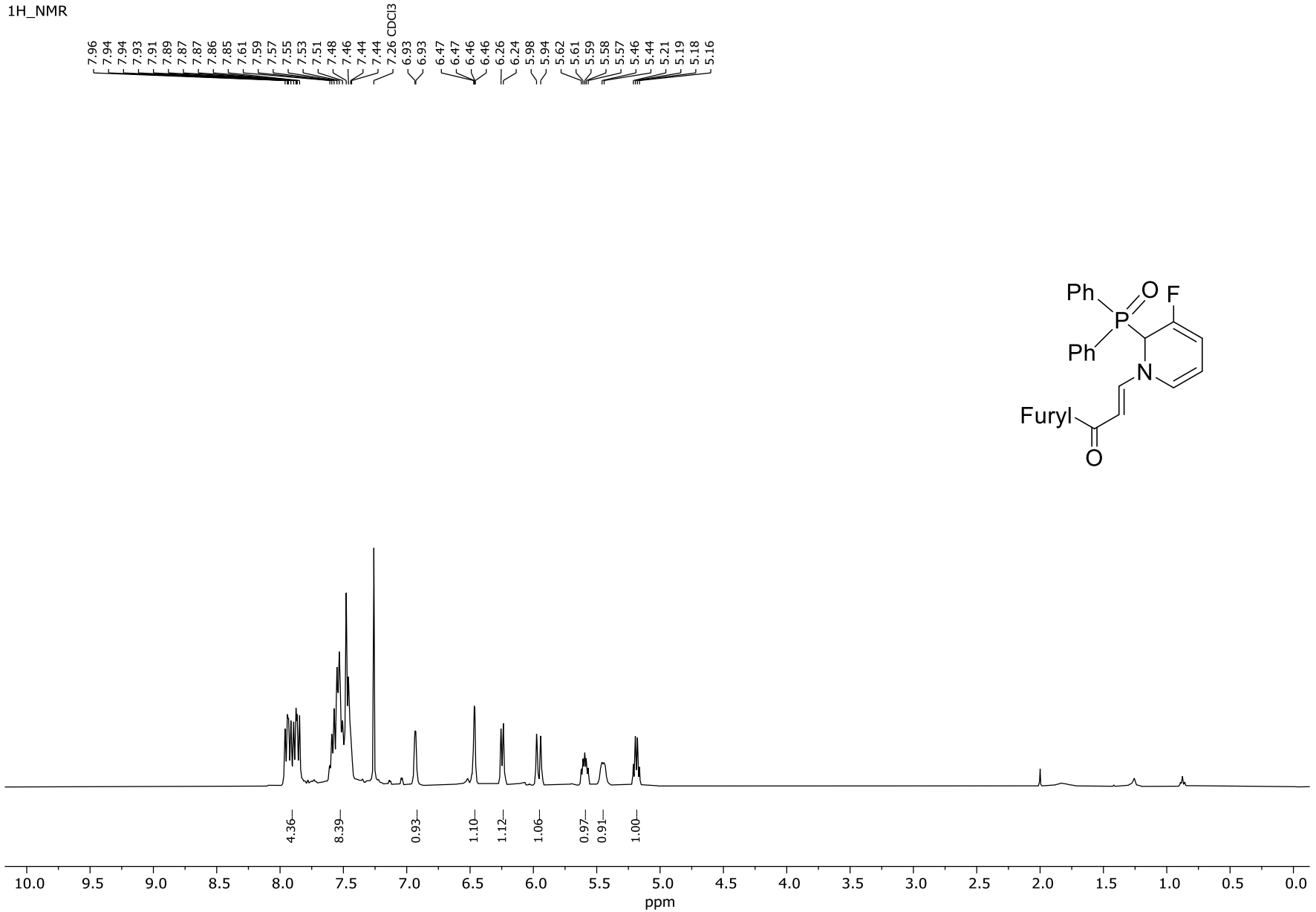

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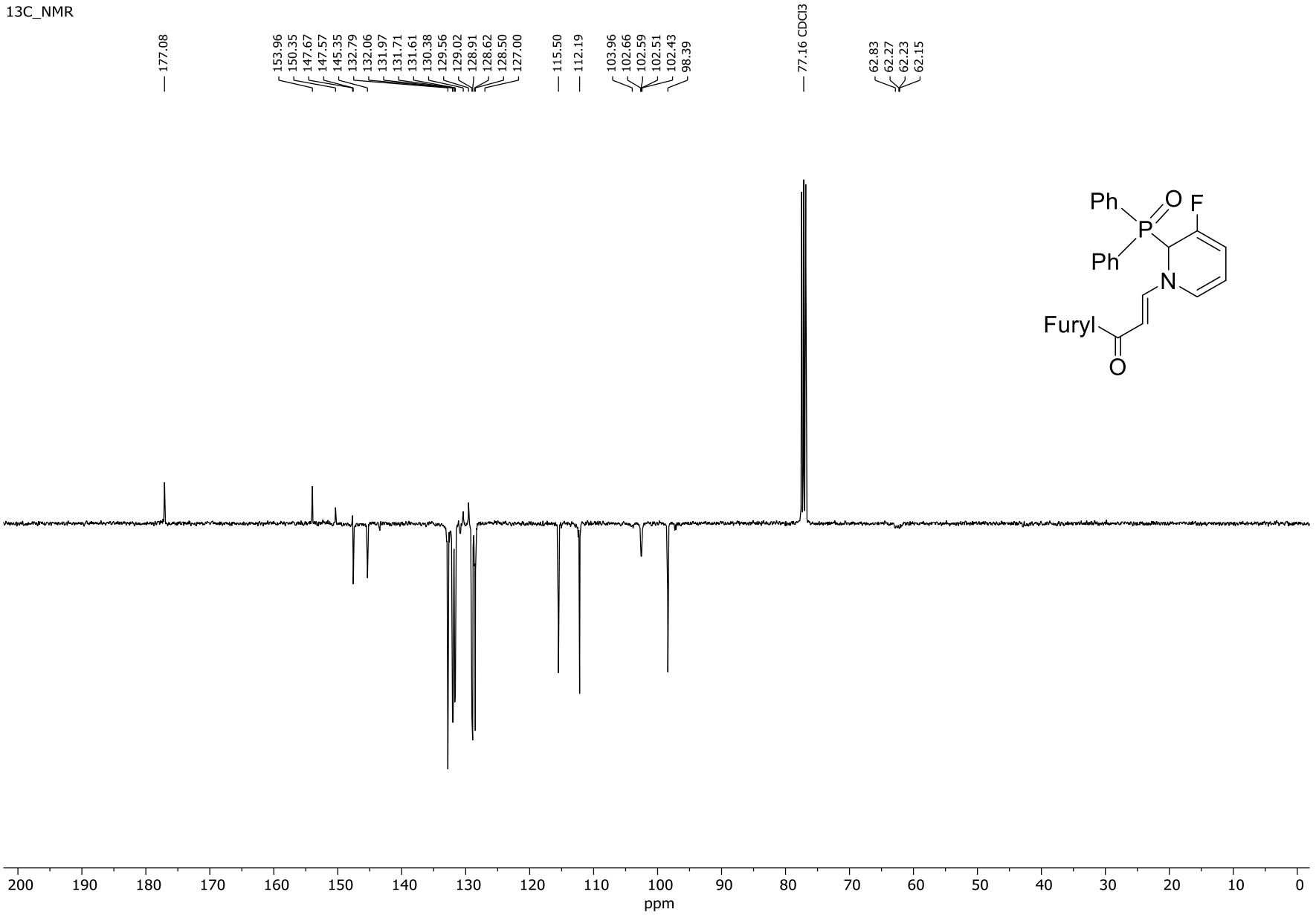

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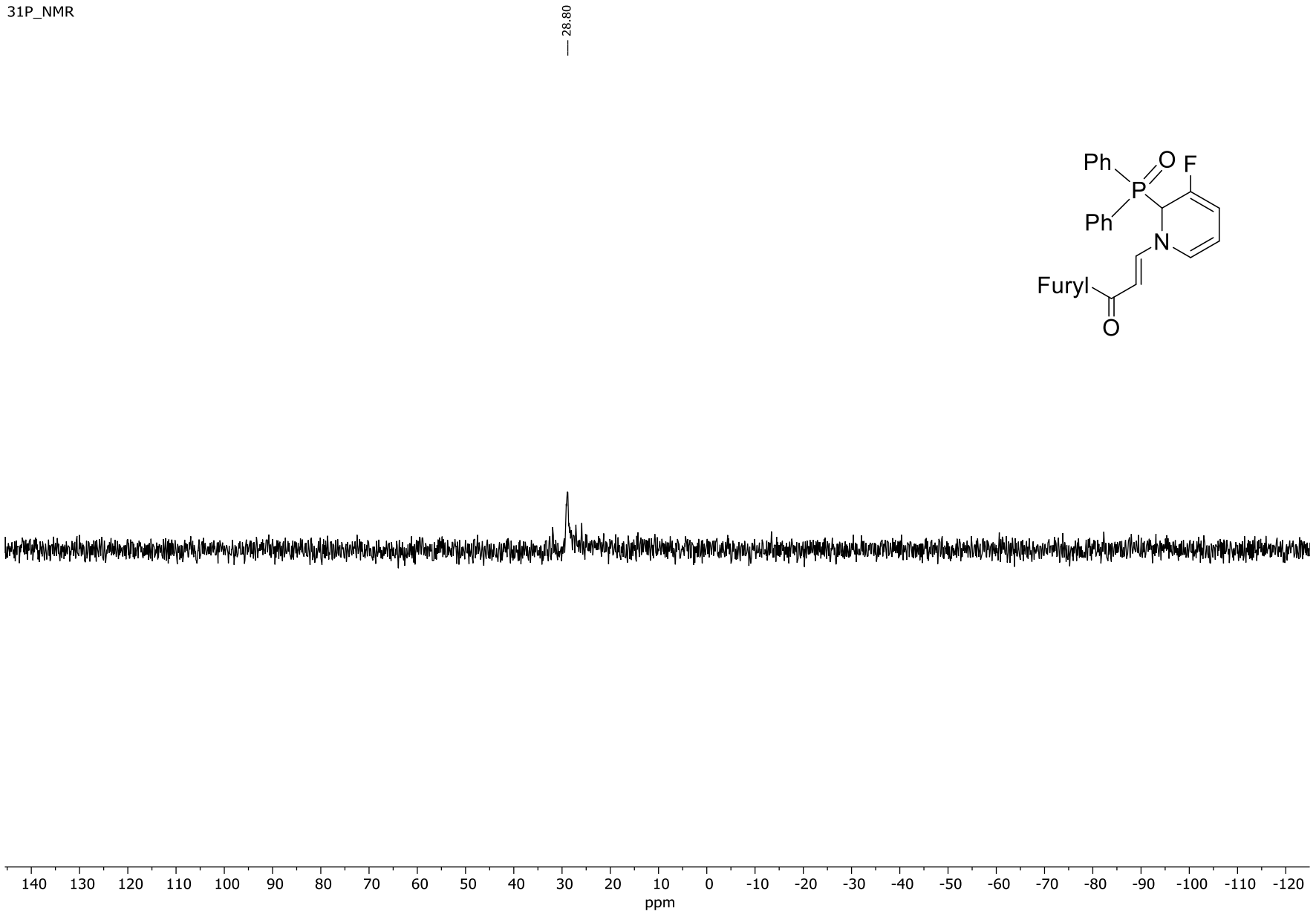
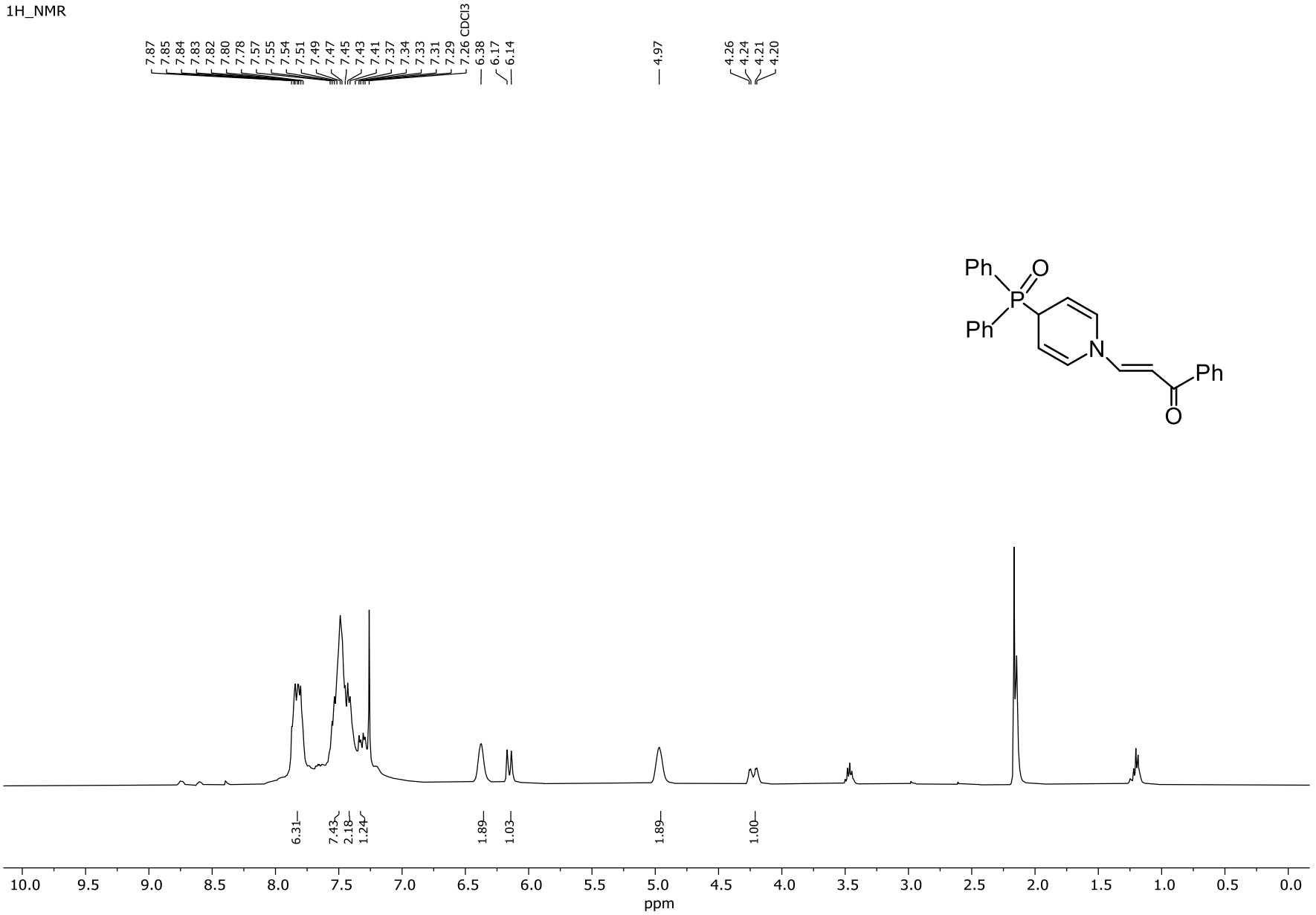


(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5a)



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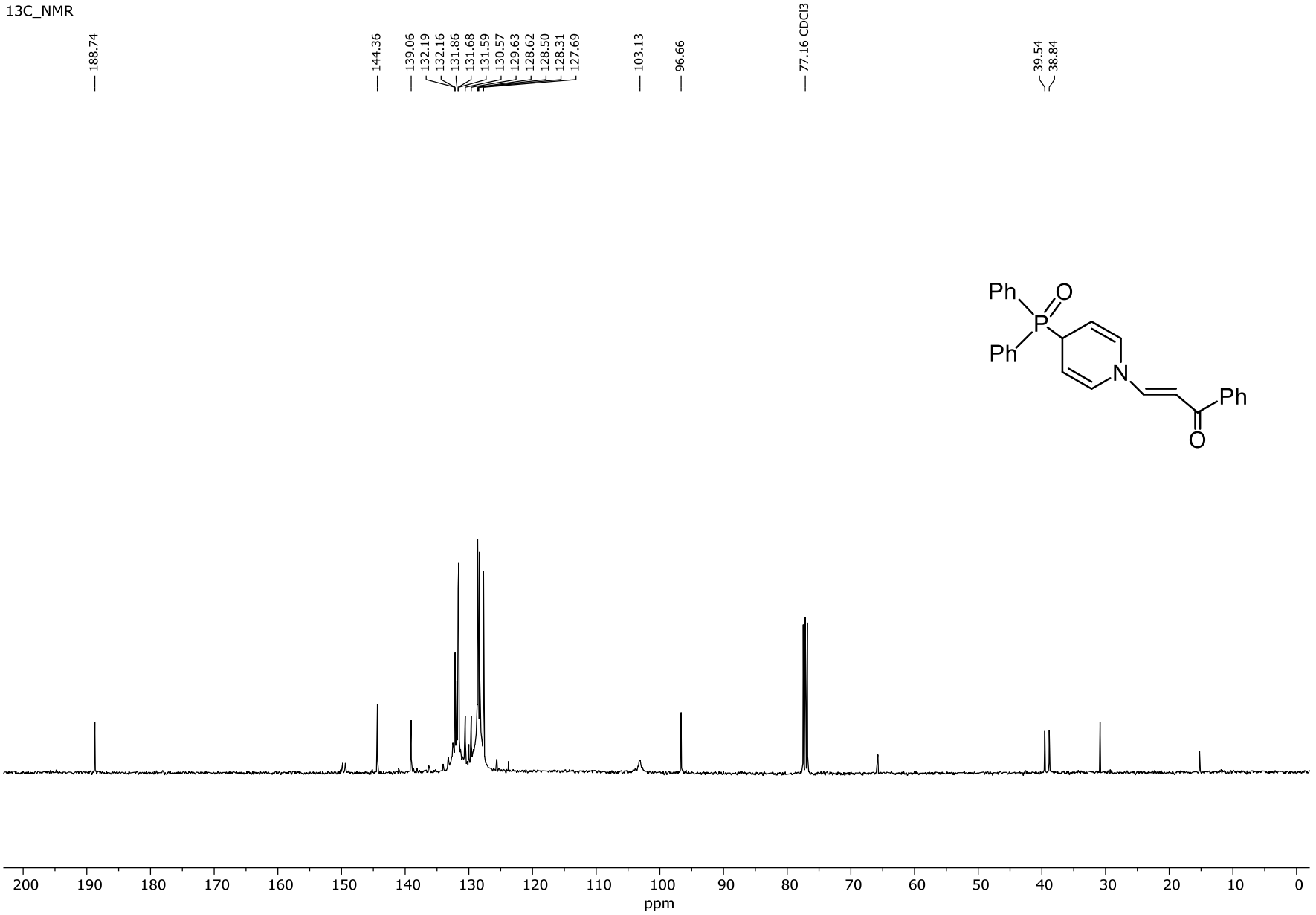
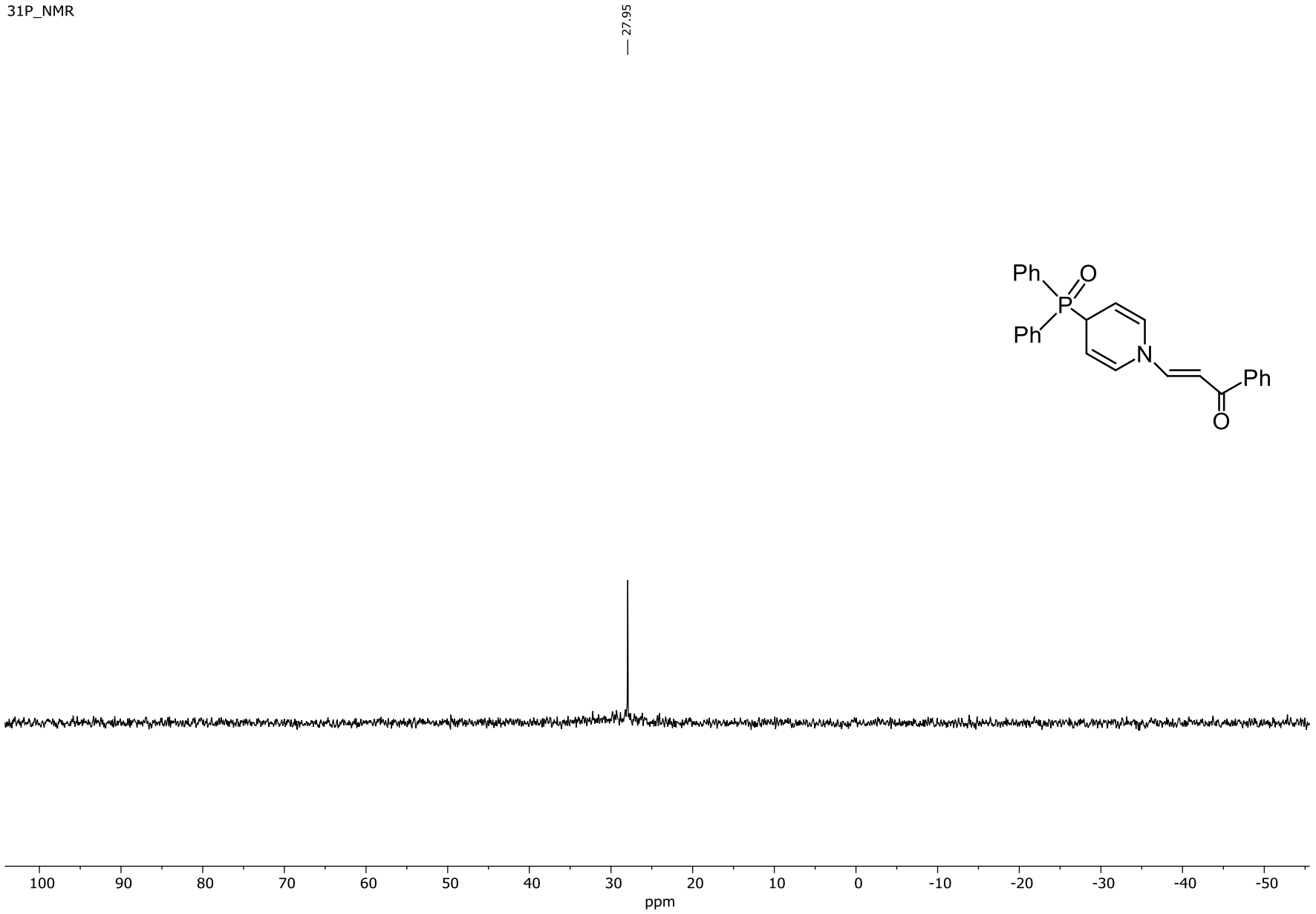
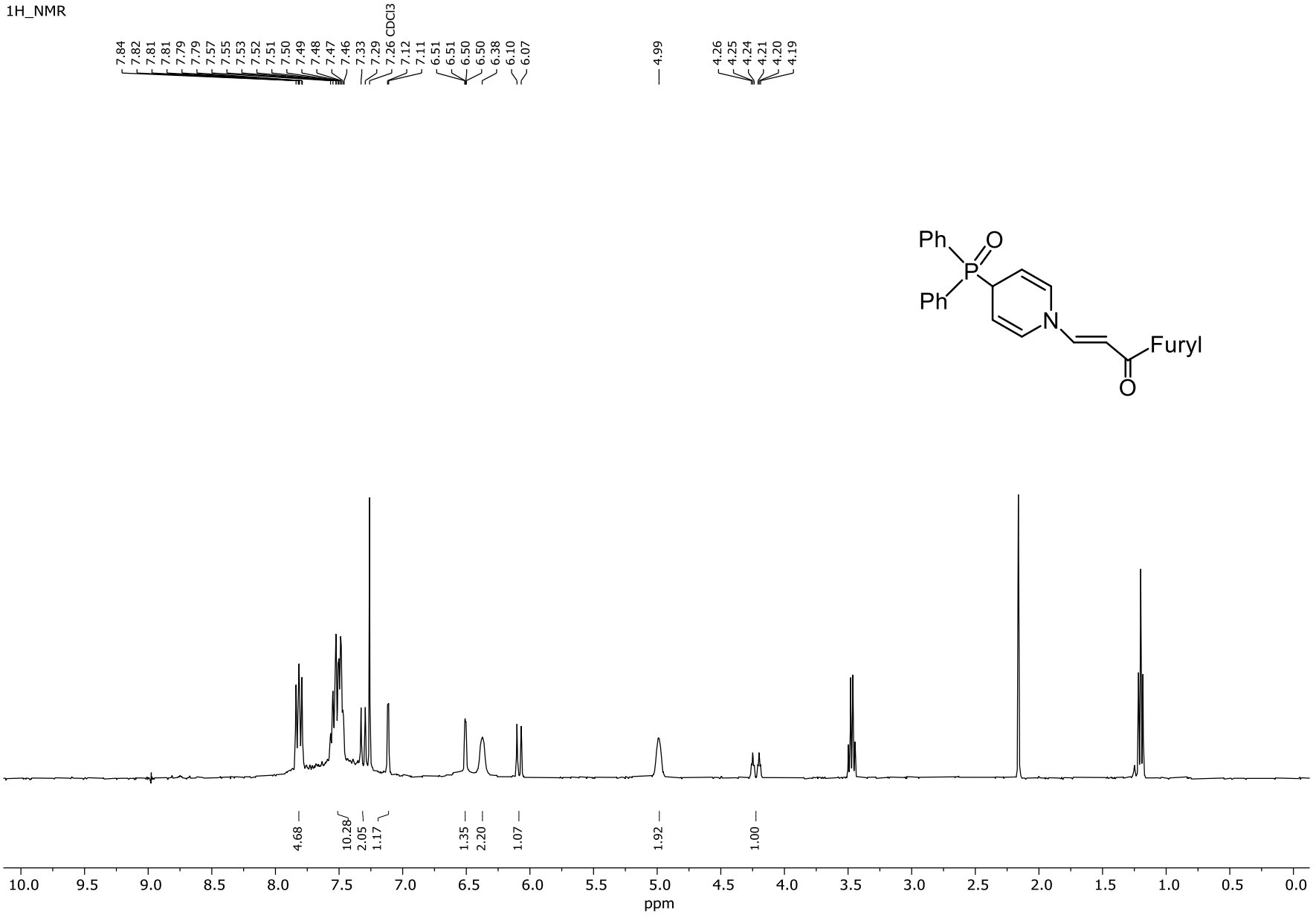


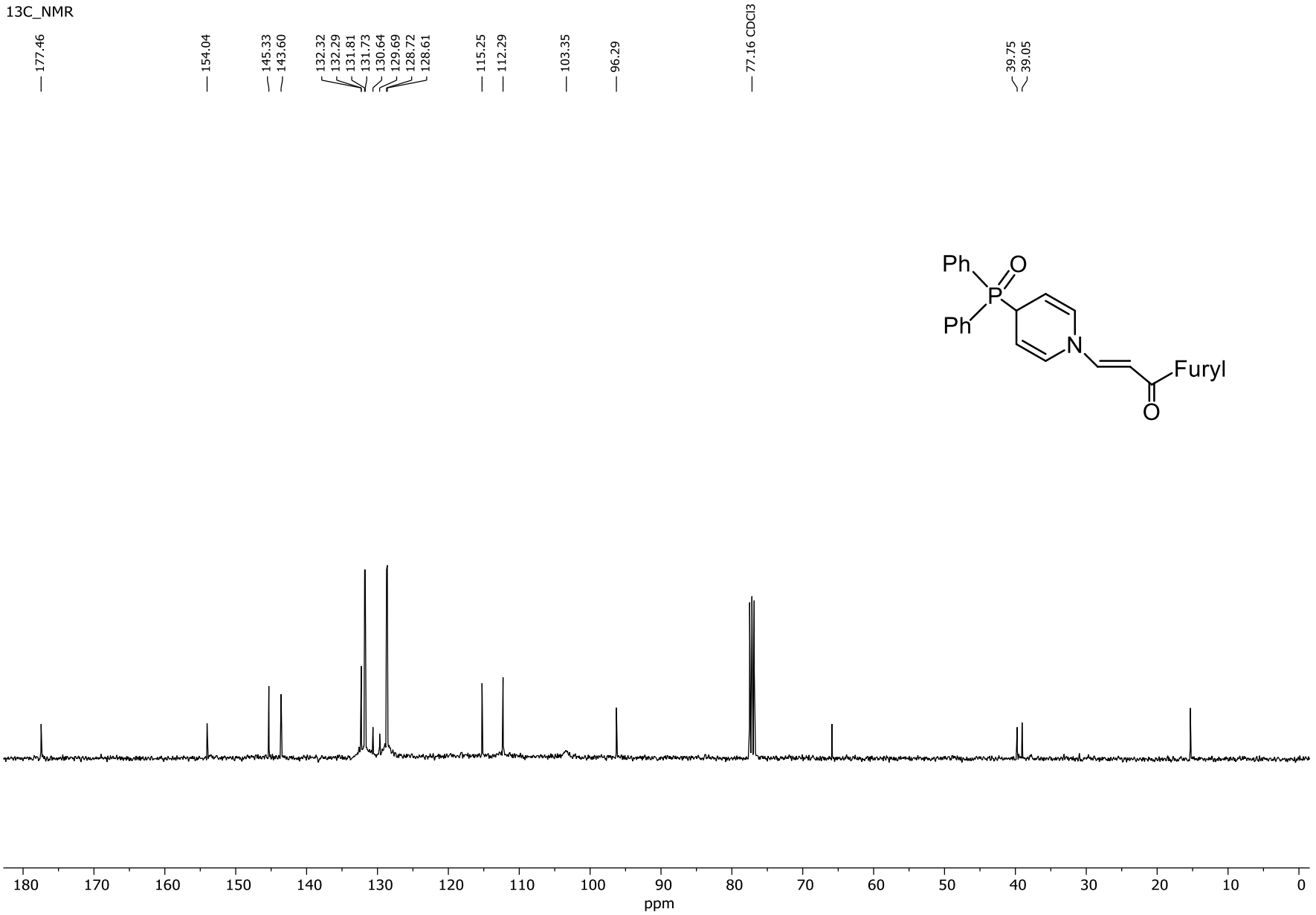
(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5a)



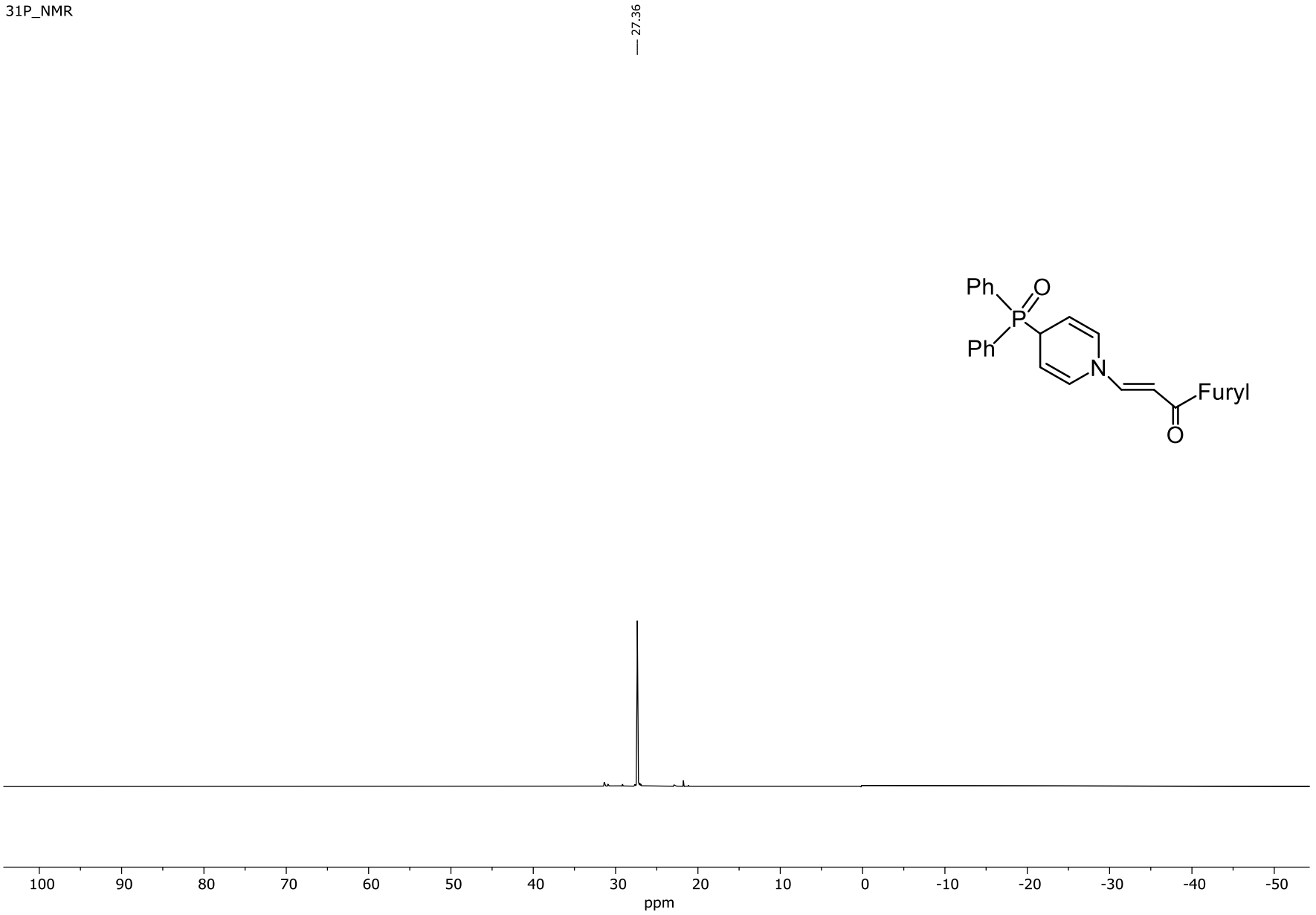
(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5b)



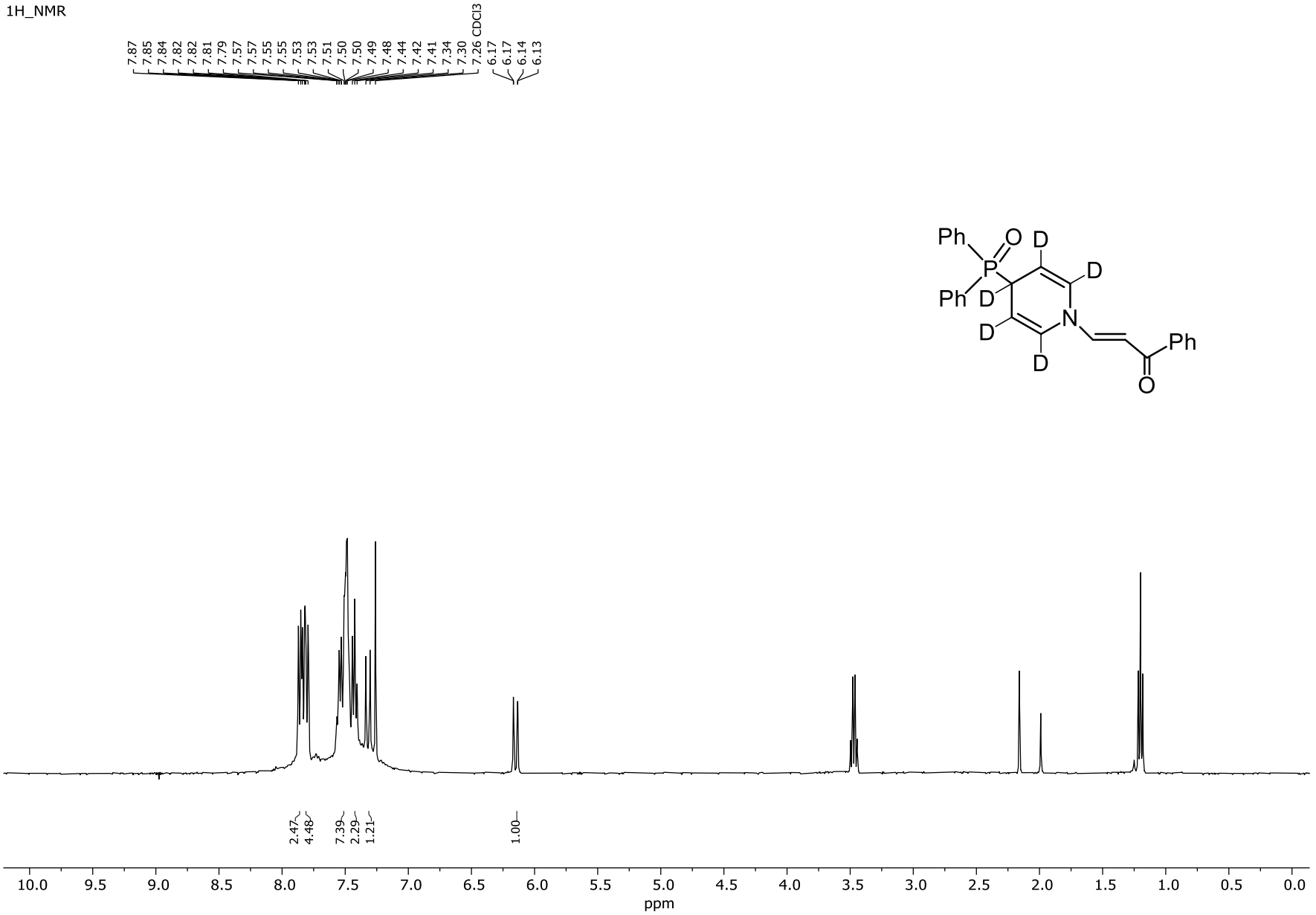
(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5b)



(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5b)



(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (5c)



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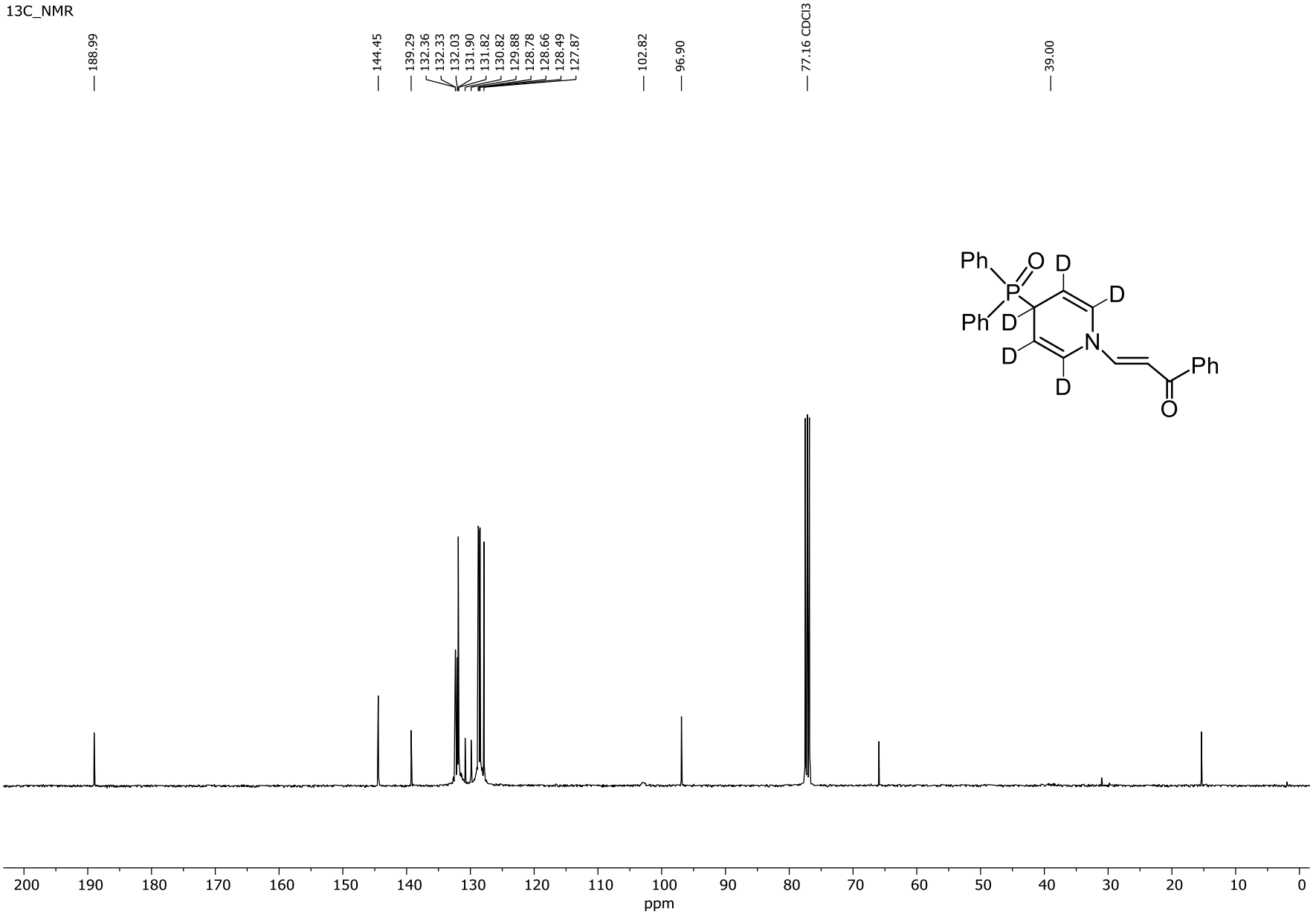
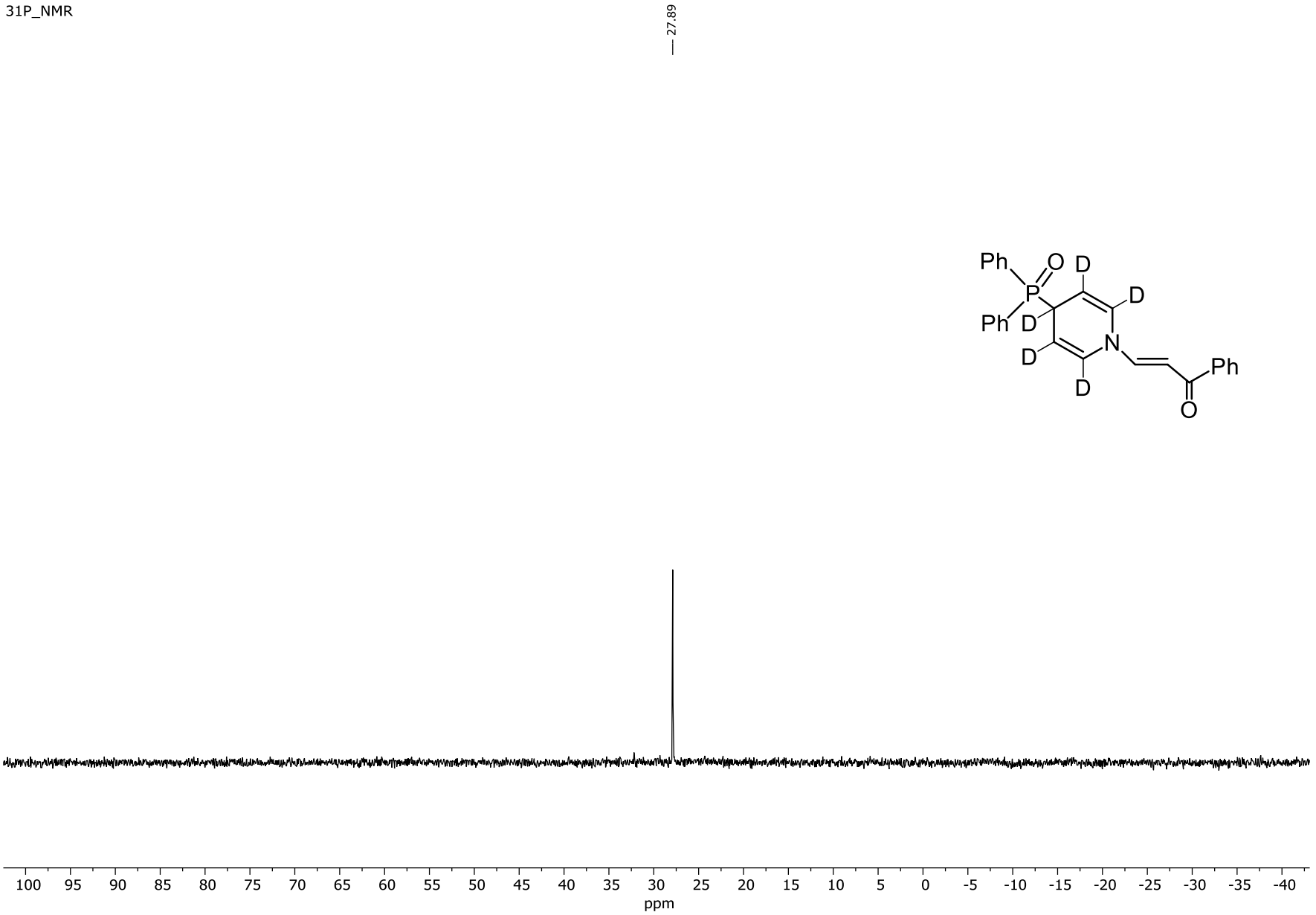
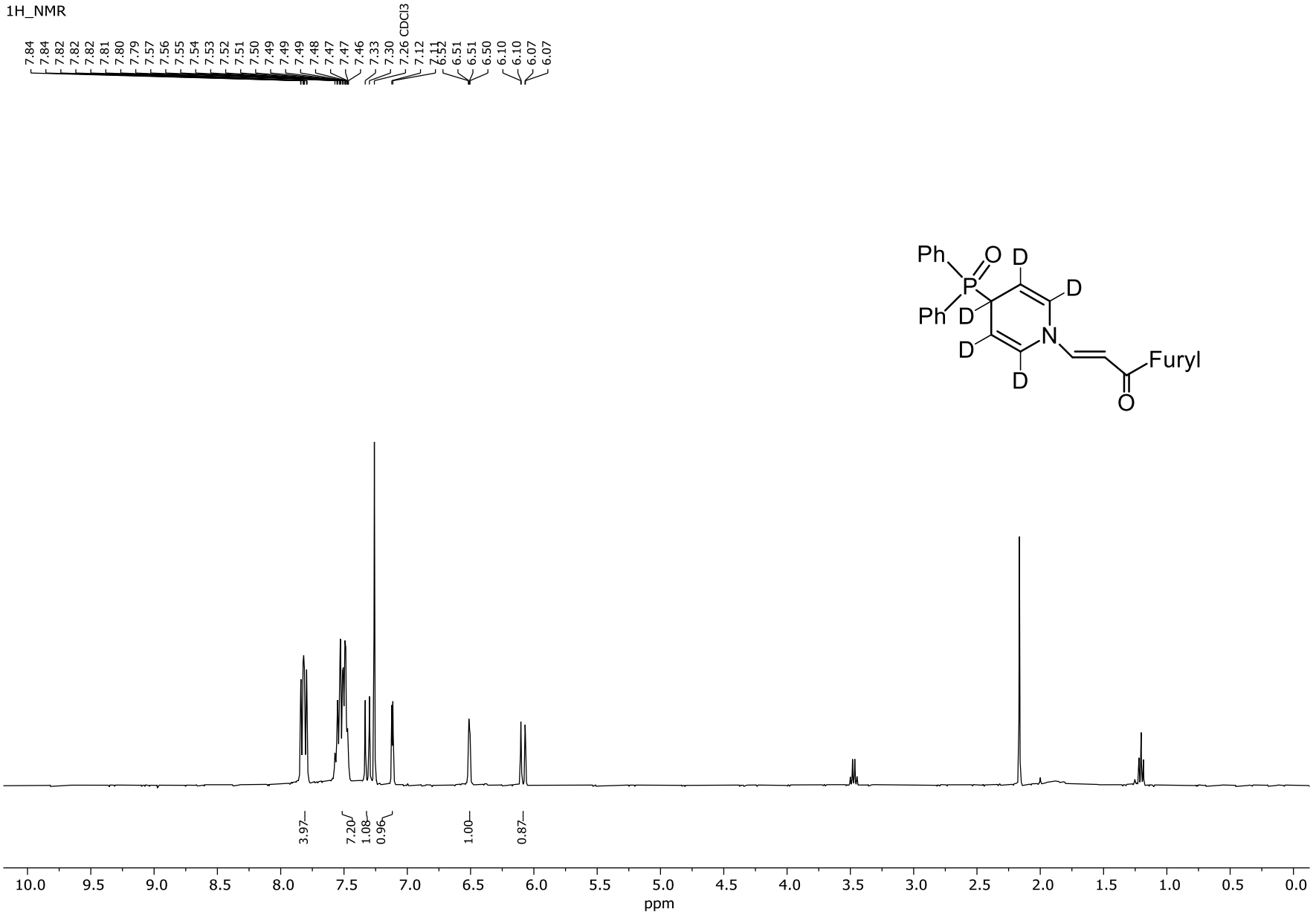


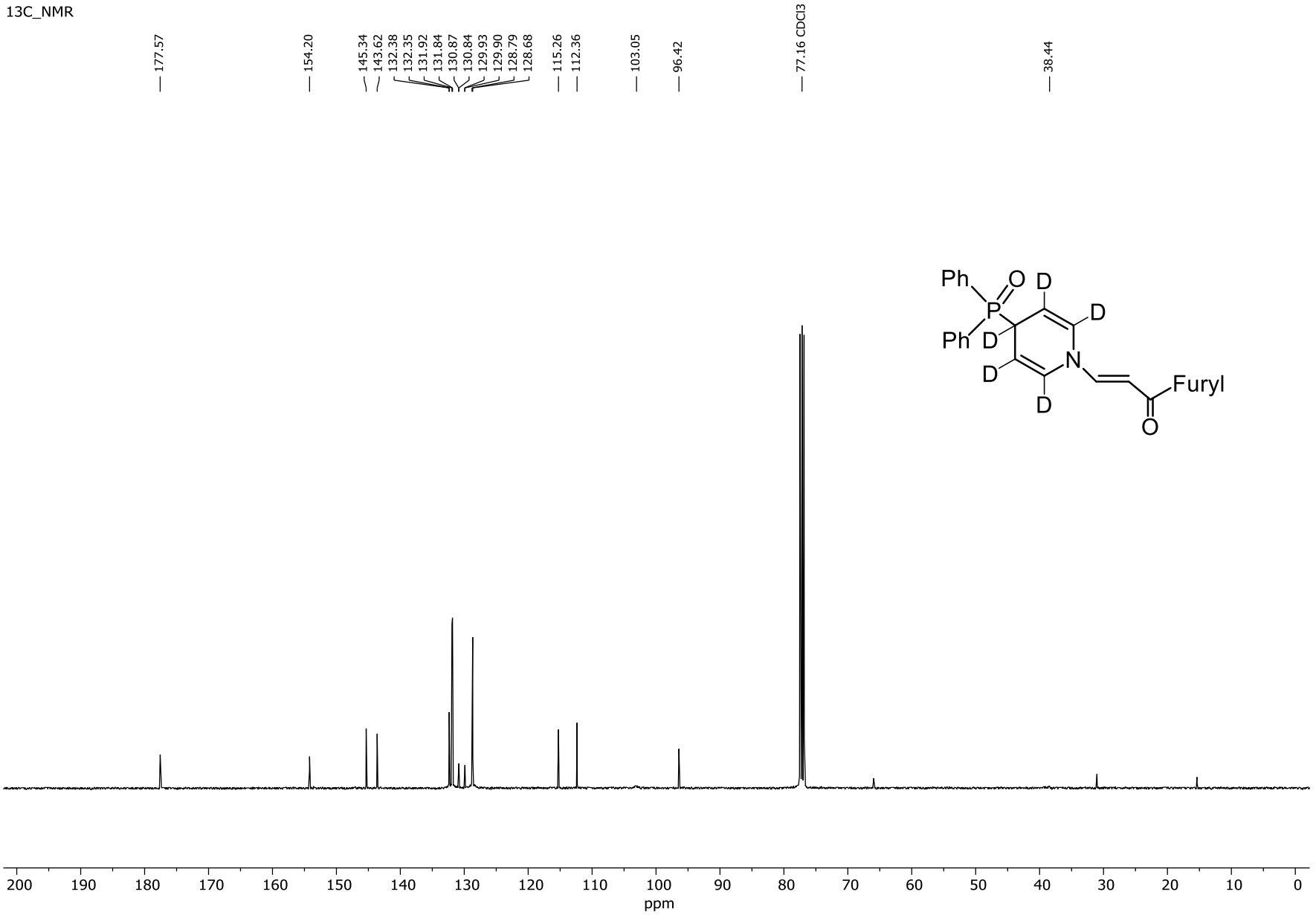
(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (5c)



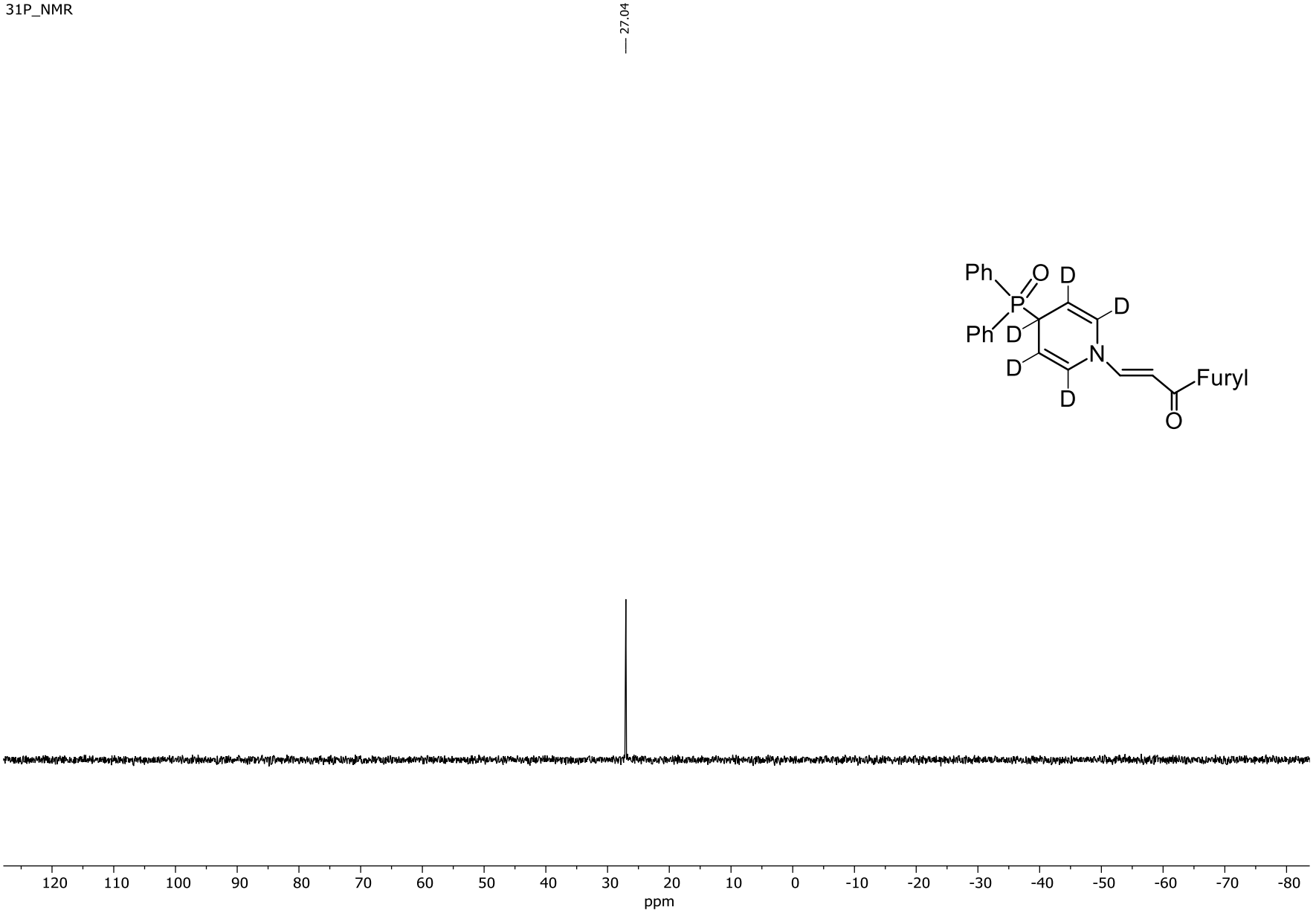
(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (5d)



(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (5d)



(2*E*)-3-[4-(Diphenylphosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-(furan-2-yl)prop-2-en-1-one (5d)



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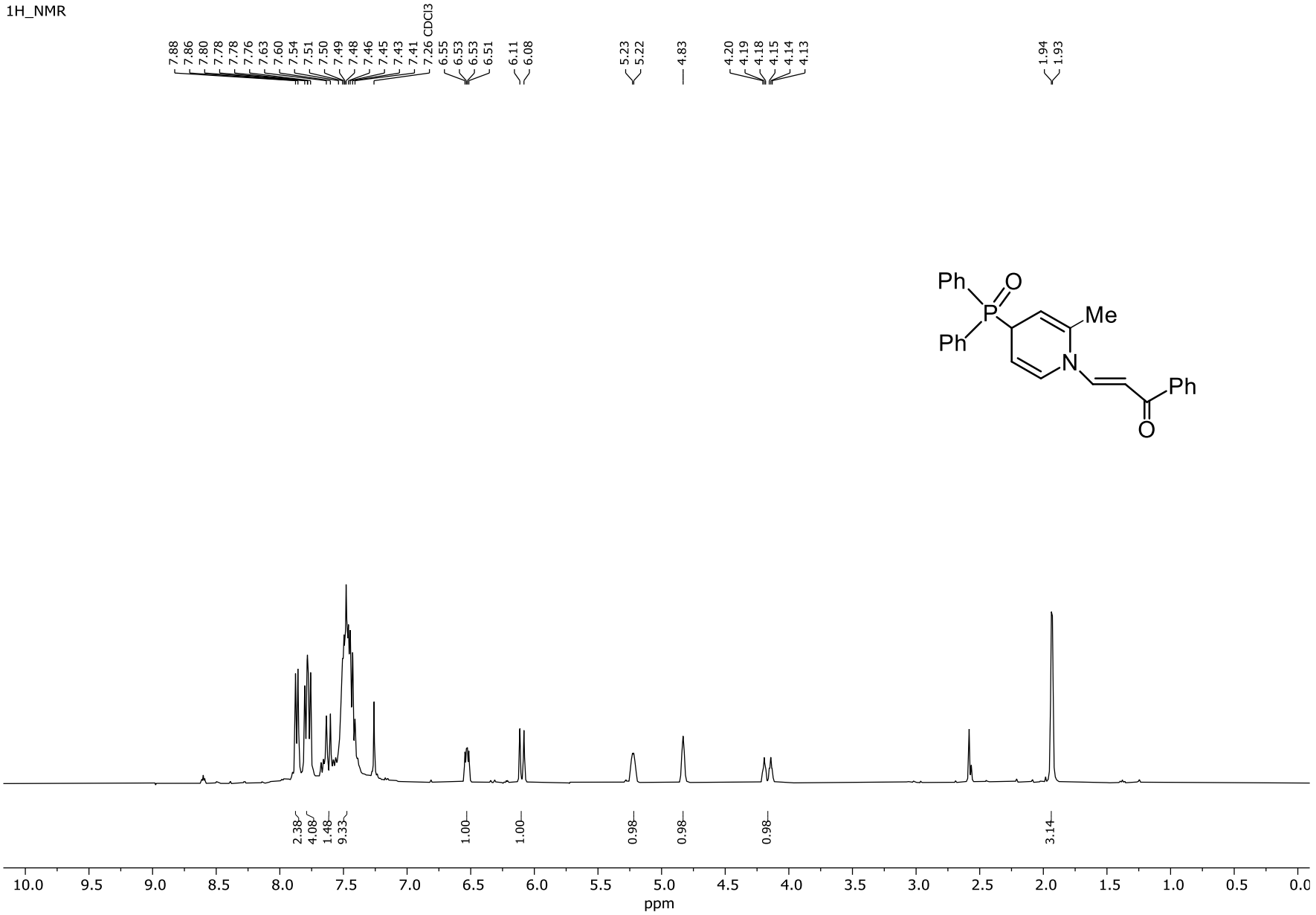
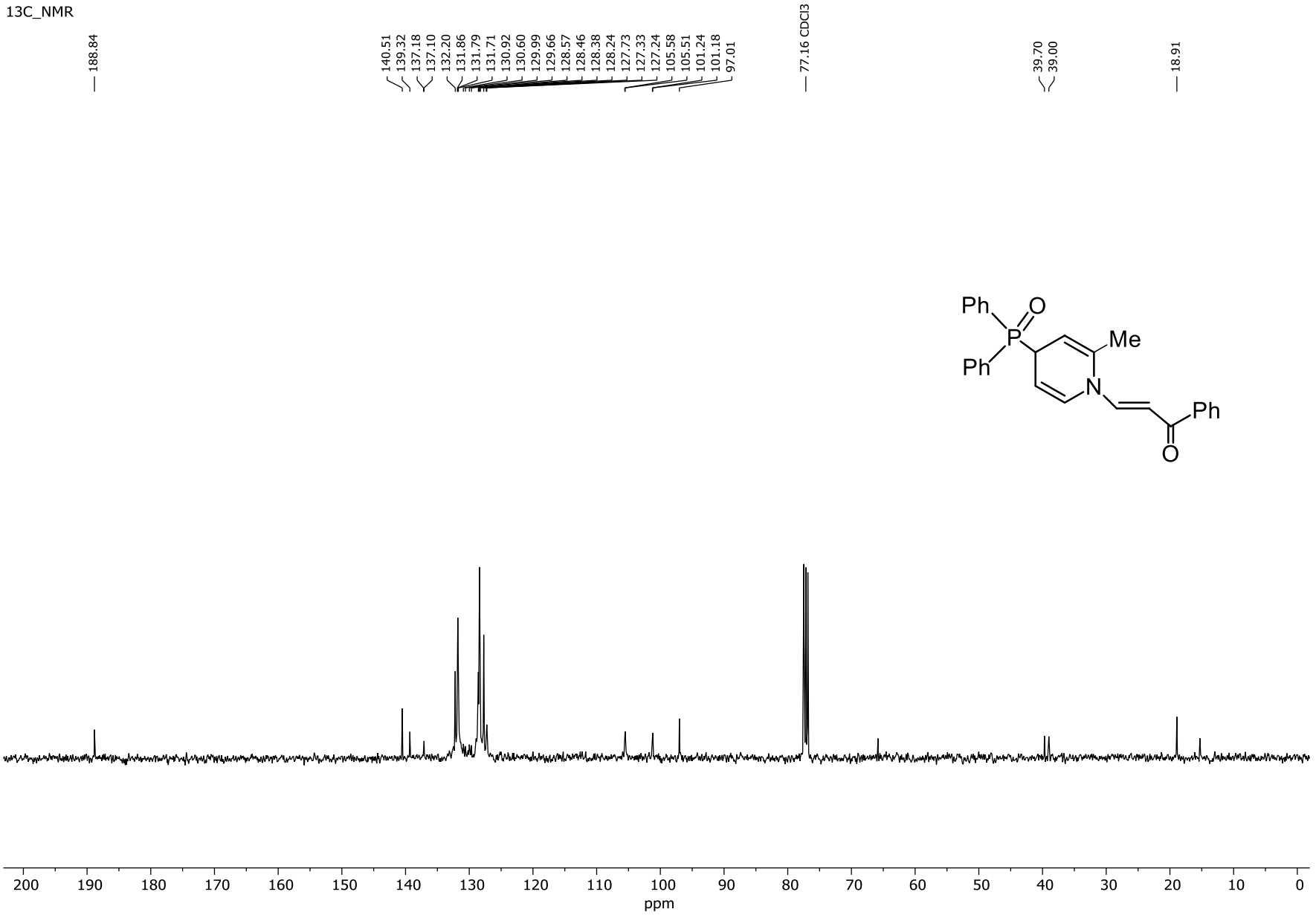
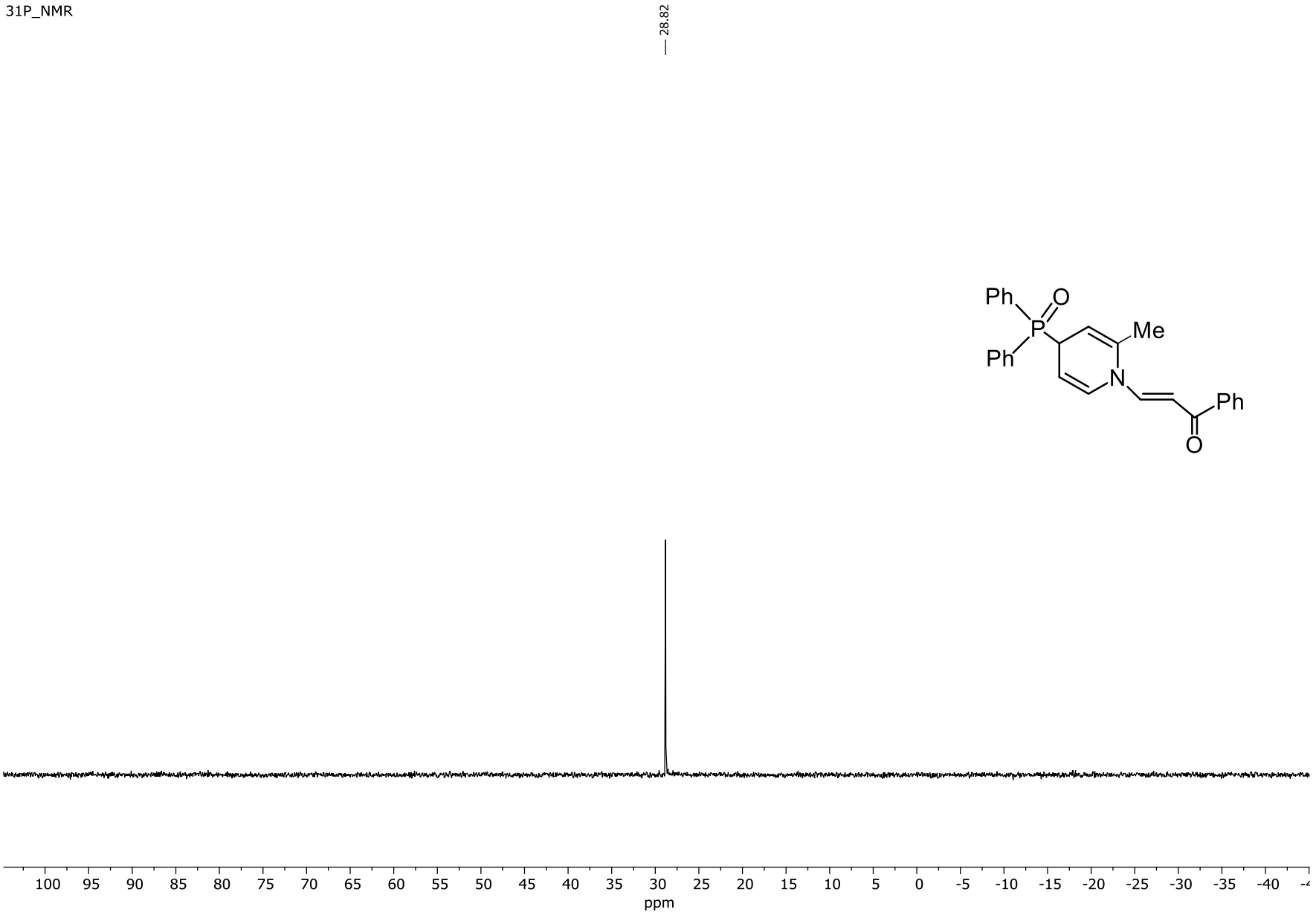


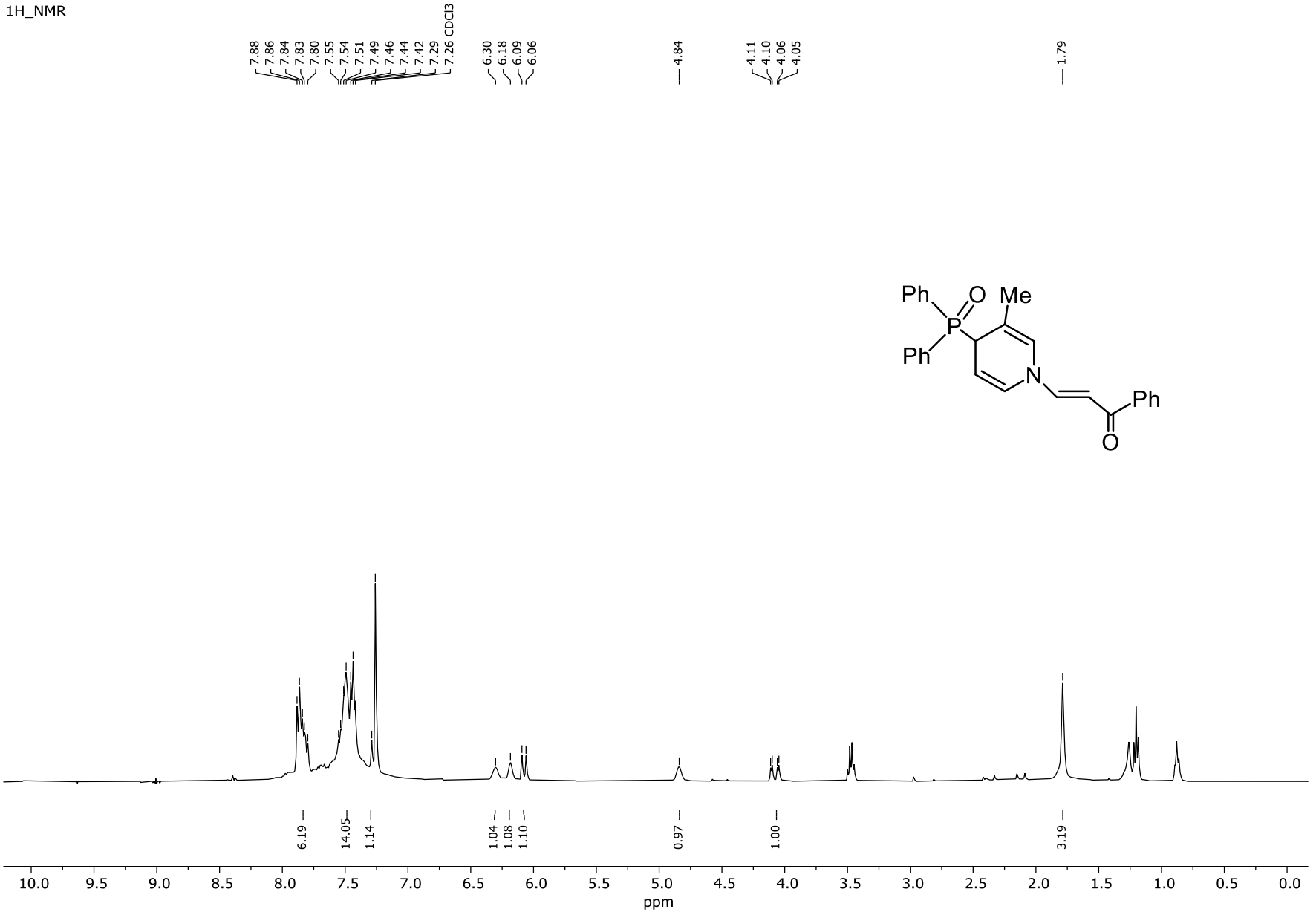
(2*E*)-3-[4-(Diphenylphosphoryl)-2-methylpyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5e)



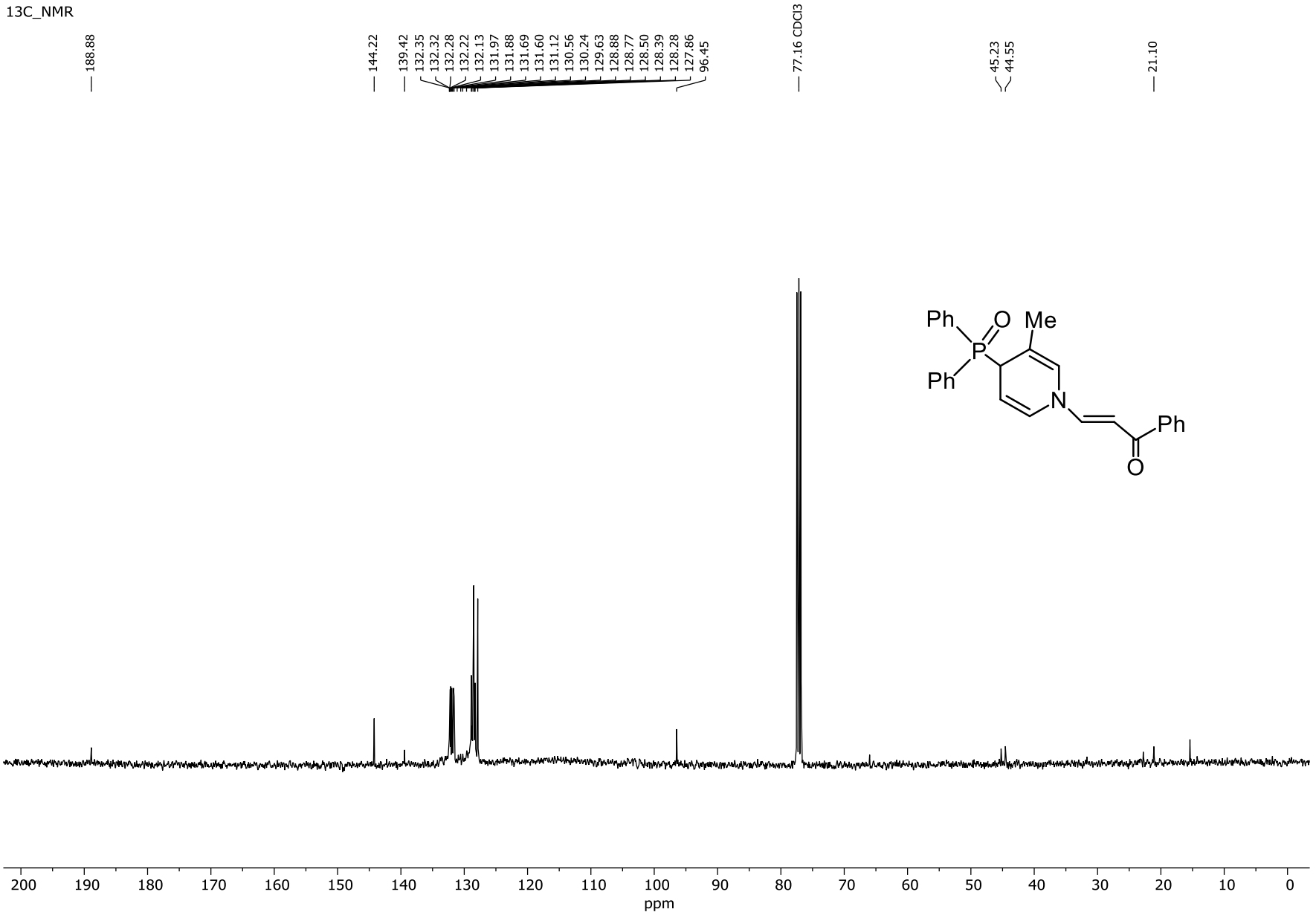
(2*E*)-3-[4-(Diphenylphosphoryl)-2-methylpyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5e)



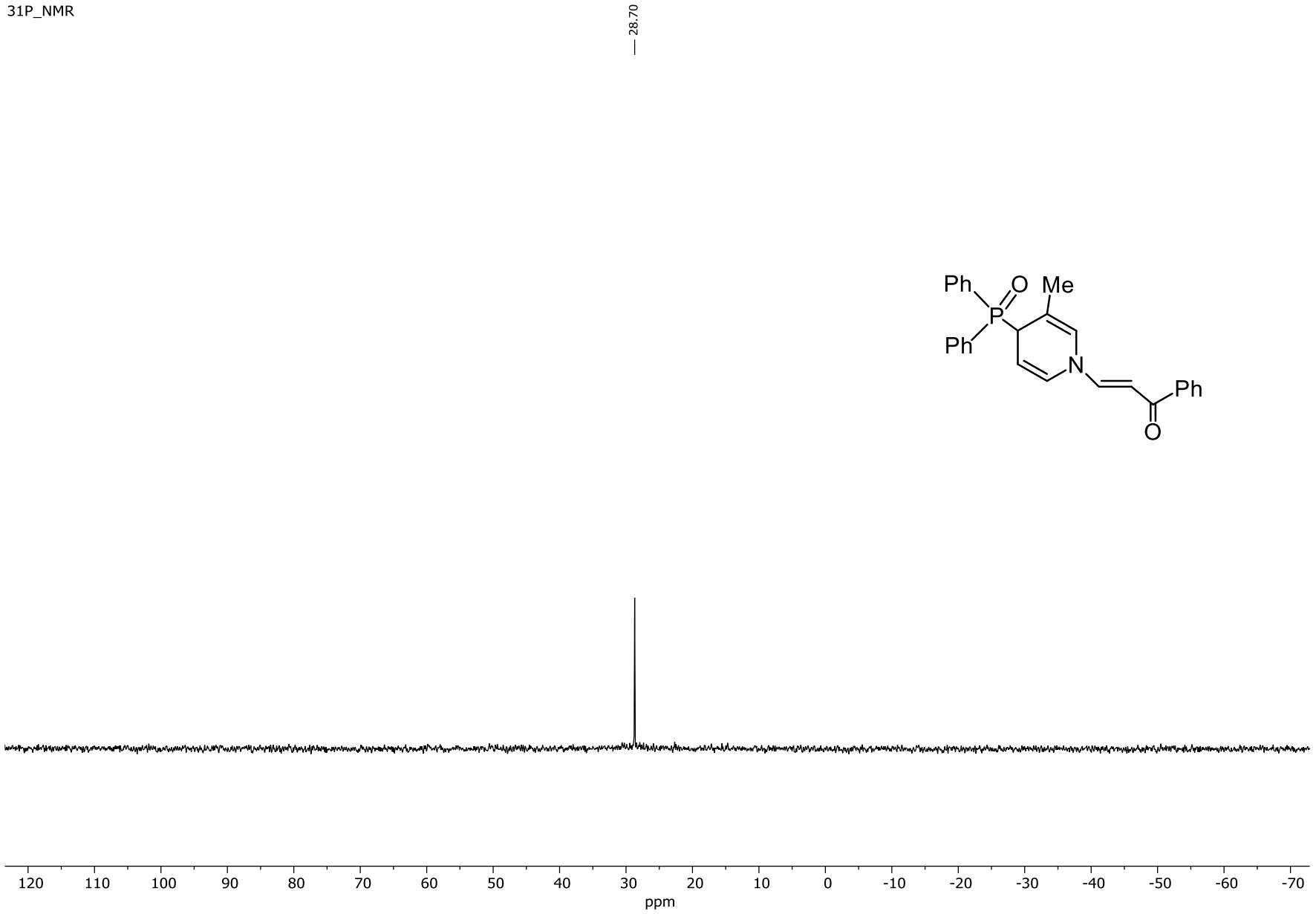
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5f)



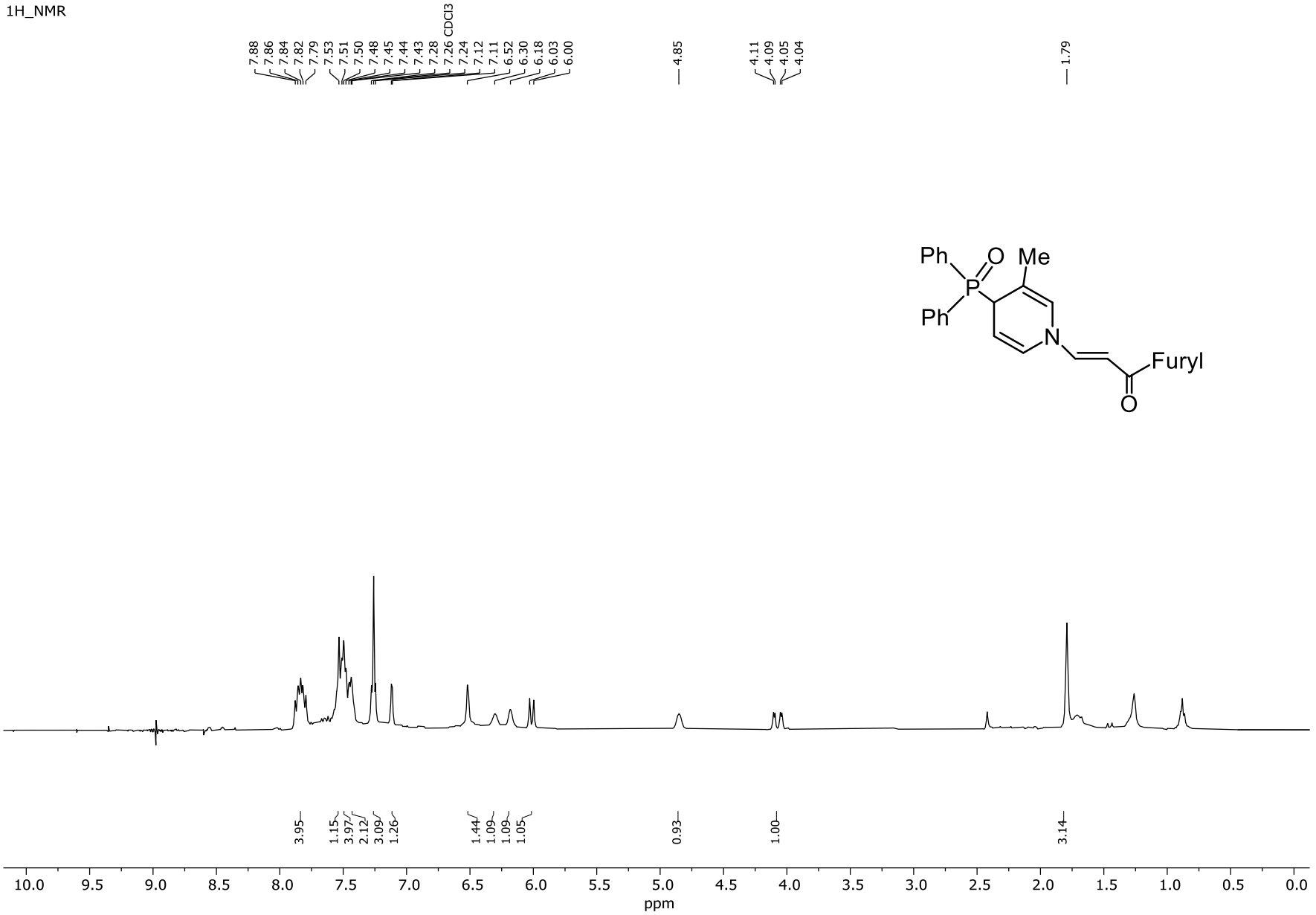
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5f)



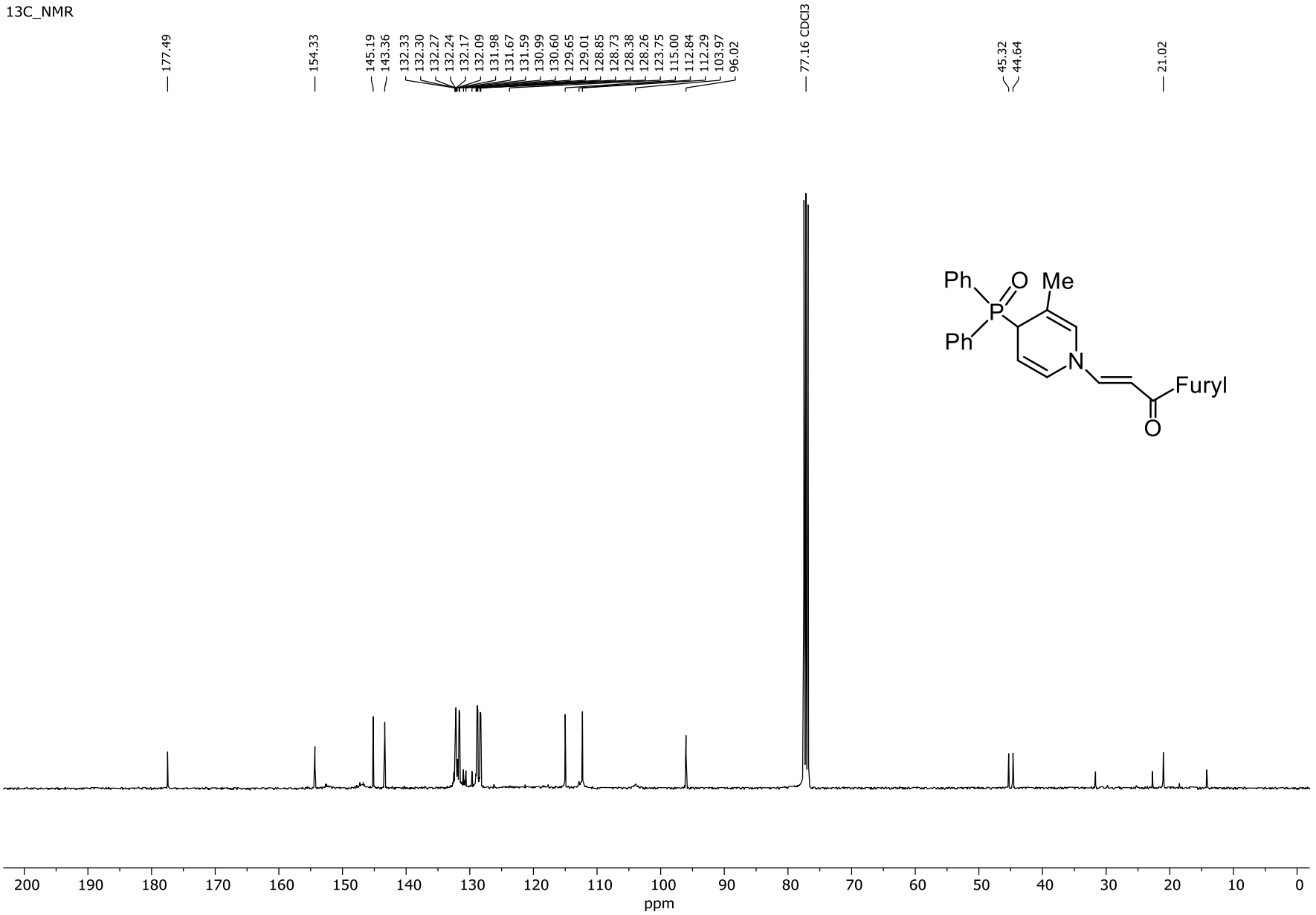
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (5f)



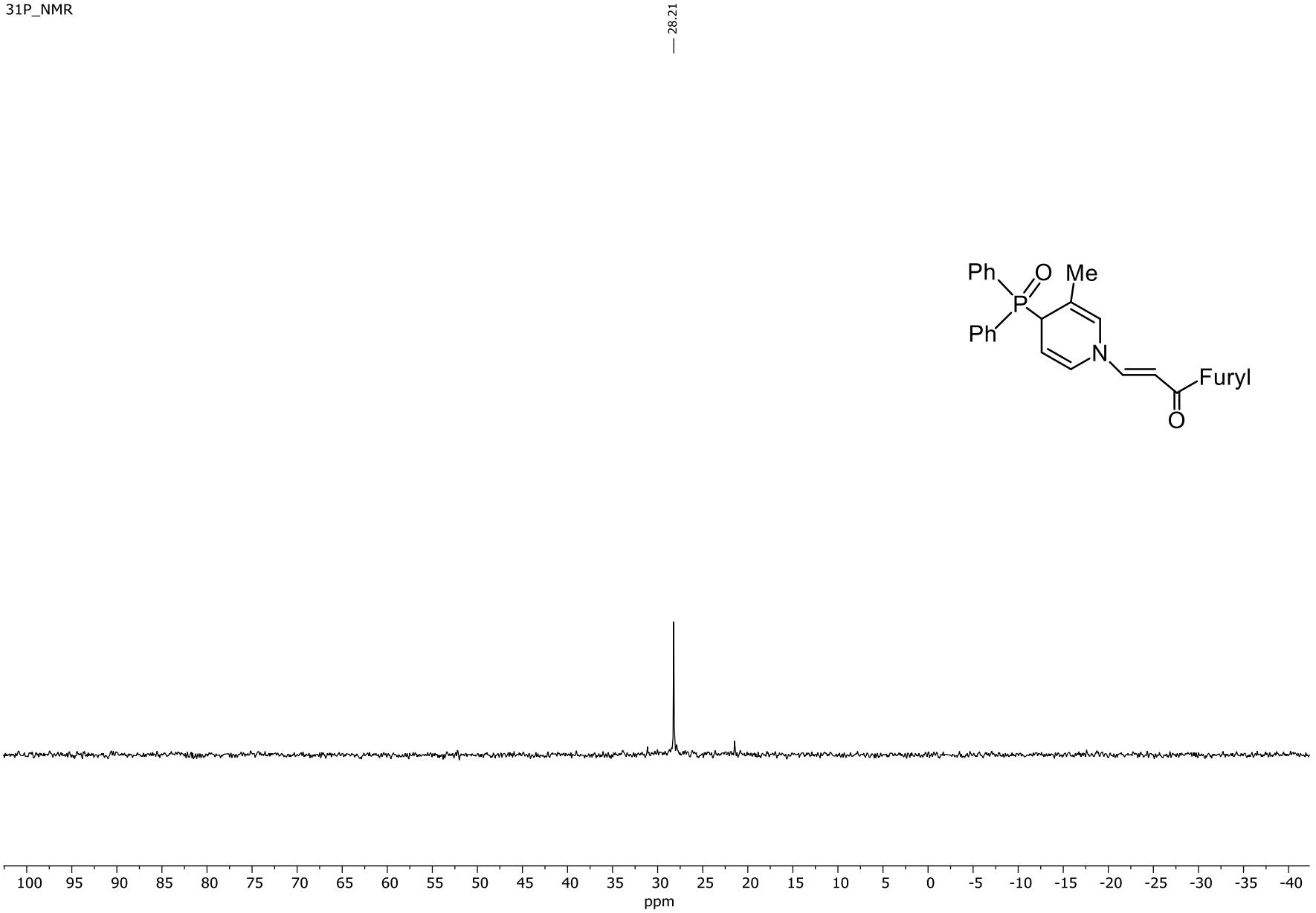
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5g)



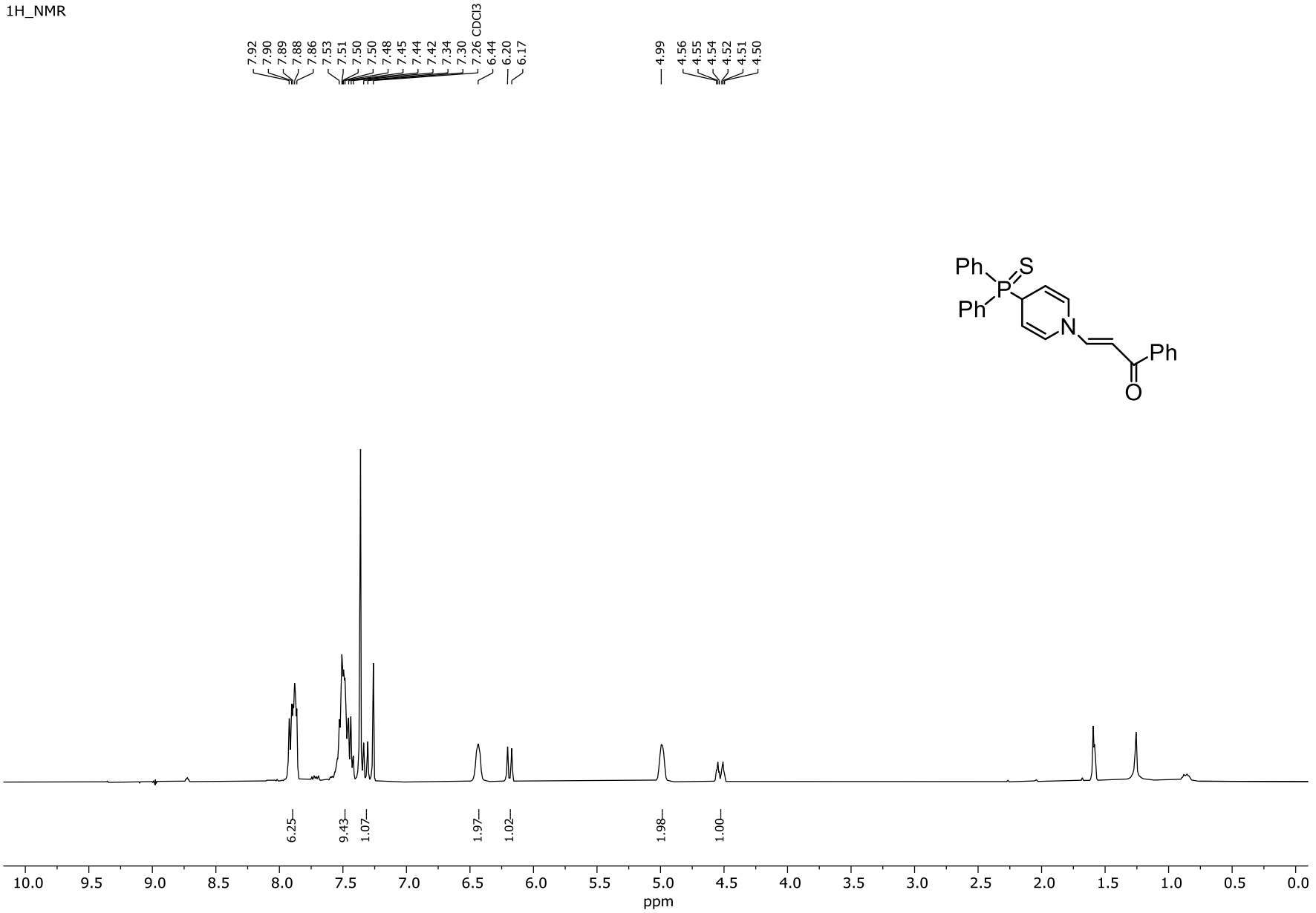
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5g)



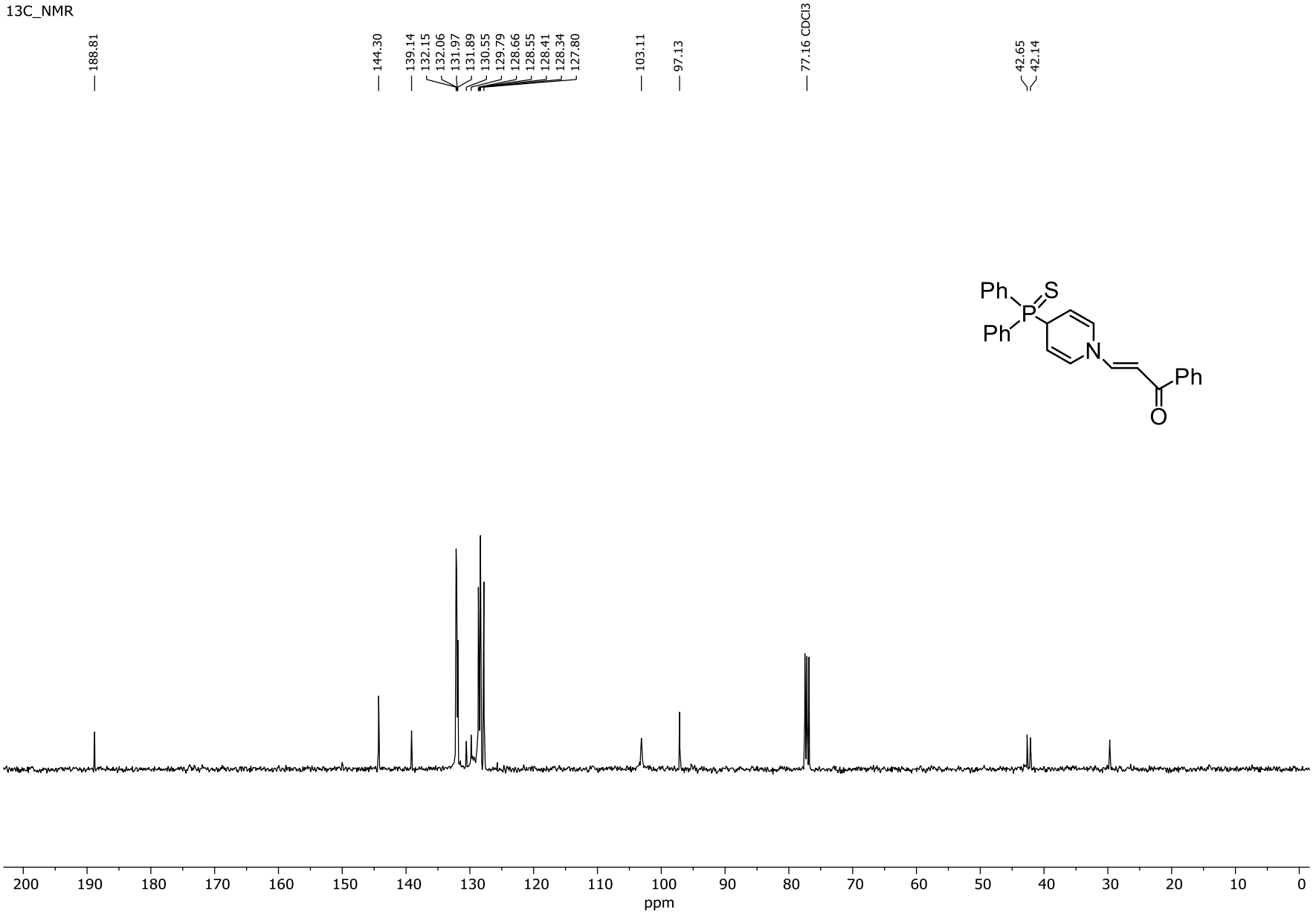
(2*E*)-3-[4-(Diphenylphosphoryl)-3-methylpyridin-1(4*H*)-yl]-1-(furan-2-yl)prop-2-en-1-one (5g)



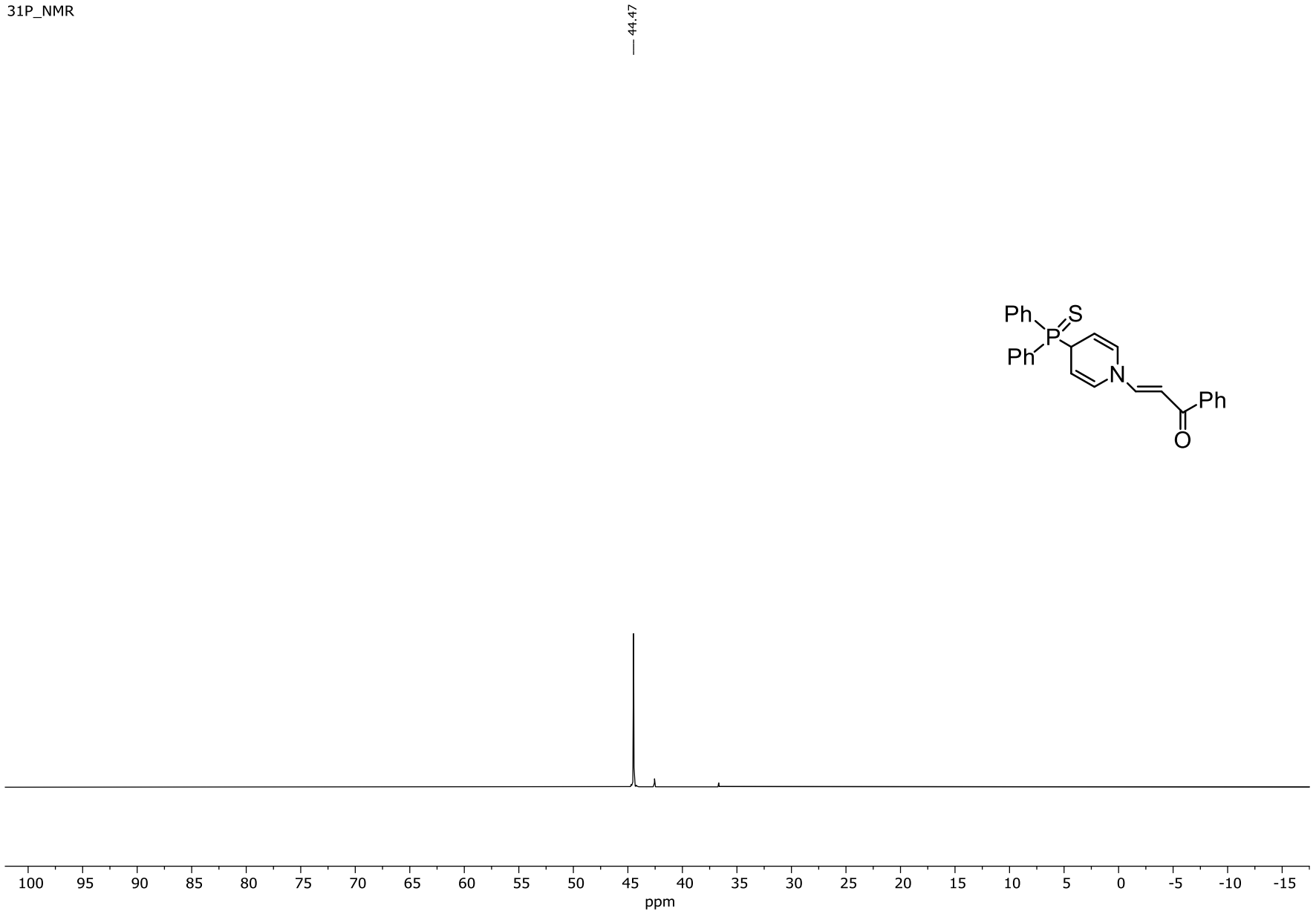
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (7a)



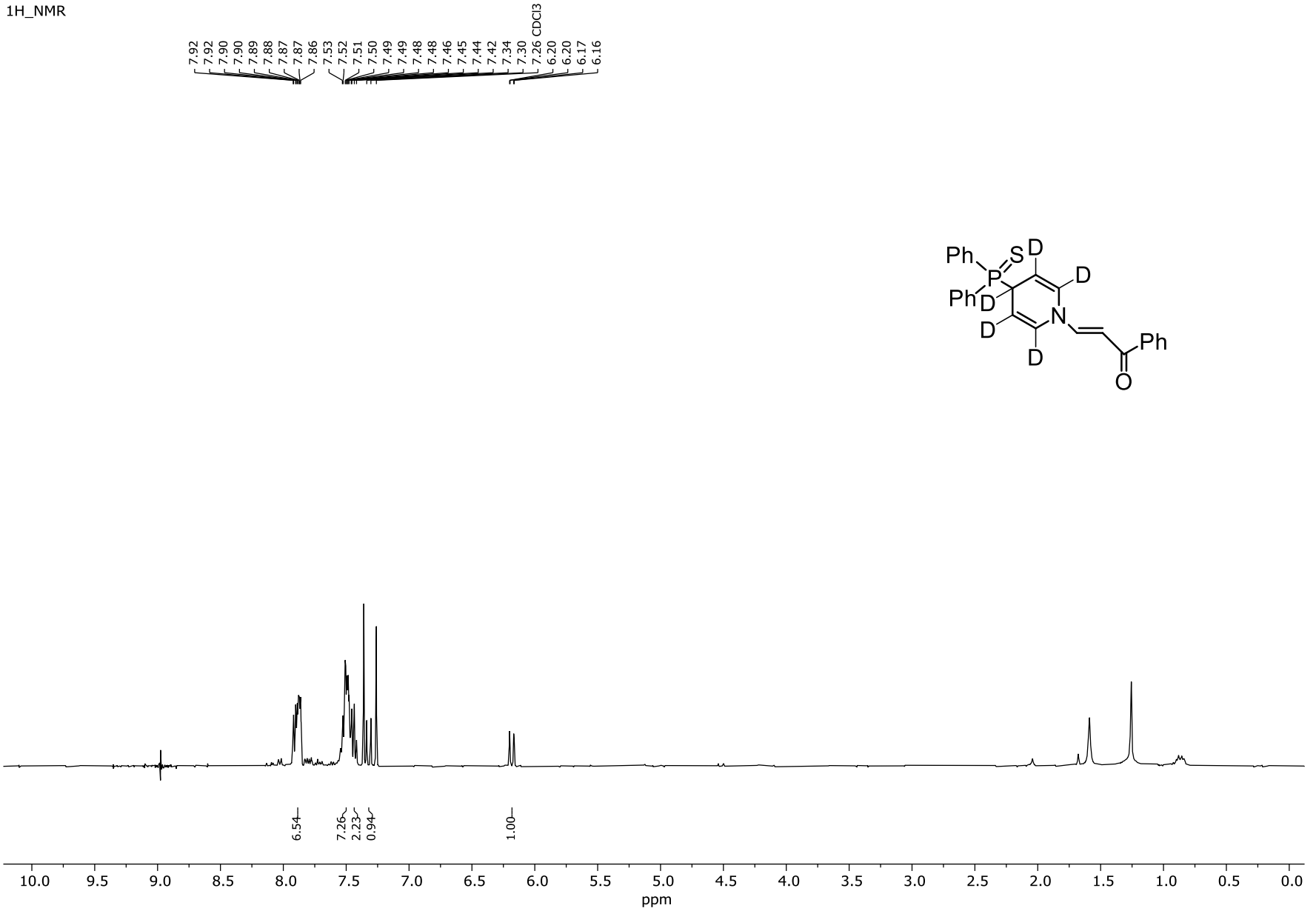
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (7a)



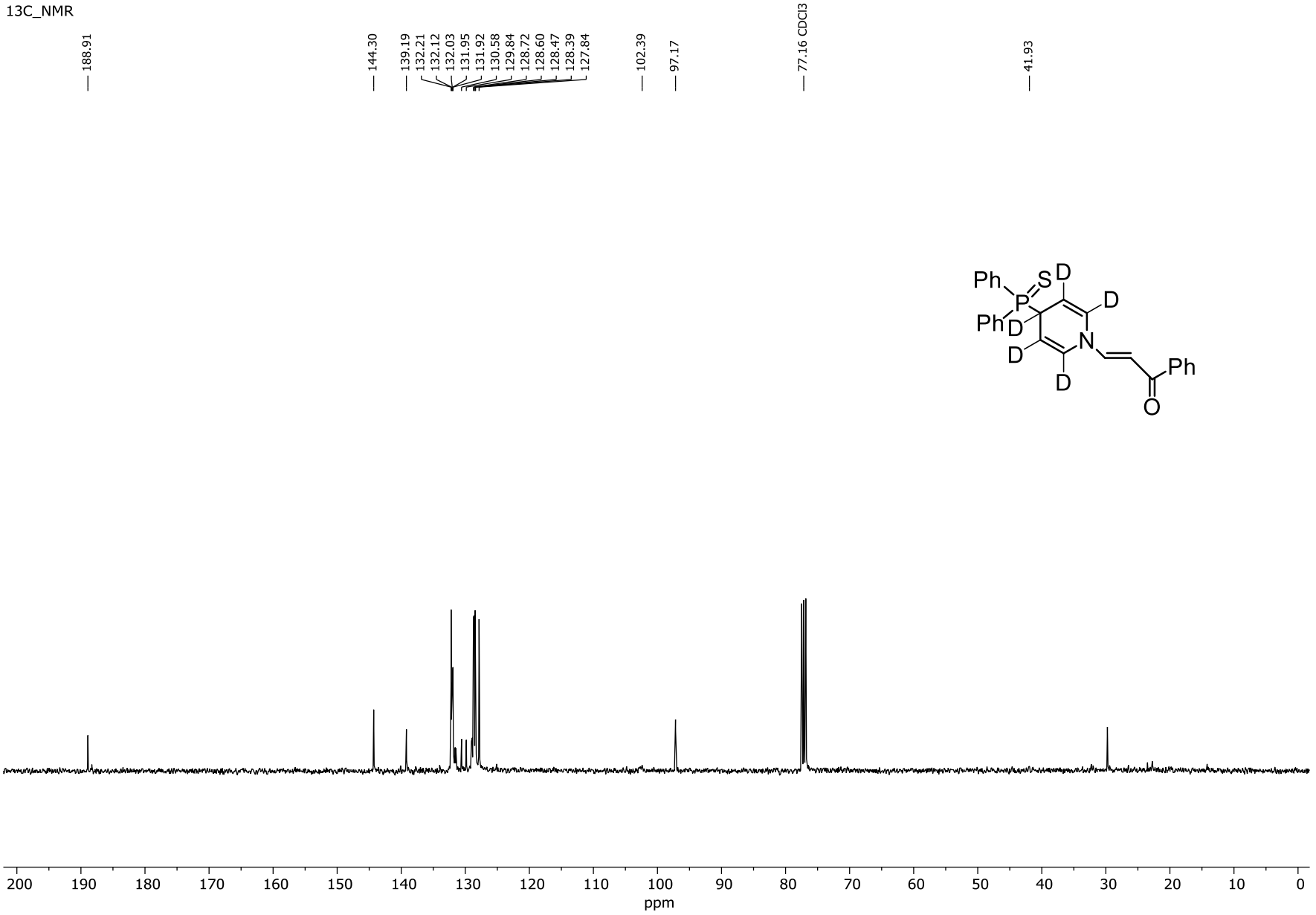
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl]-1-phenylprop-2-en-1-one (7a)



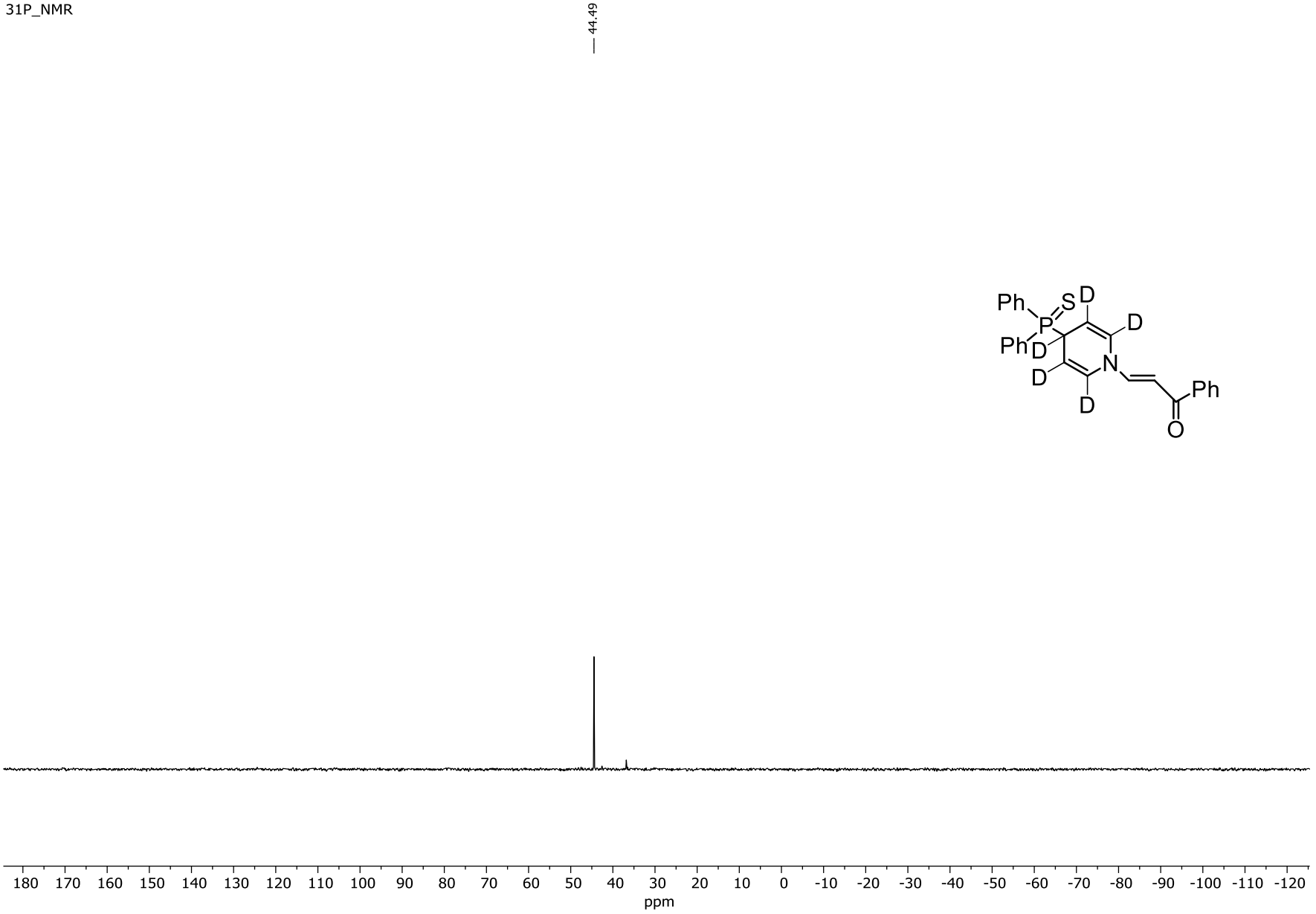
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (7b)



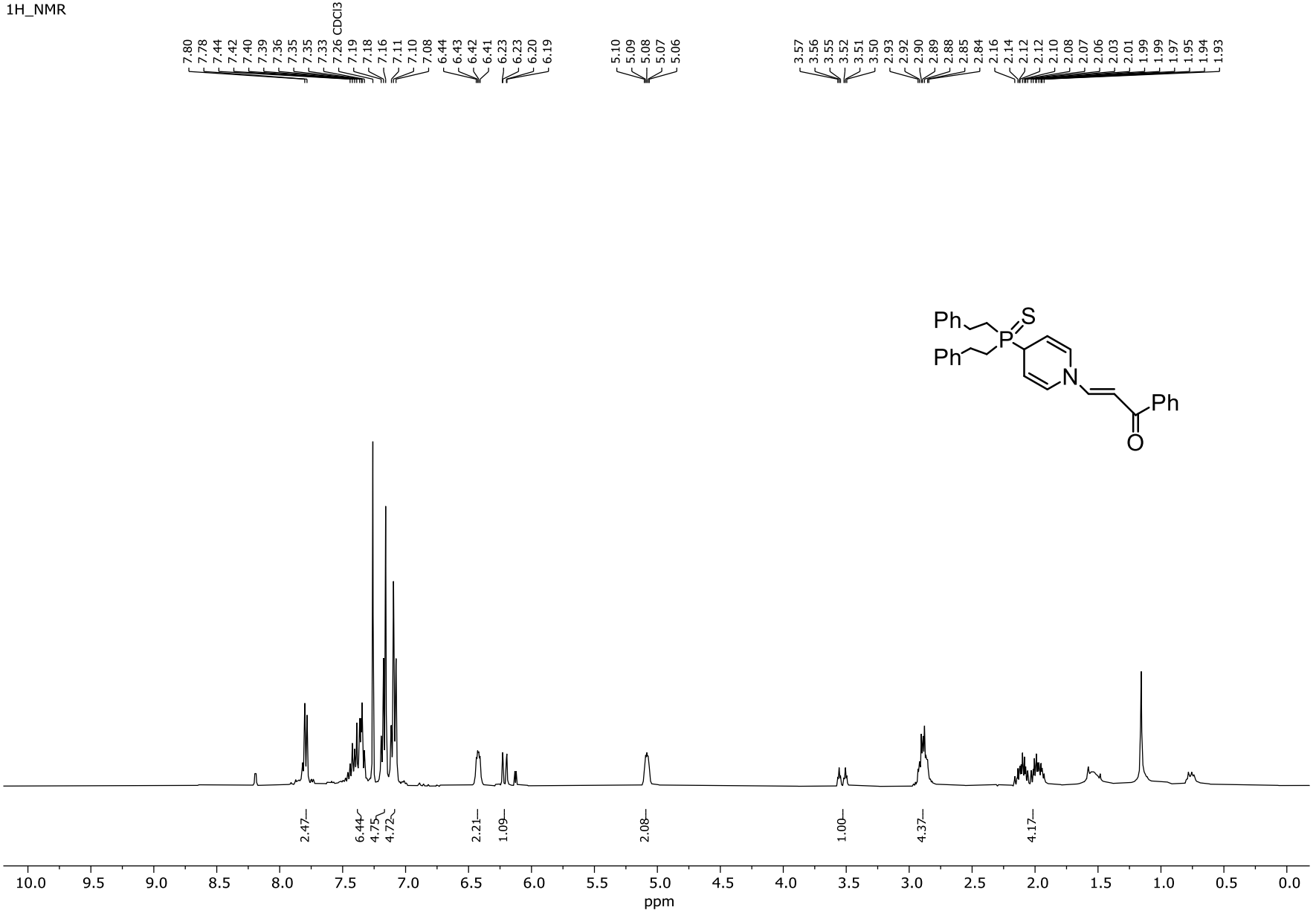
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (7b)



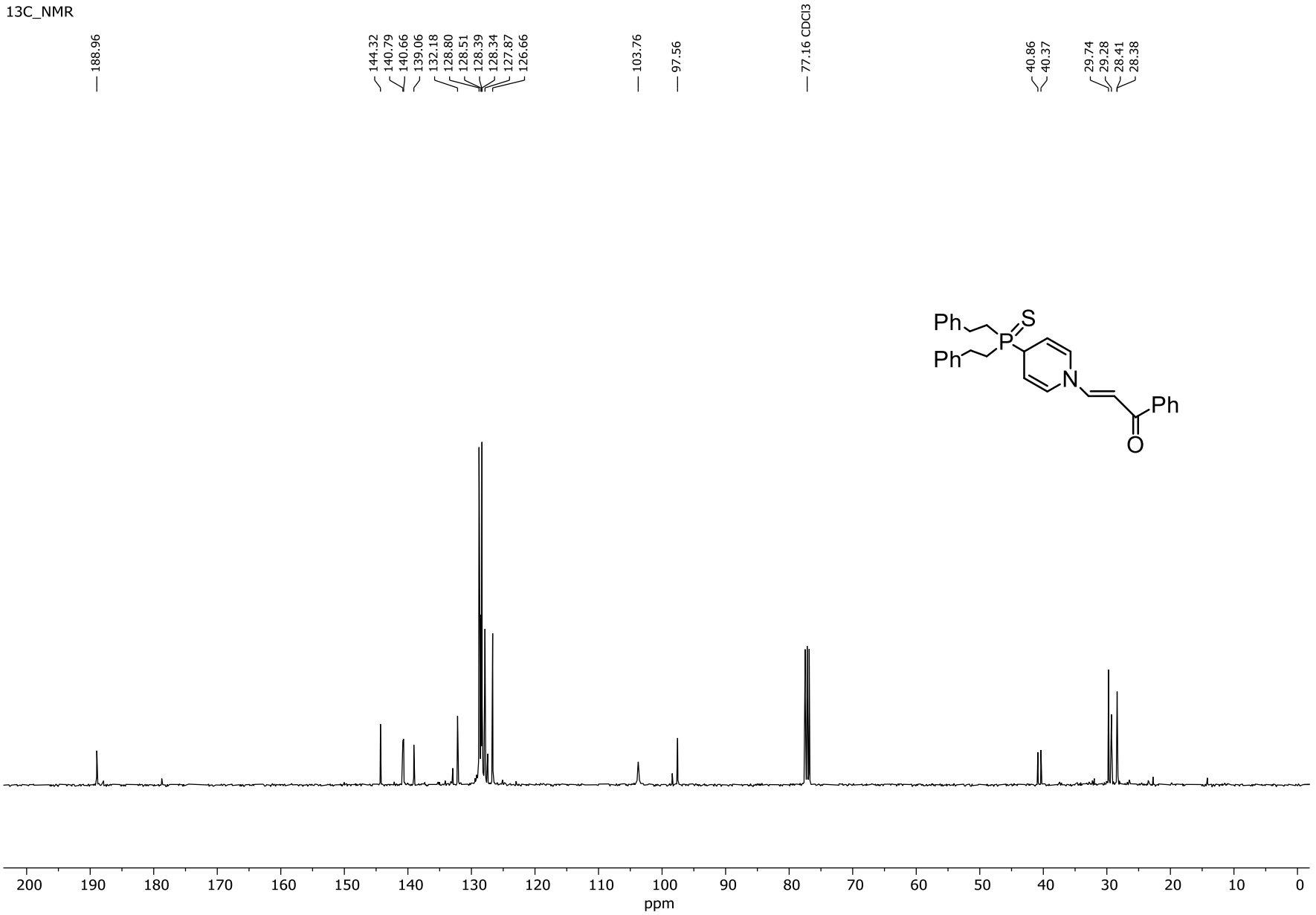
(2*E*)-3-[4-(Diphenylthiophosphoryl)pyridin-1(4*H*)-yl-2,3,4,5,6-d_5]-1-phenylprop-2-en-1-one (7b)



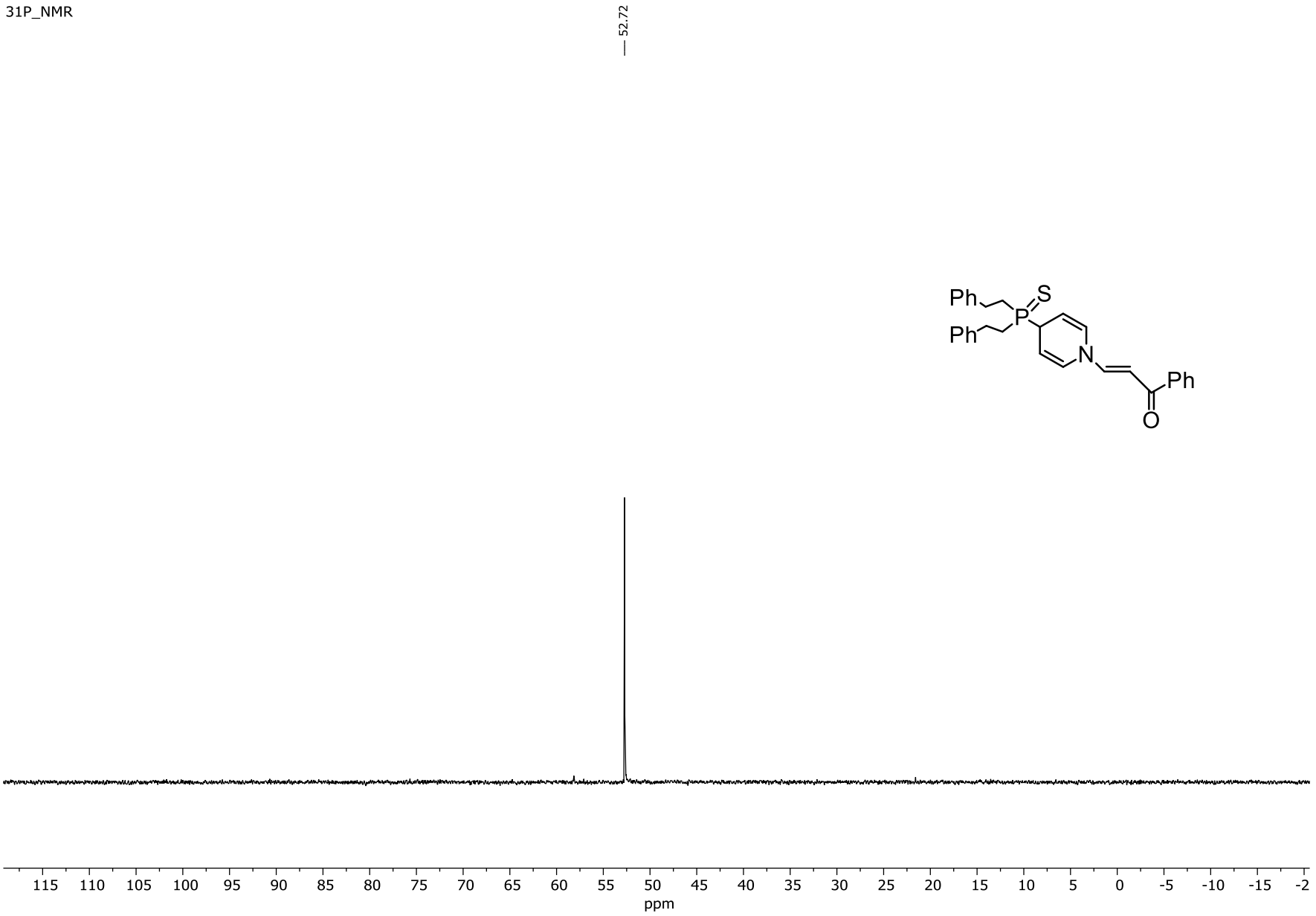
(2*E*)-3-{4-[Bis(2-phenylethyl)thiophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7c)



(2*E*)-3-{4-[Bis(2-phenylethyl)thiophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7c)



(2*E*)-3-{4-[Bis(2-phenylethyl)thiophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7c)



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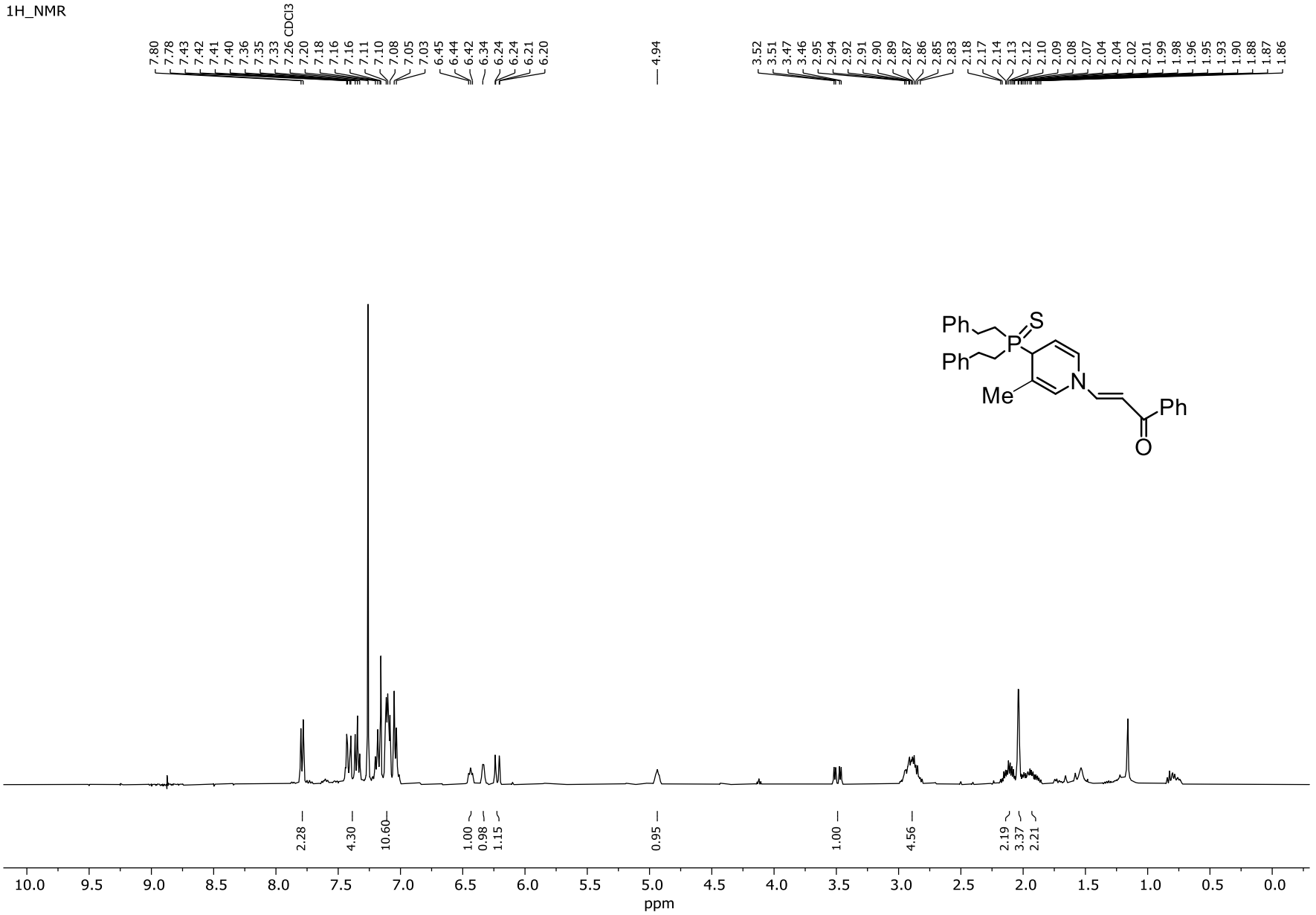

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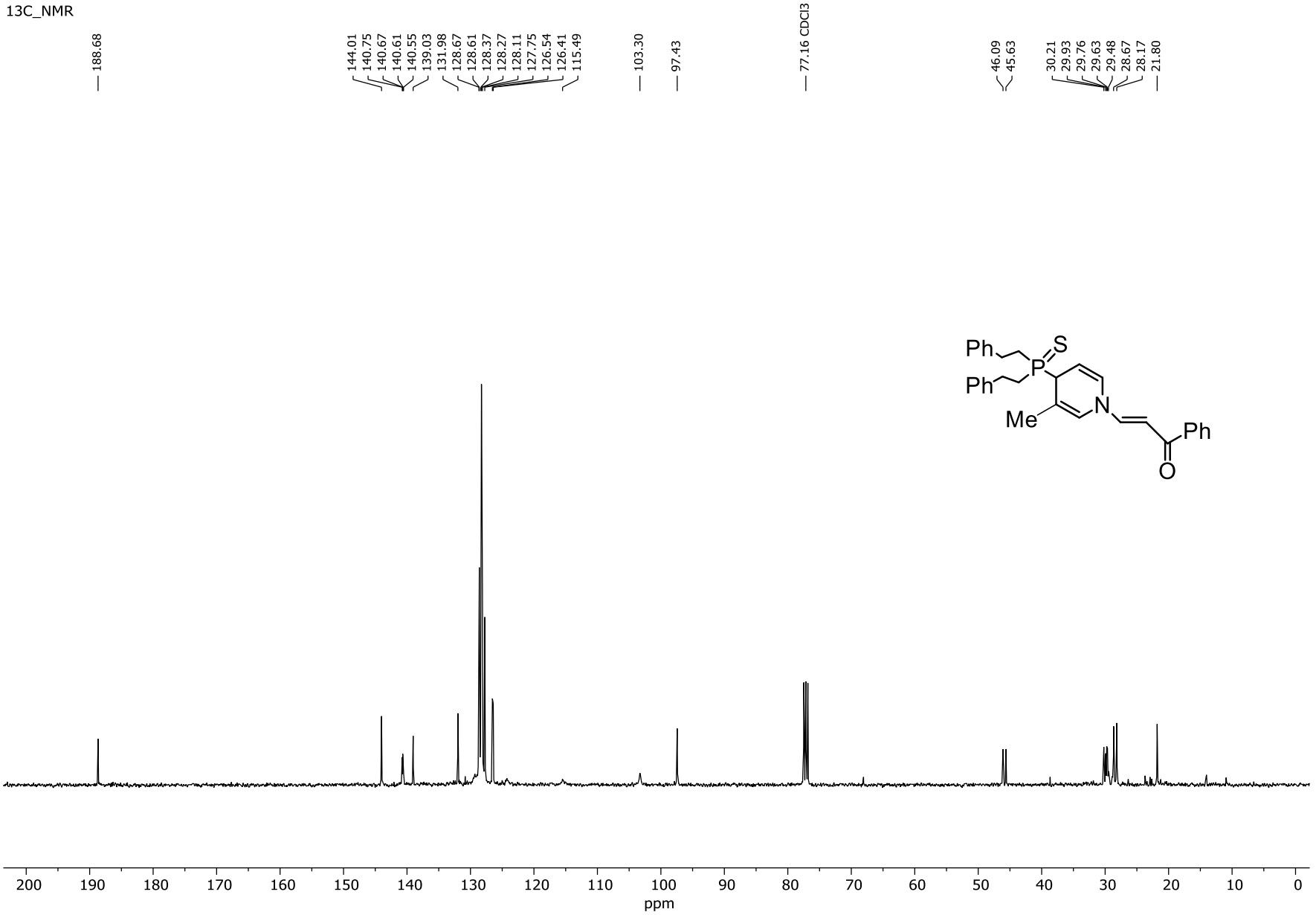

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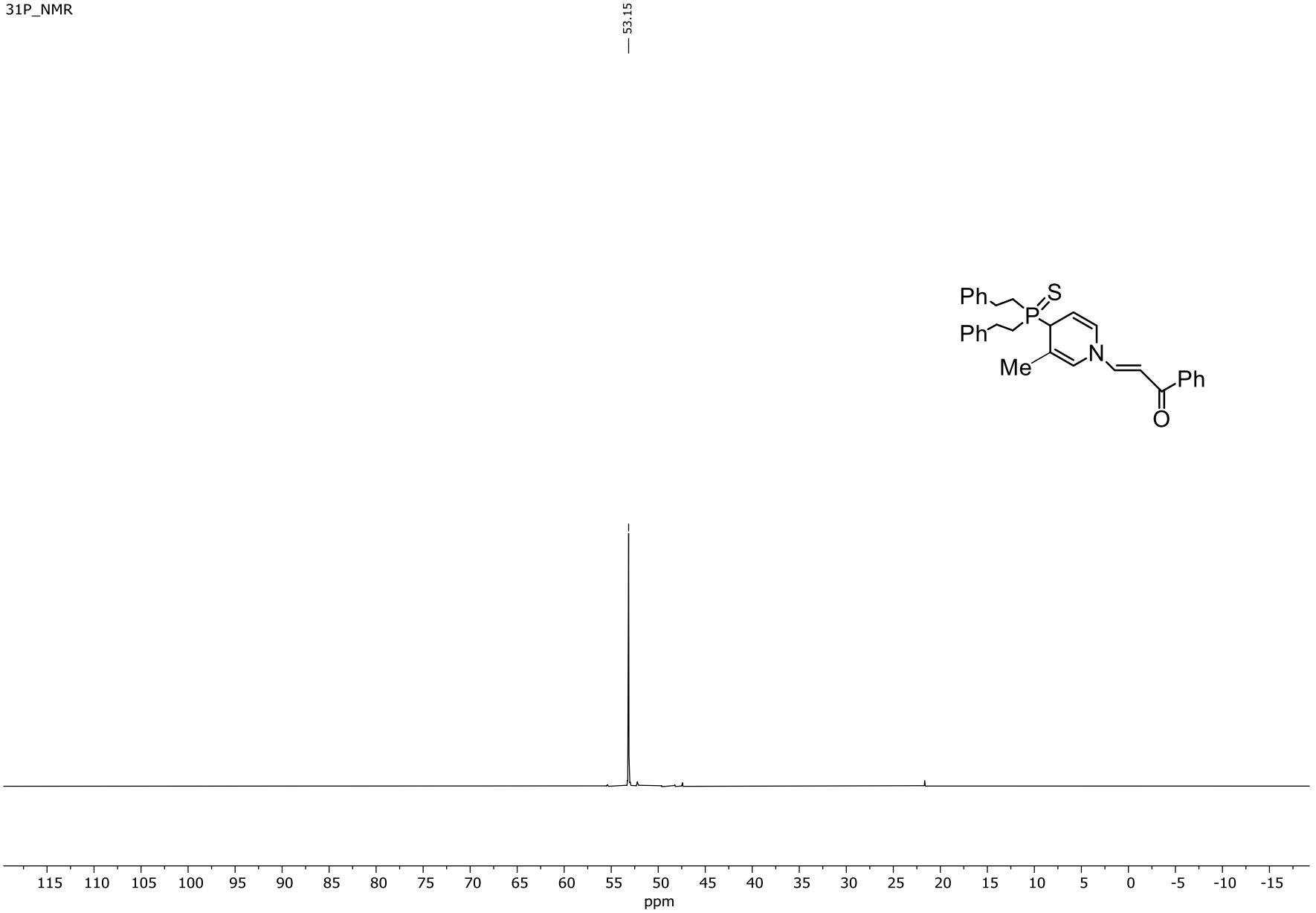
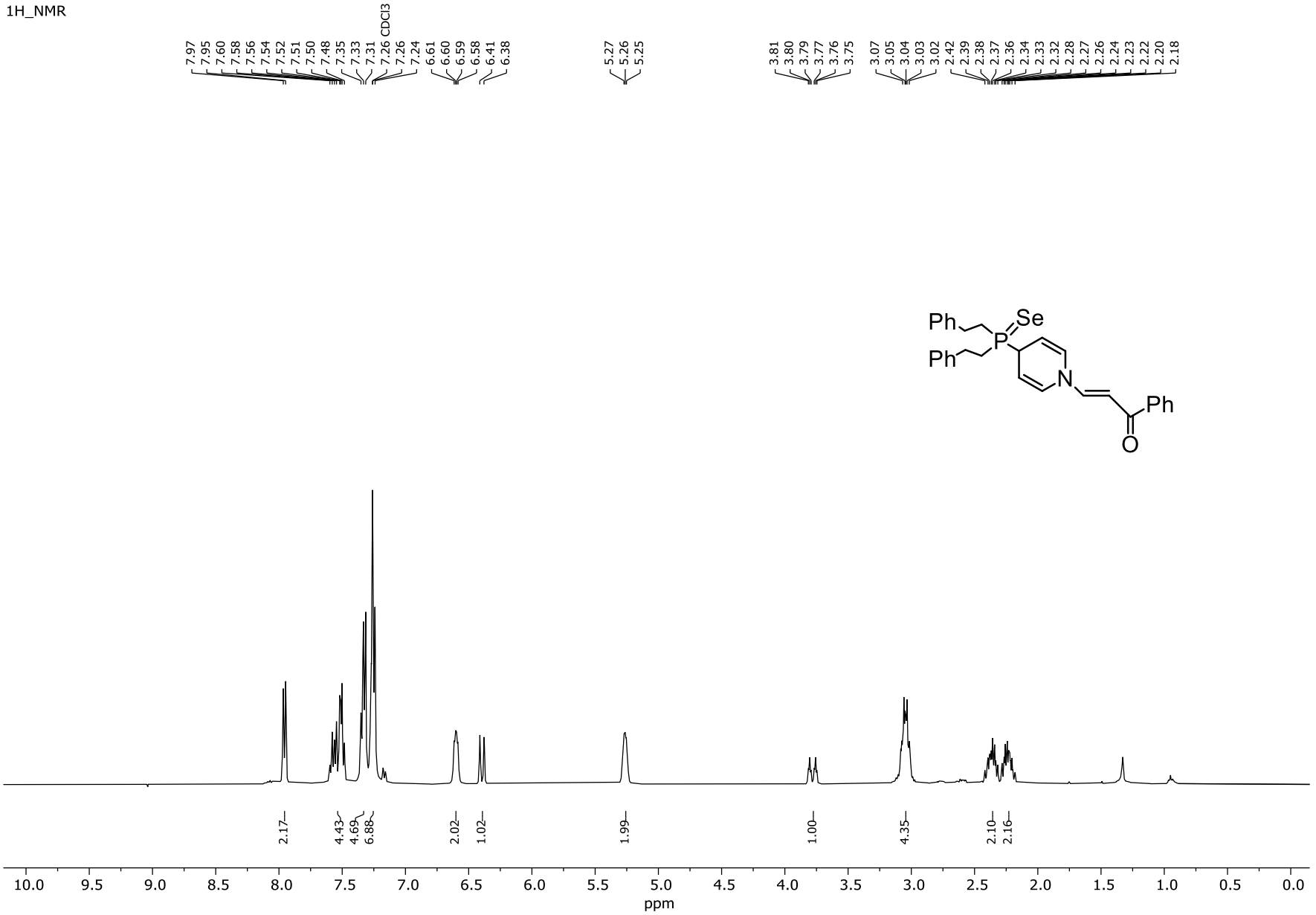
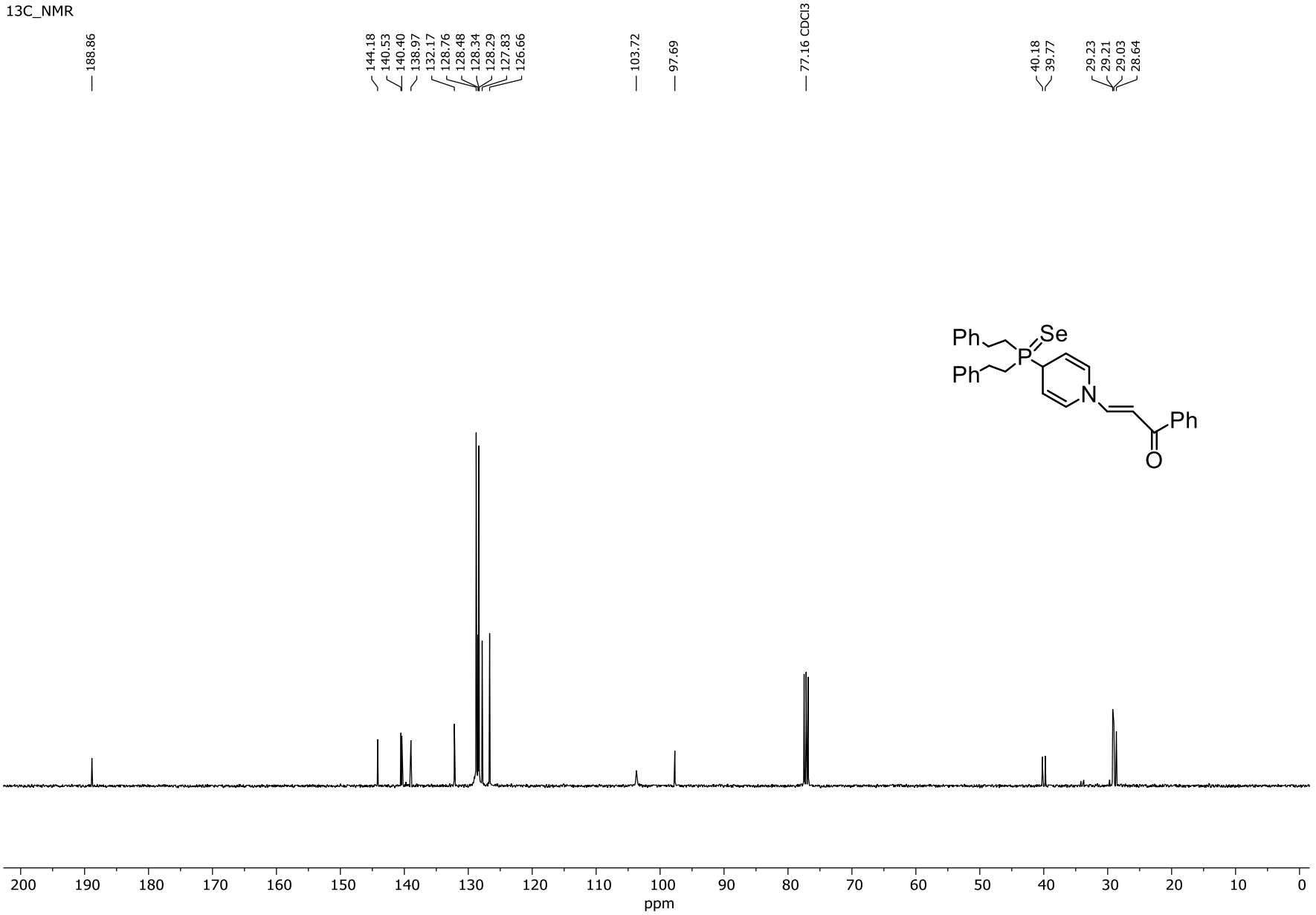


(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7f)



(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7f)



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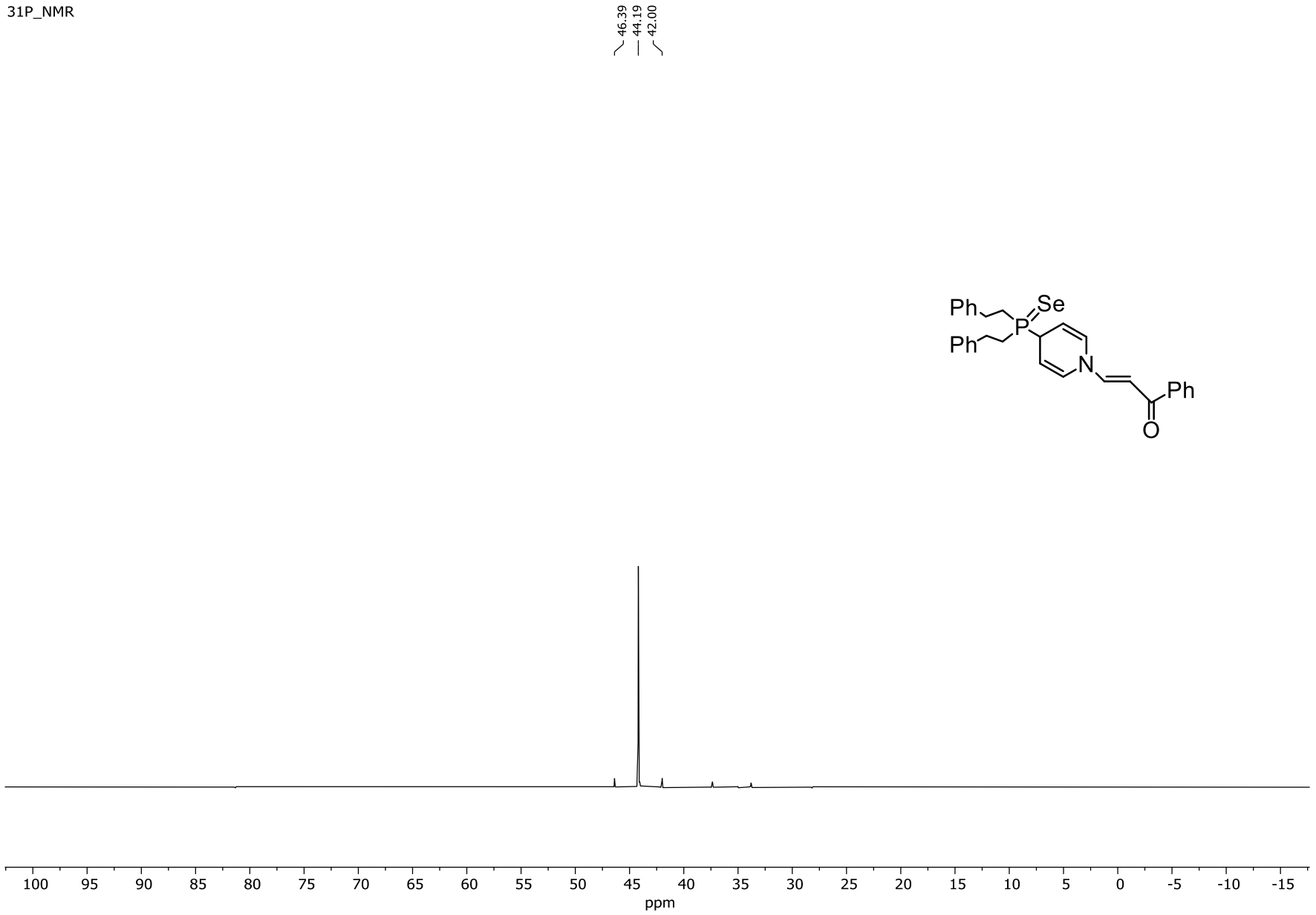
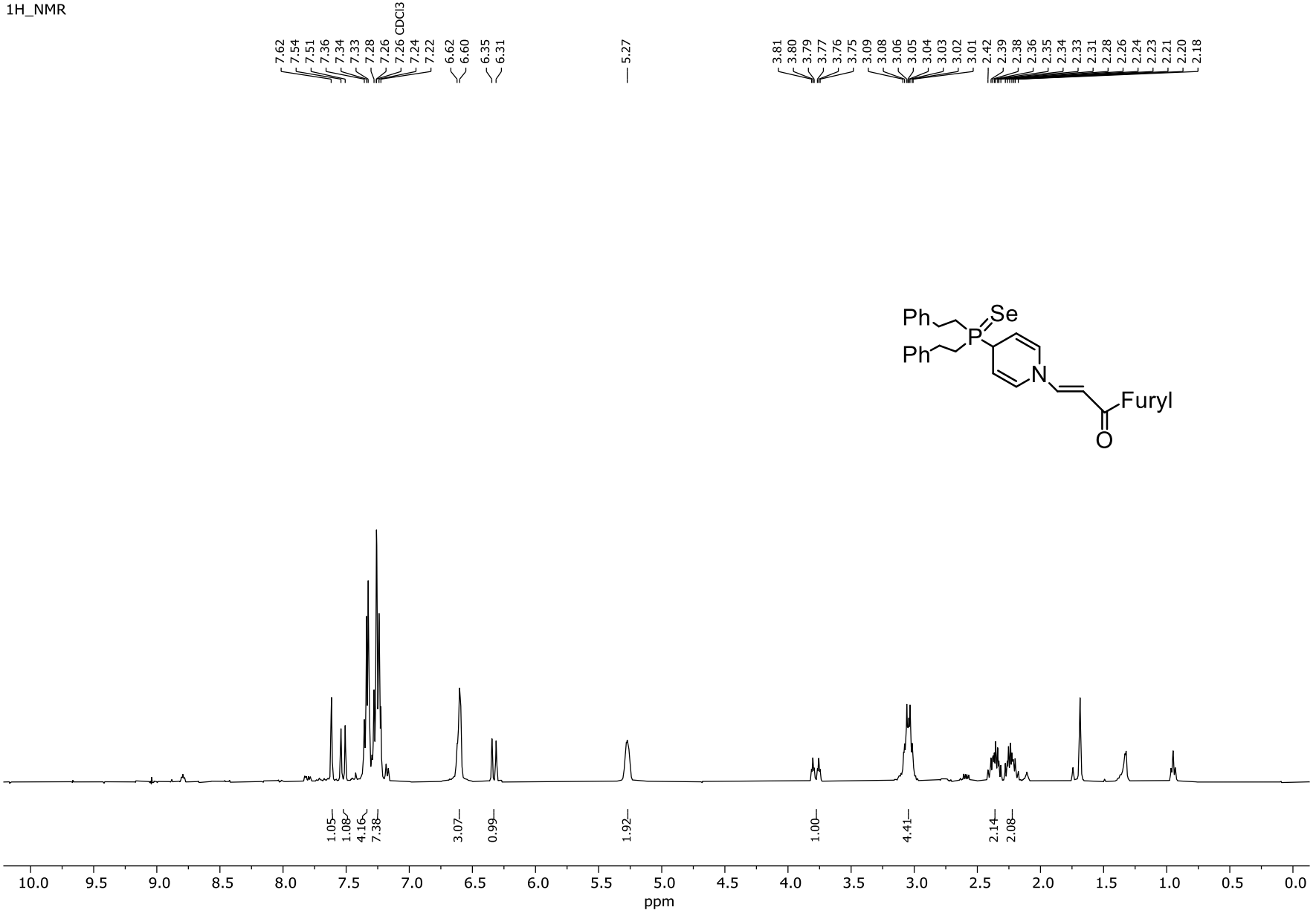


(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl}-1-(furan-2-yl)prop-2-en-1-one (7g)



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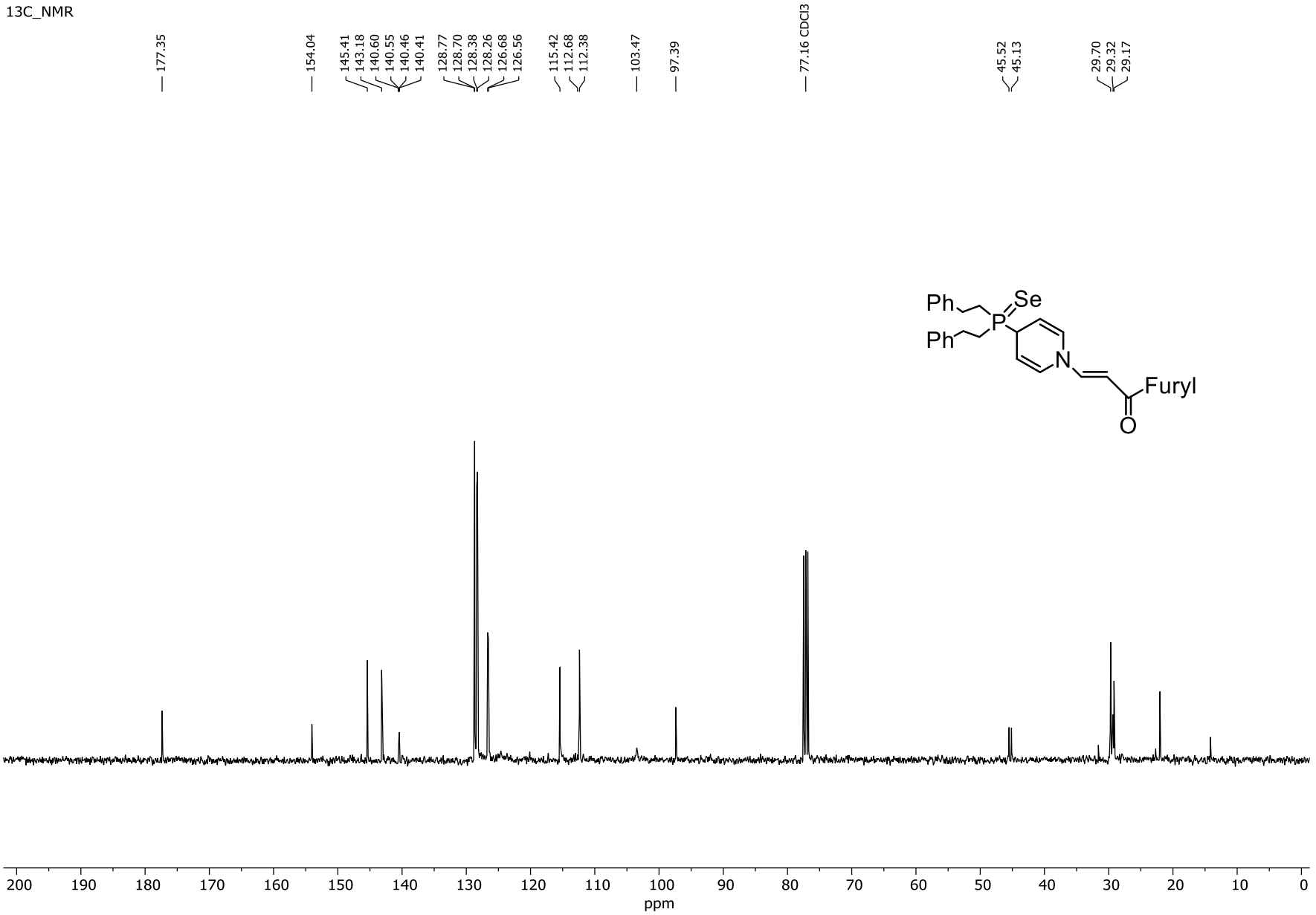

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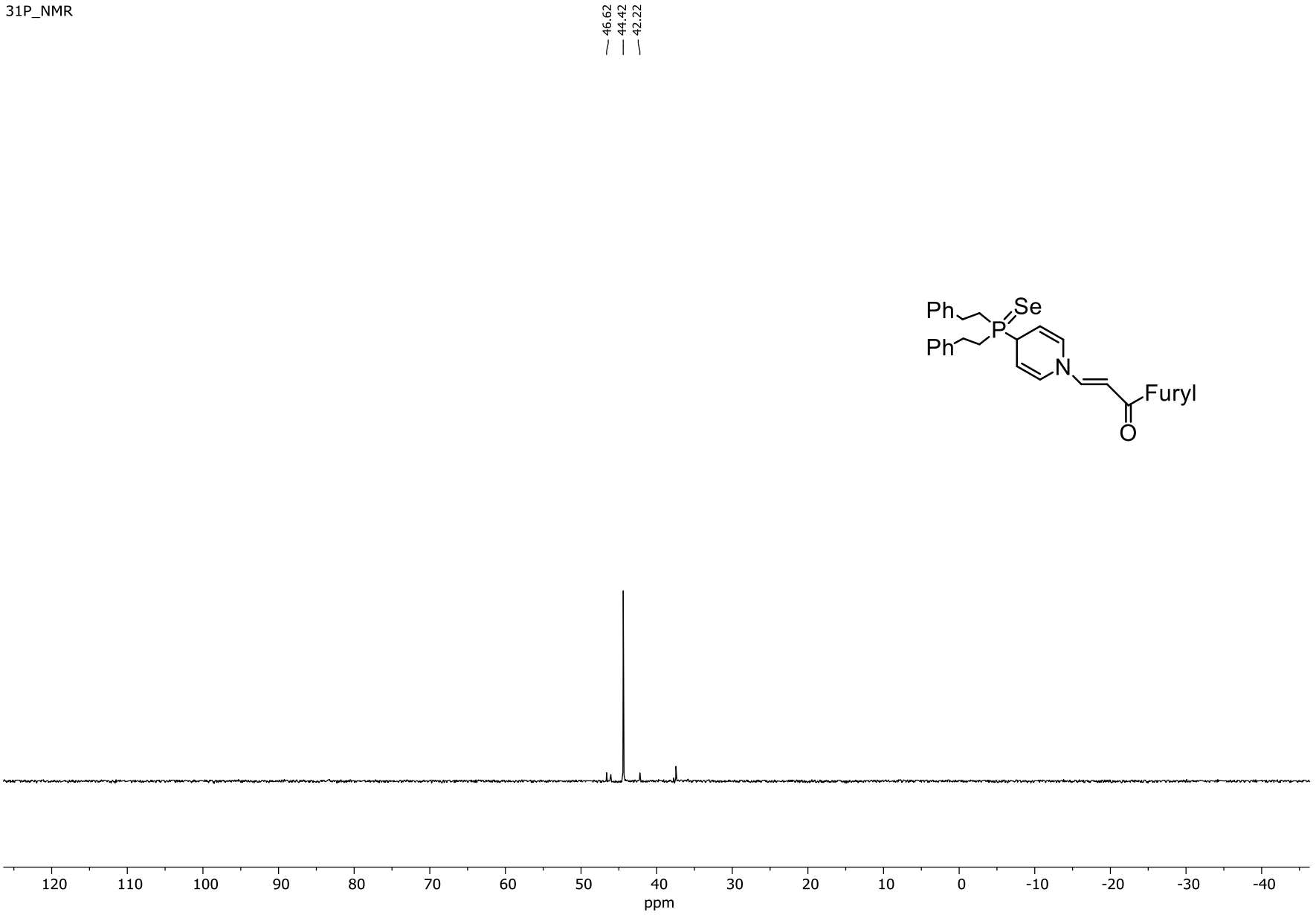
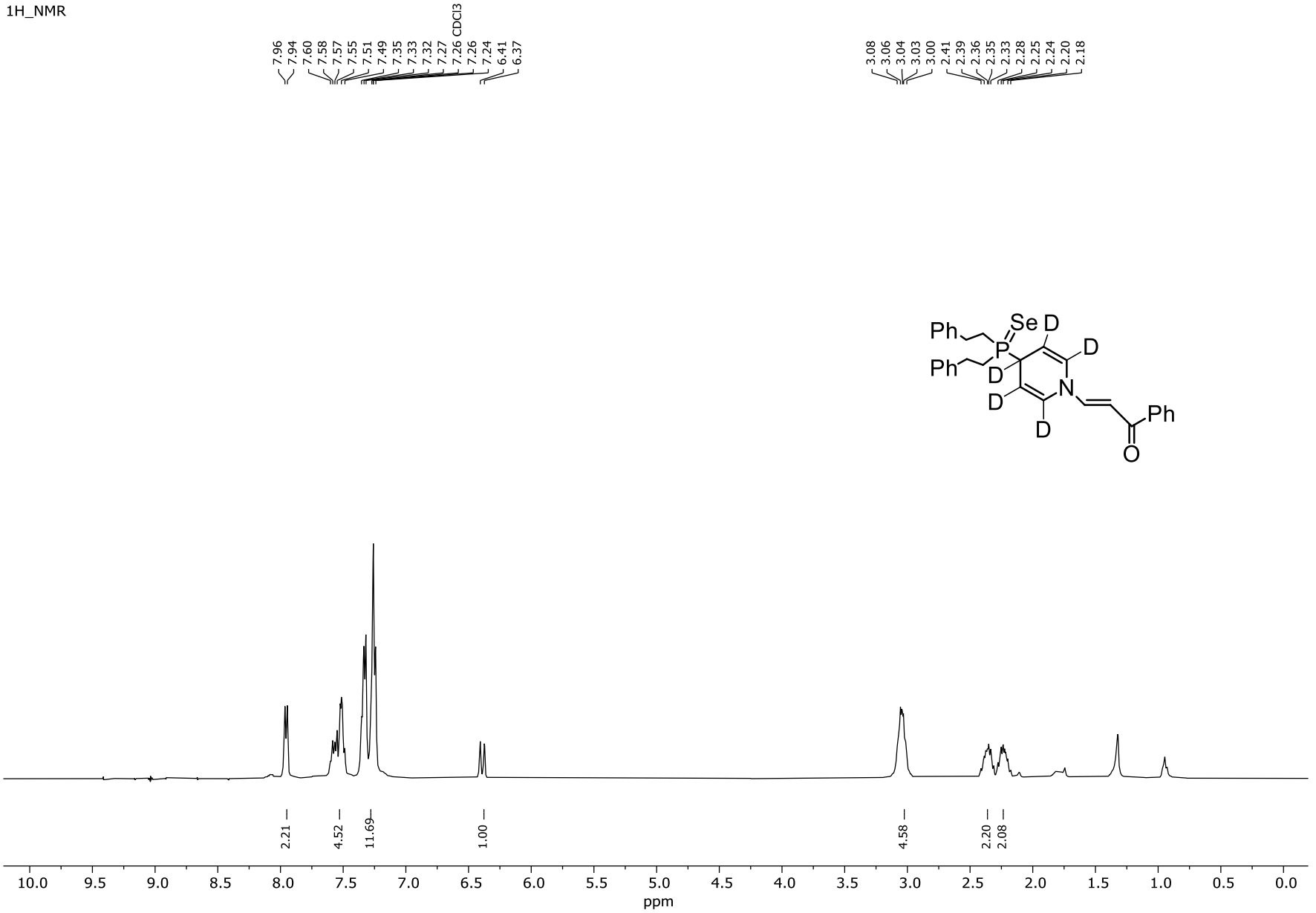
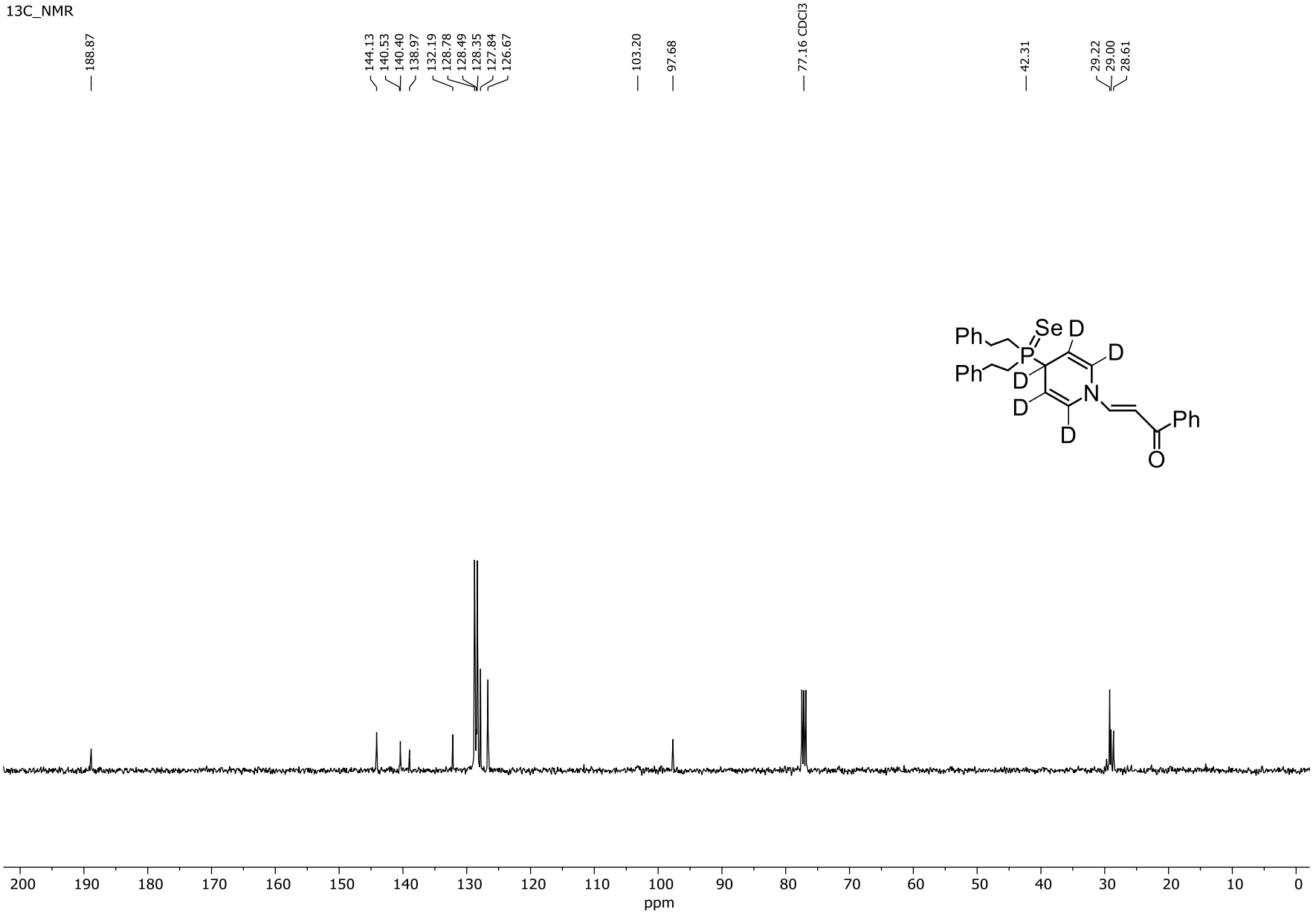


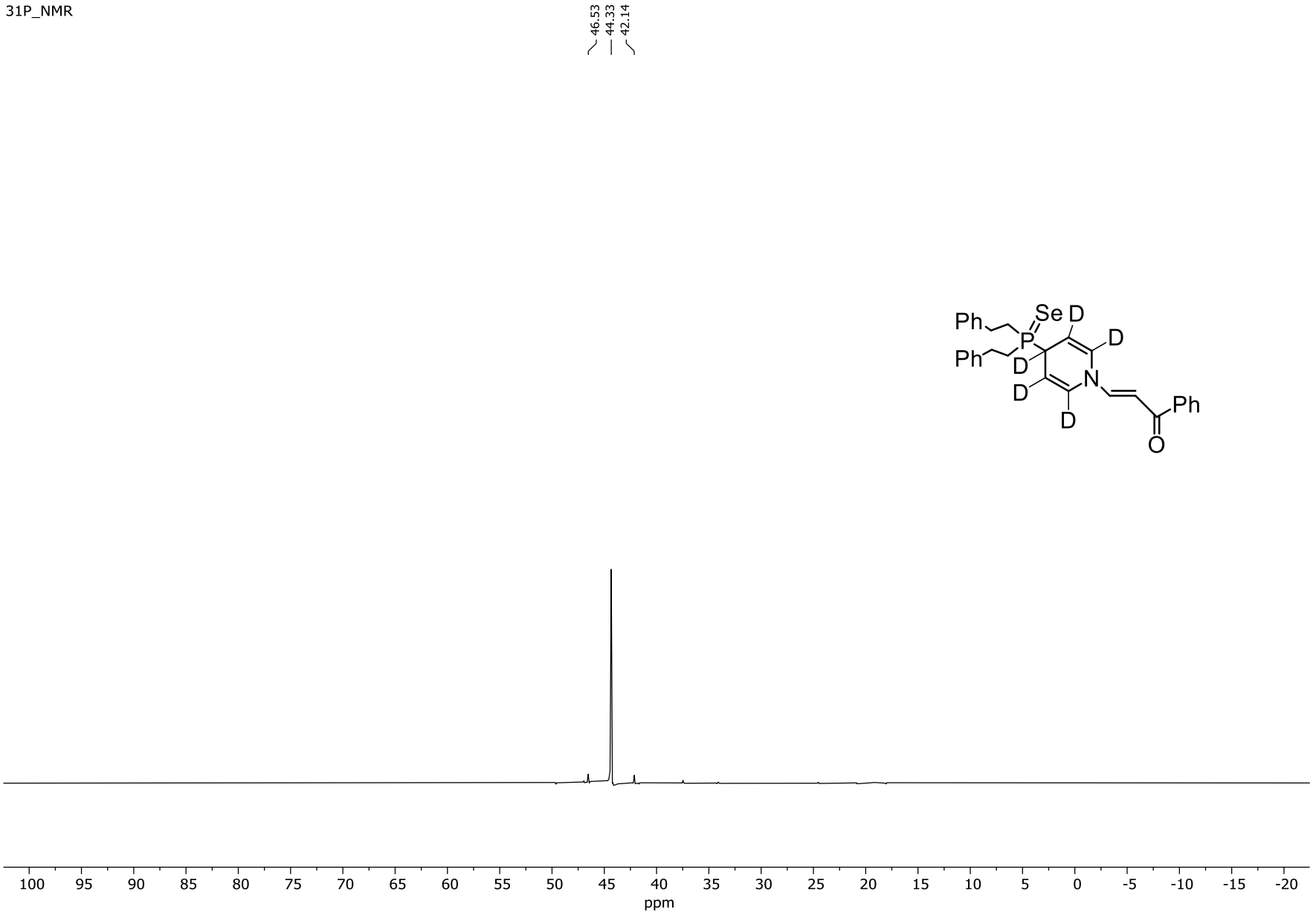
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-phenylprop-2-en-1-one (7h)



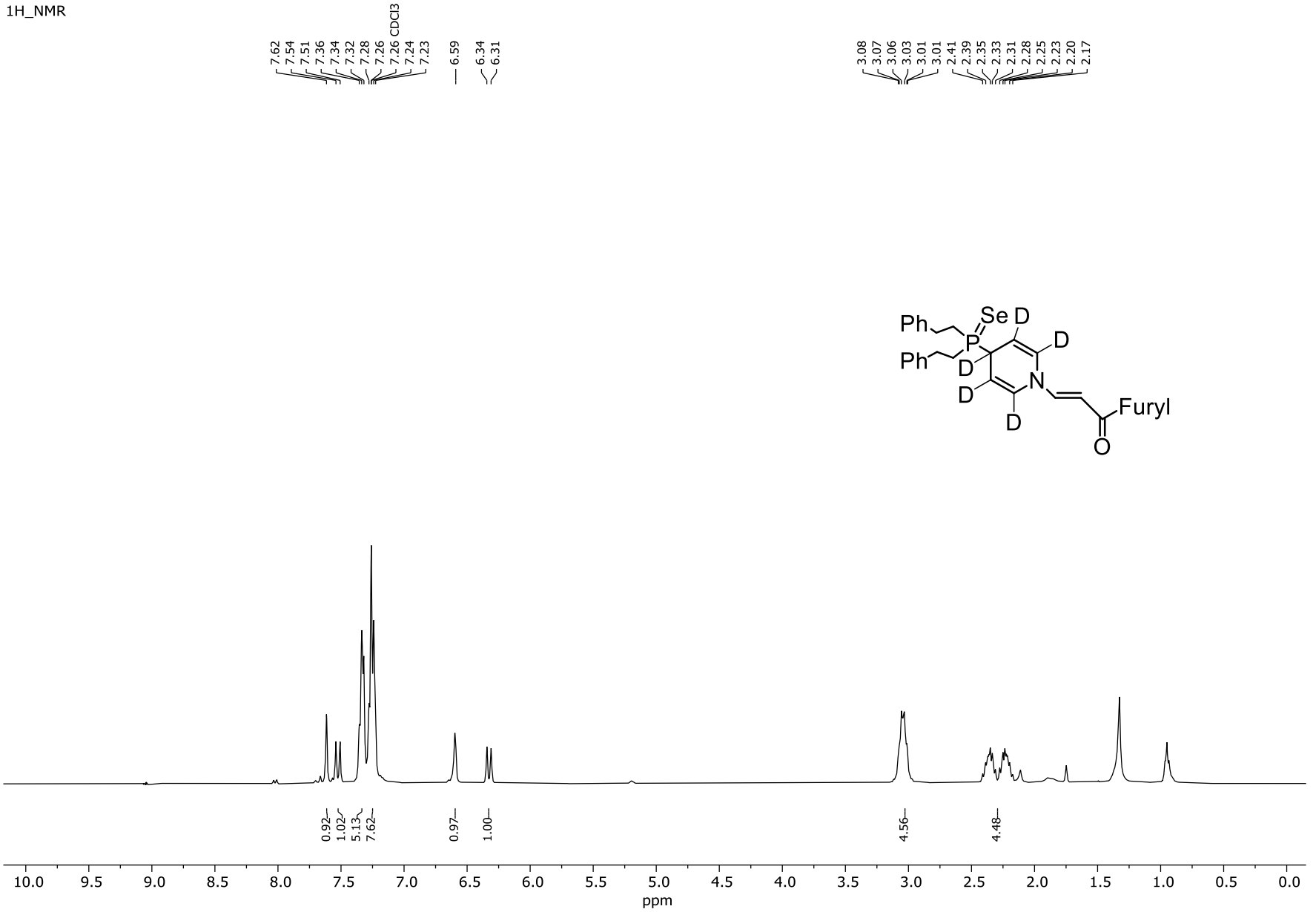
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-phenylprop-2-en-1-one (7h)



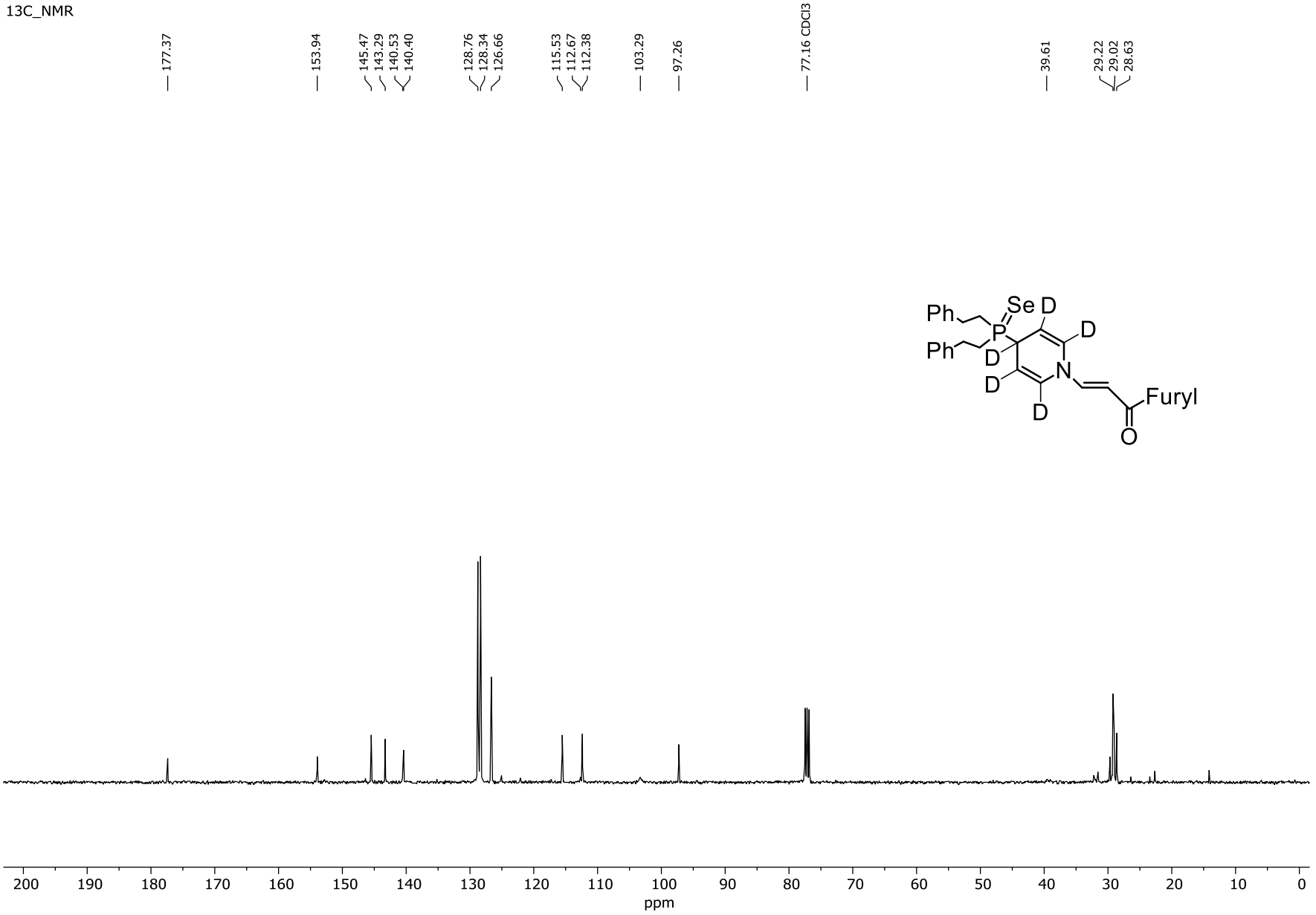
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-phenylprop-2-en-1-one (7h)



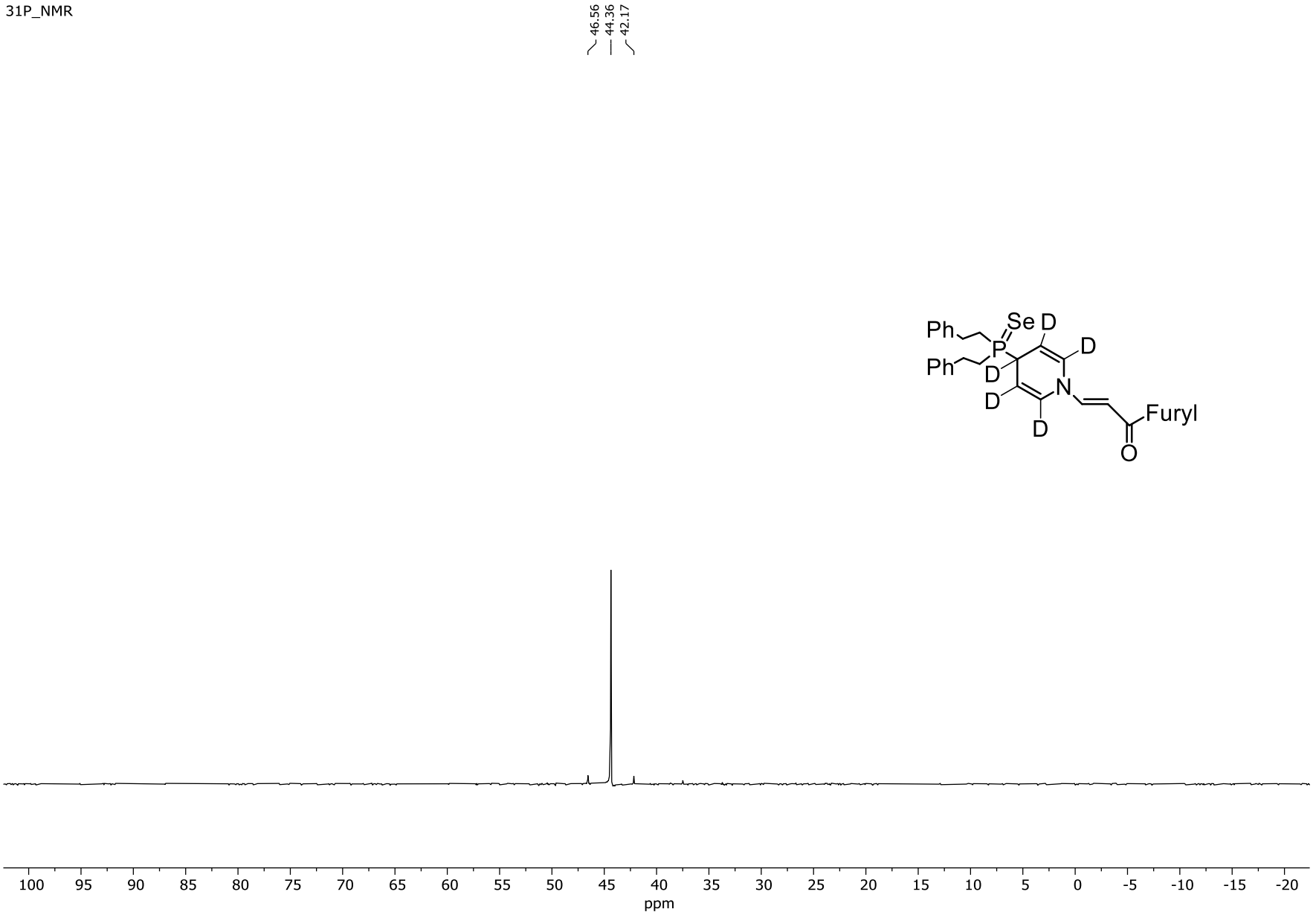
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-(furan-2-yl)prop-2-en-1-one (7i)



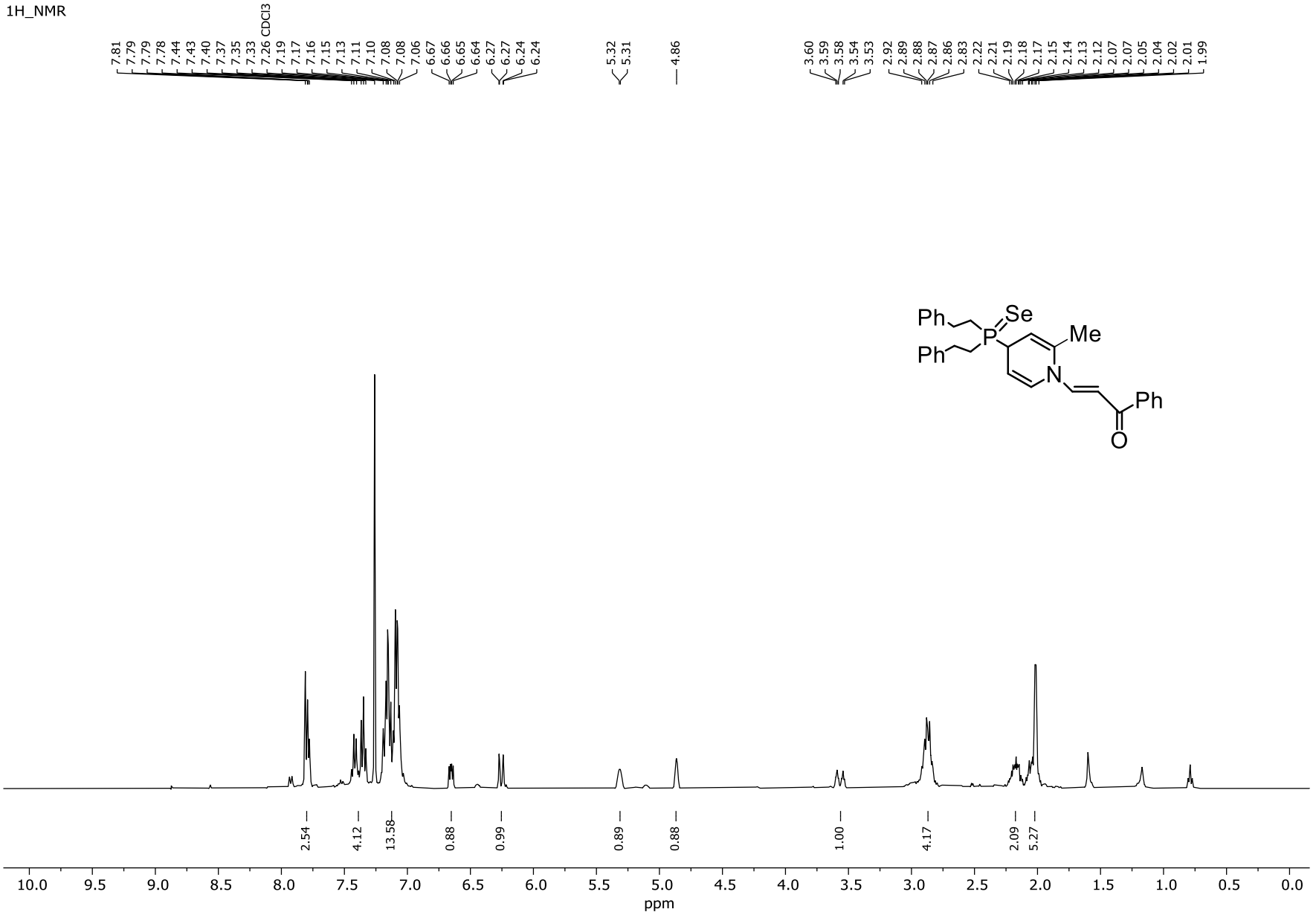
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-(furan-2-yl)prop-2-en-1-one (7i)



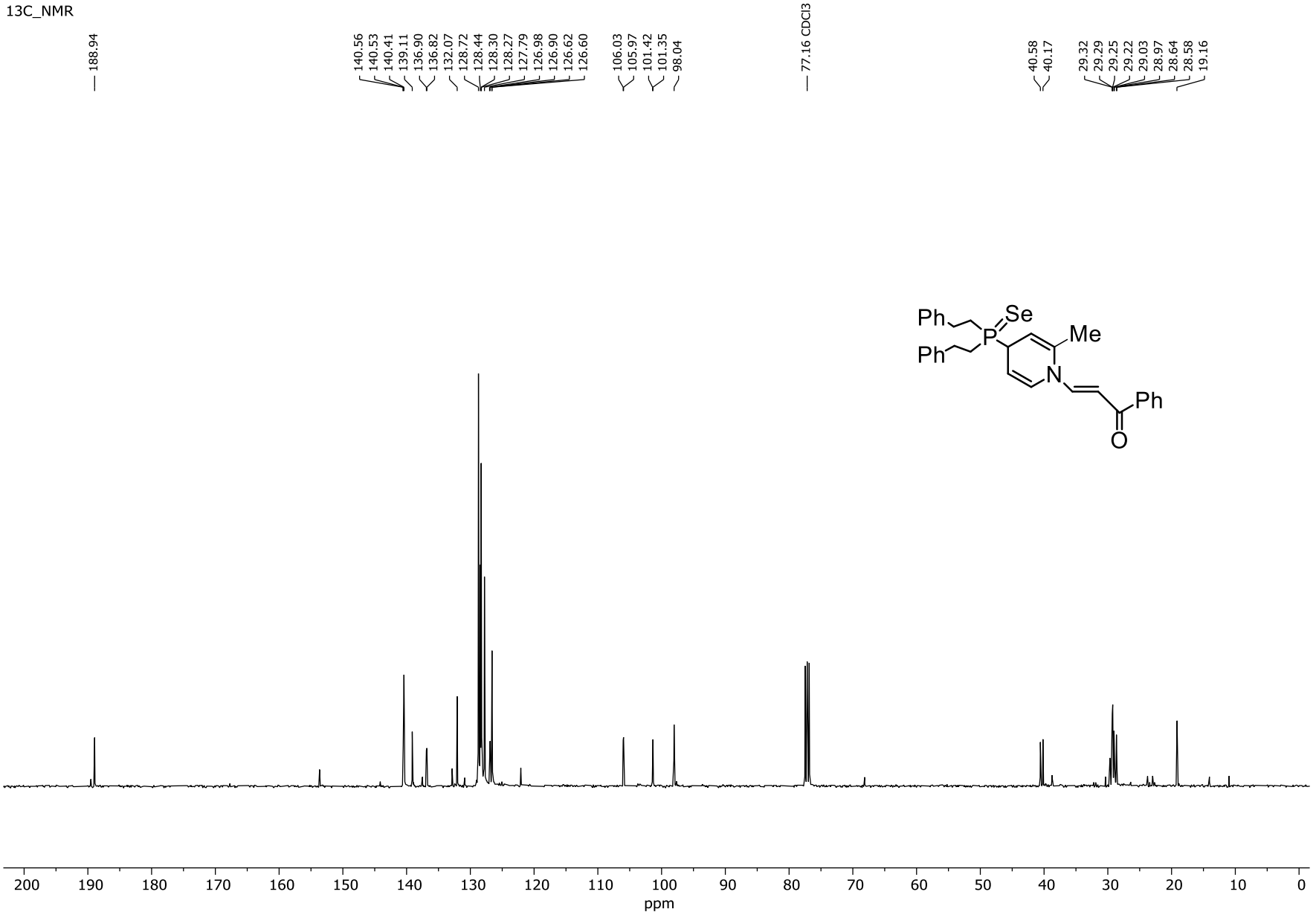
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]pyridin-1(4*H*)-yl-2,3,4,5,6-d_5}-1-(furan-2-yl)prop-2-en-1-one (7i)



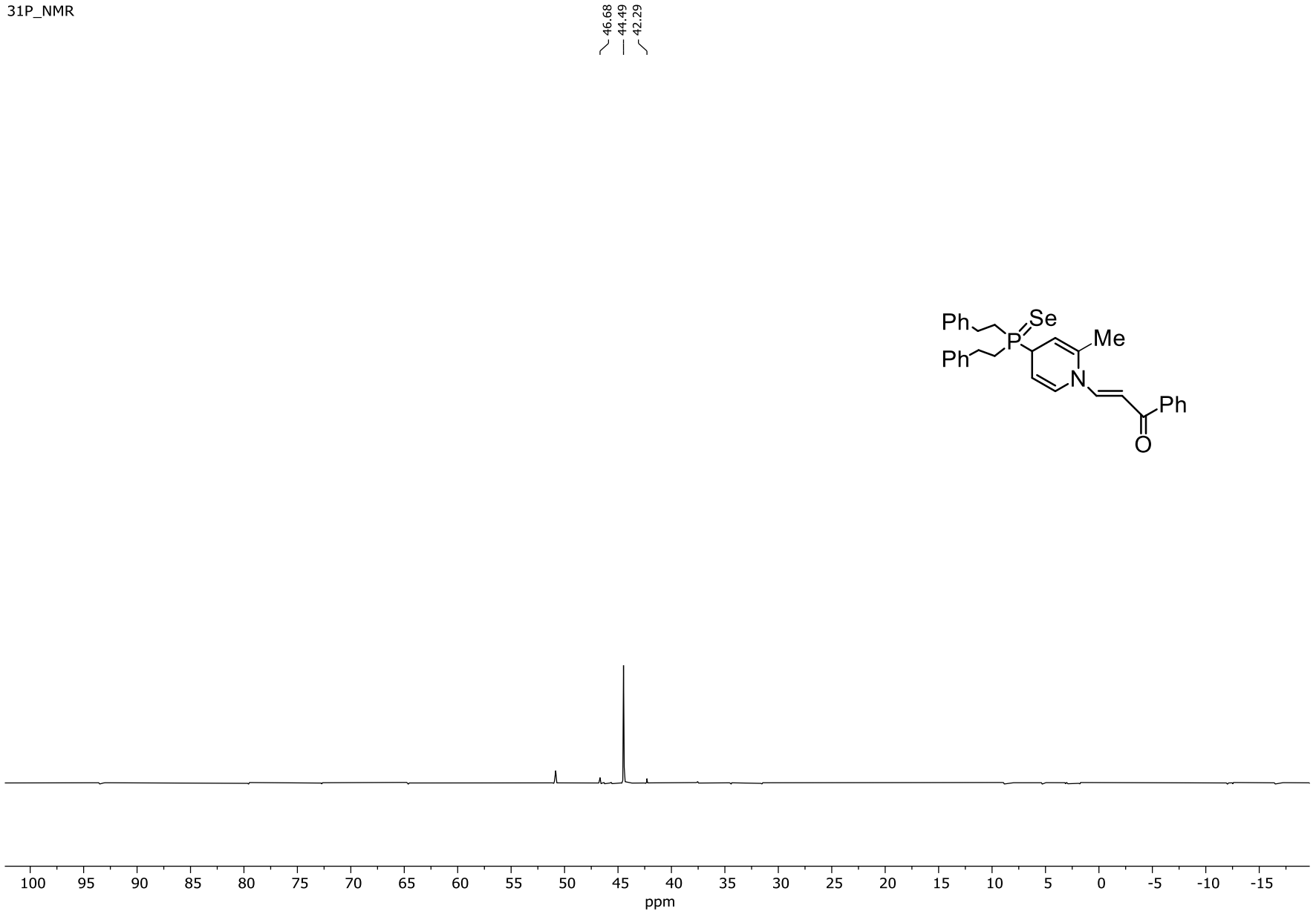
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-2-methylpyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7j)



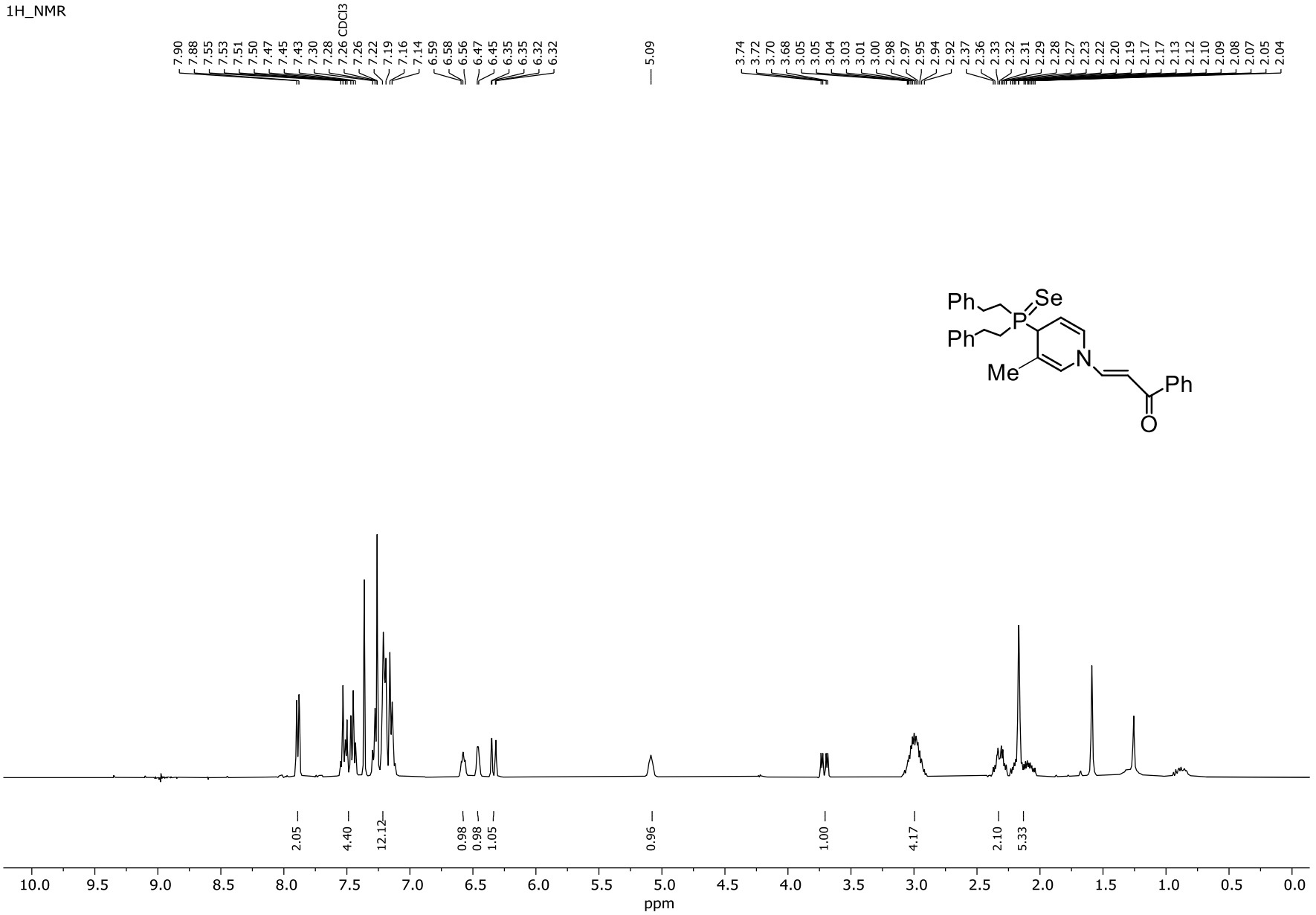
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-2-methylpyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7j)



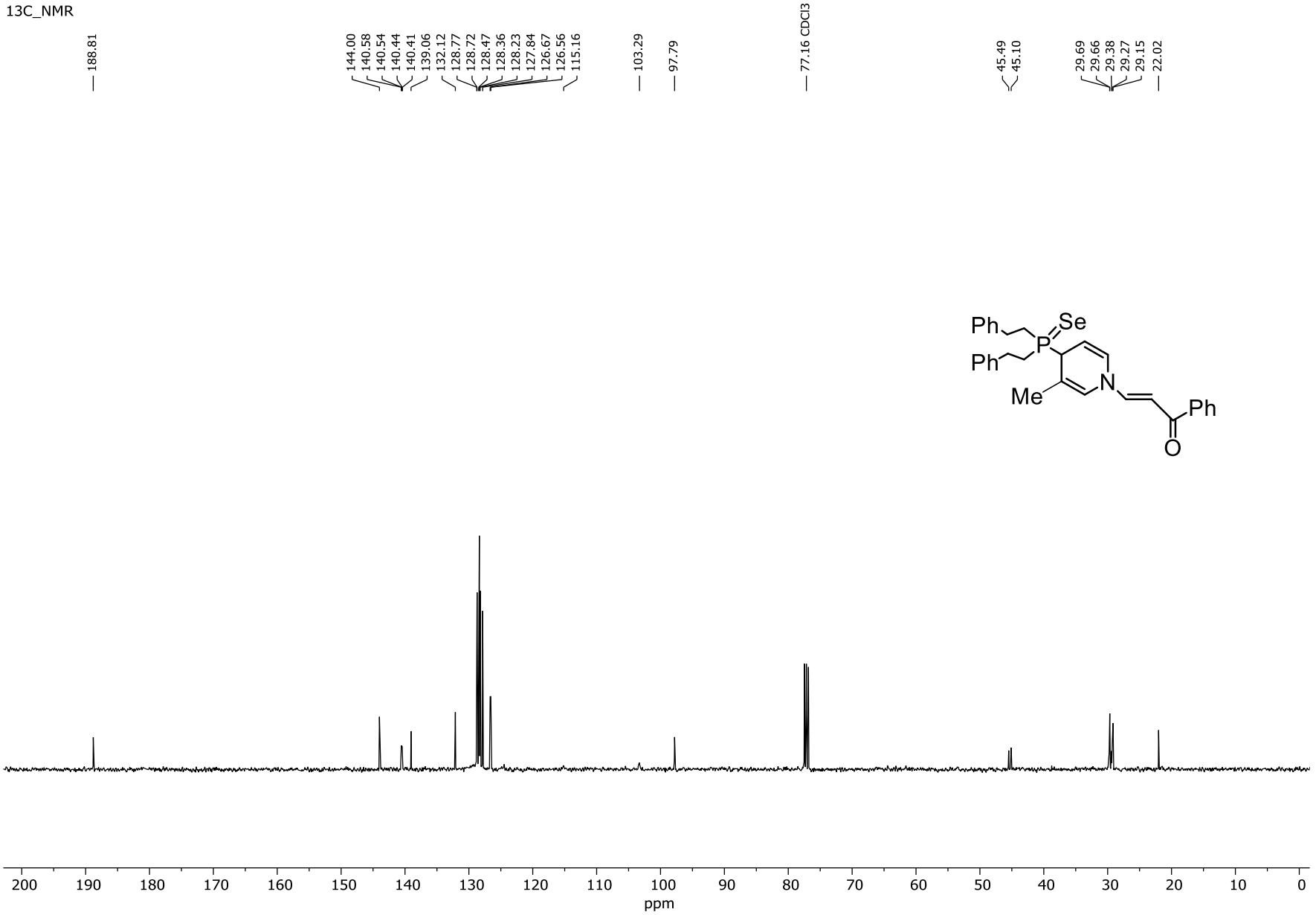
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-2-methylpyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7j)



(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7k)



(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7k)



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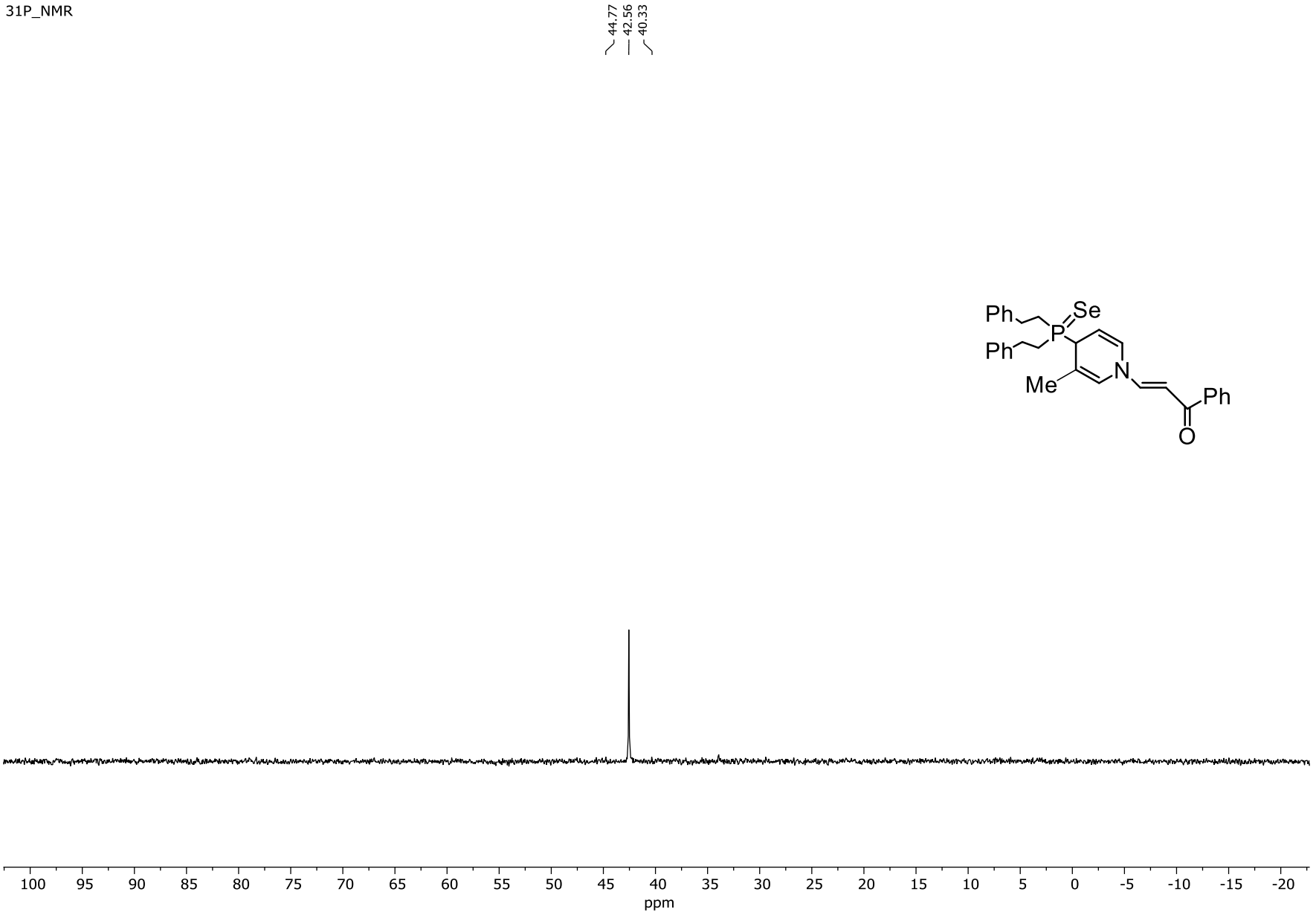
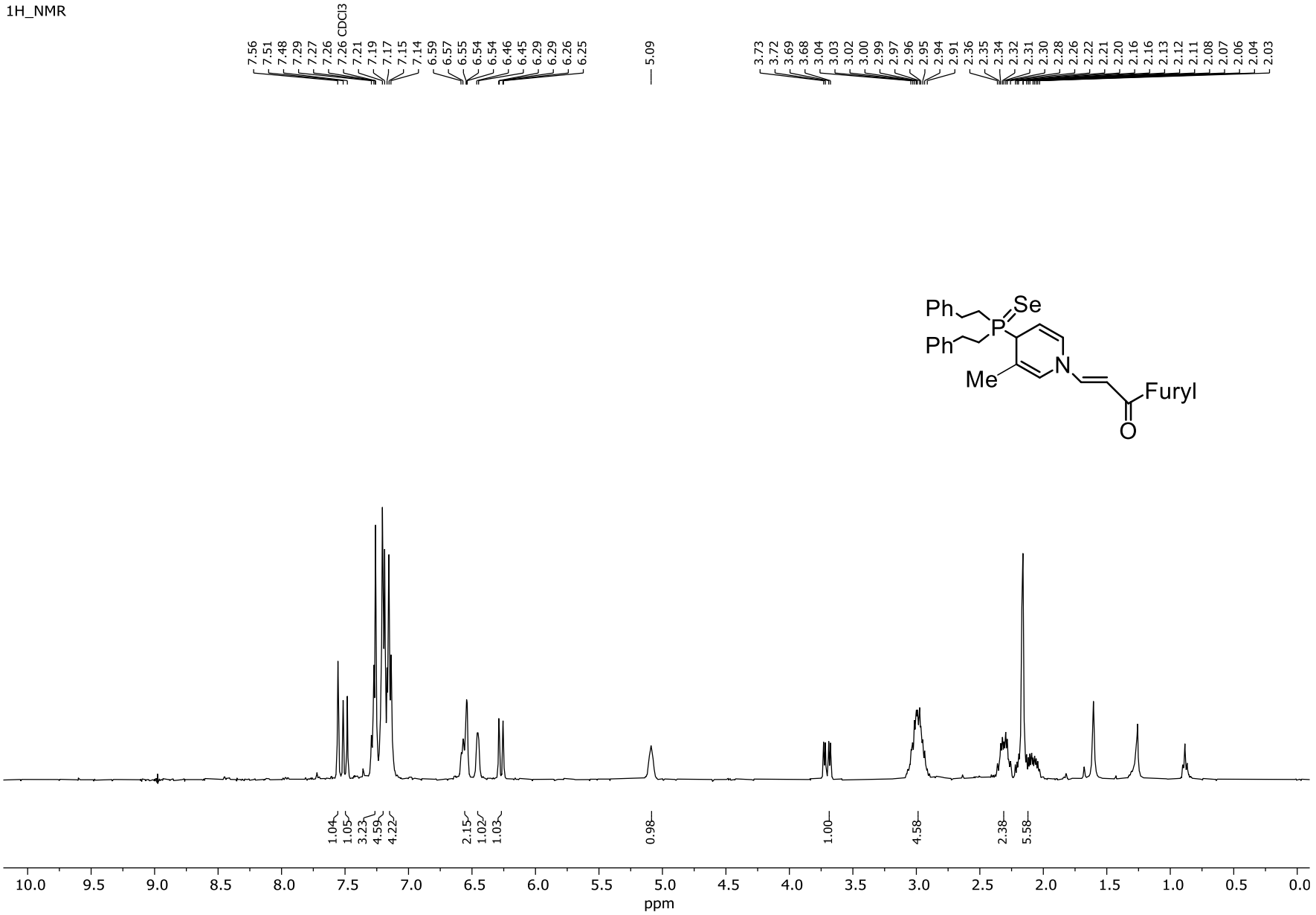
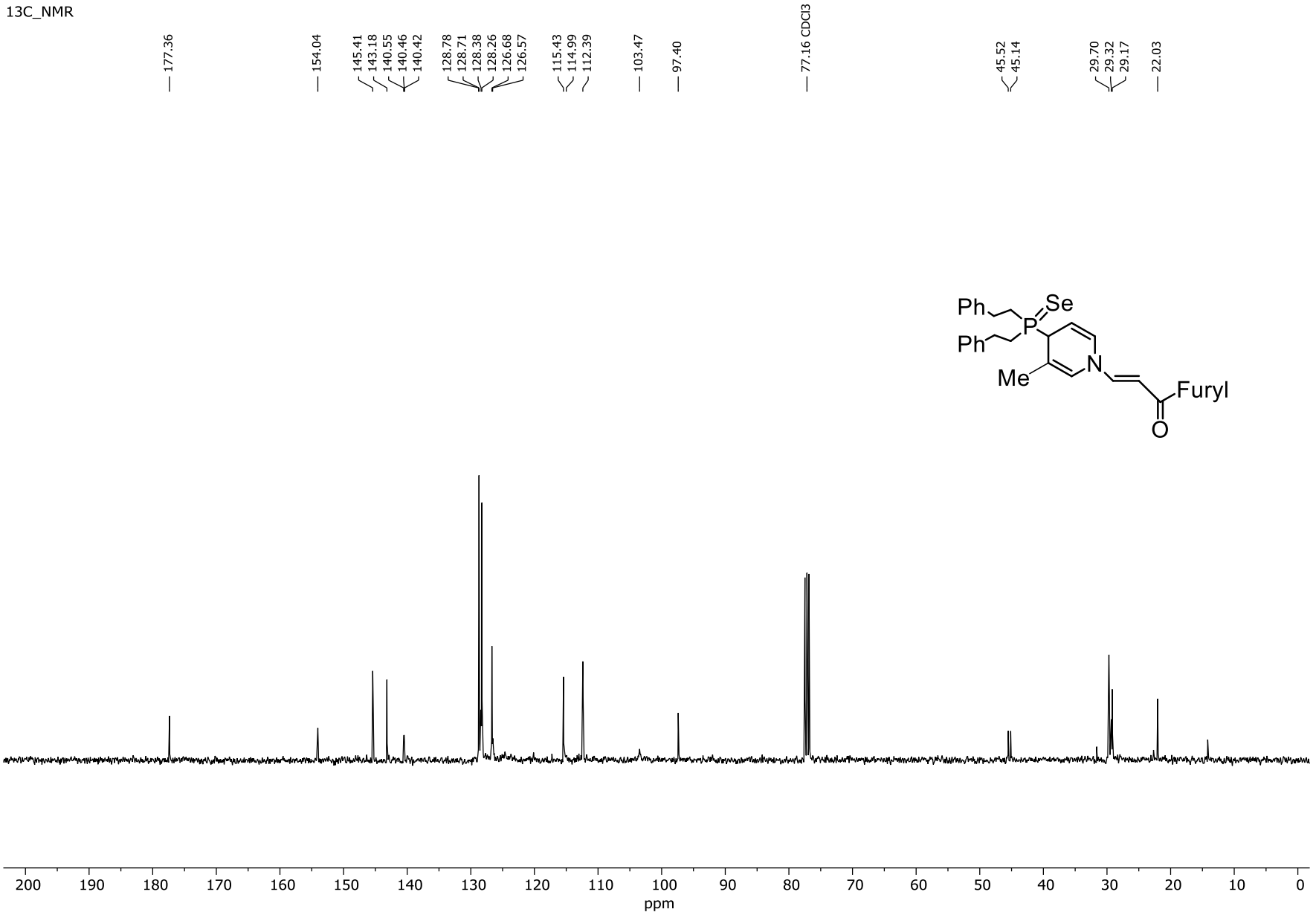


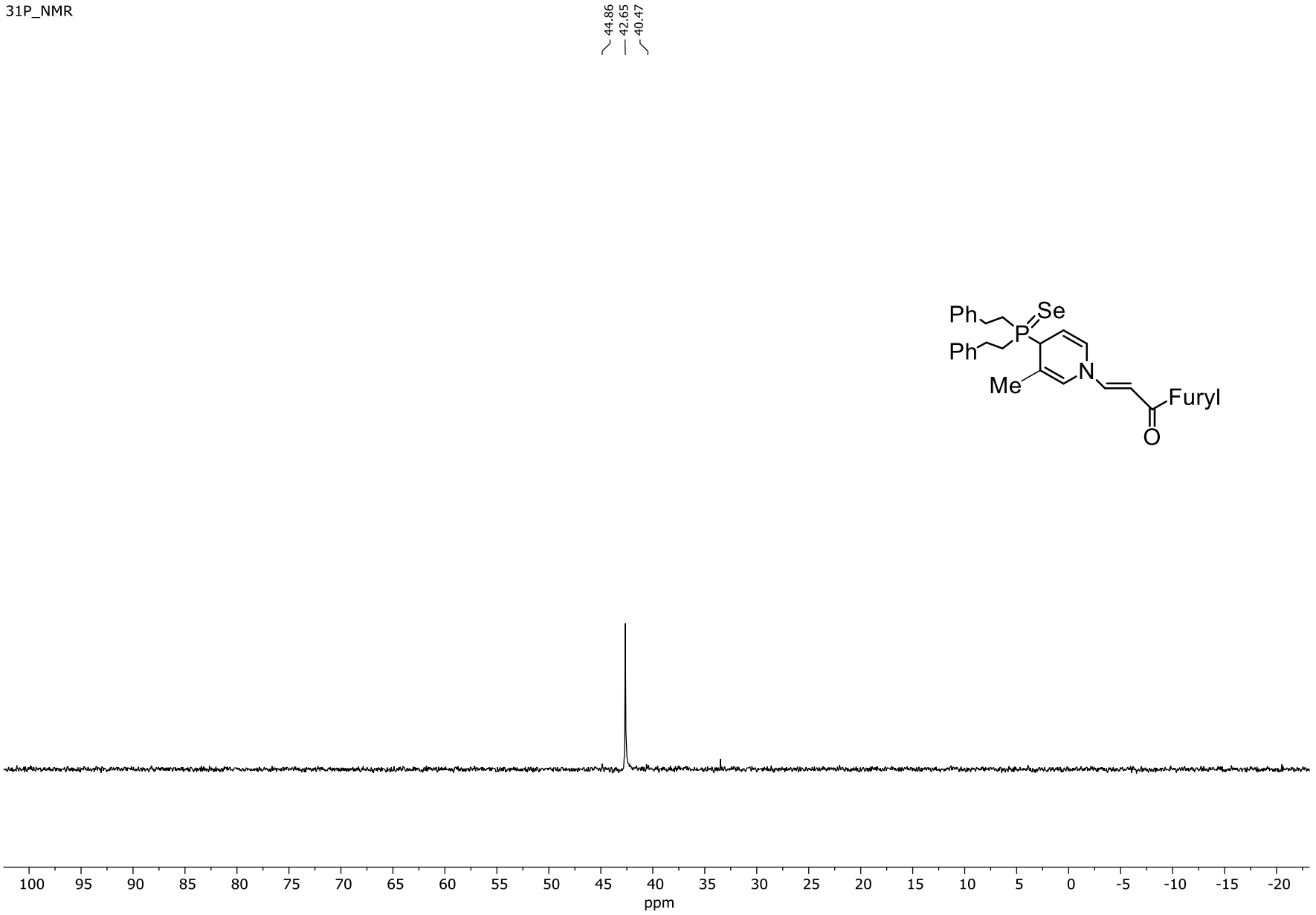
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridin-1(4*H*)-yl}-1-(furan-2-yl)prop-2-en-1-one (7l)



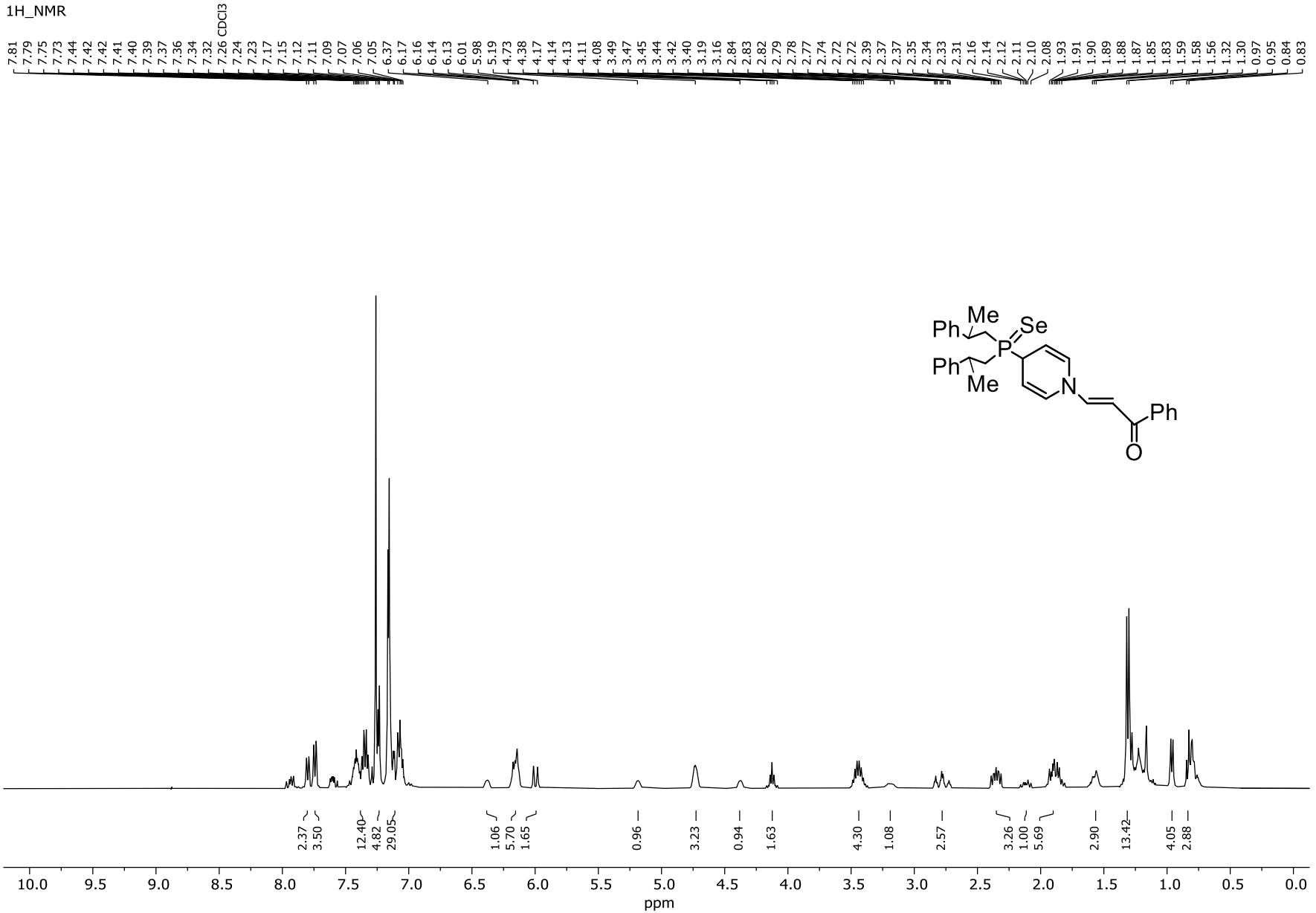
(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridin-1(4*H*)-yl}-1-(furan-2-yl)prop-2-en-1-one (7l)



(2*E*)-3-{4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridin-1(4*H*)-yl}-1-(furan-2-yl)prop-2-en-1-one (7l)



(2*E*)-3-{4-[Bis(2-phenylpropyl)selenophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7n)



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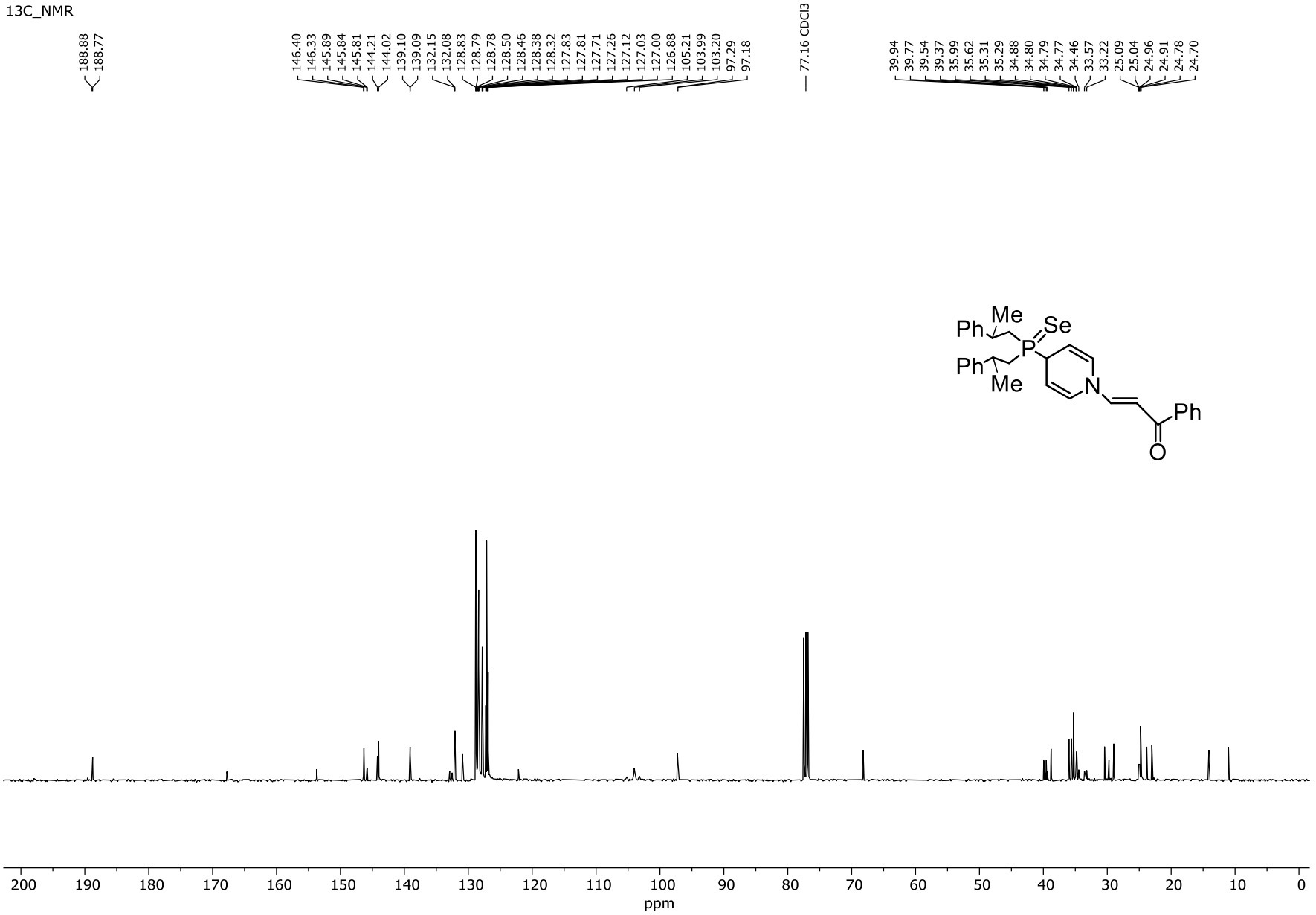
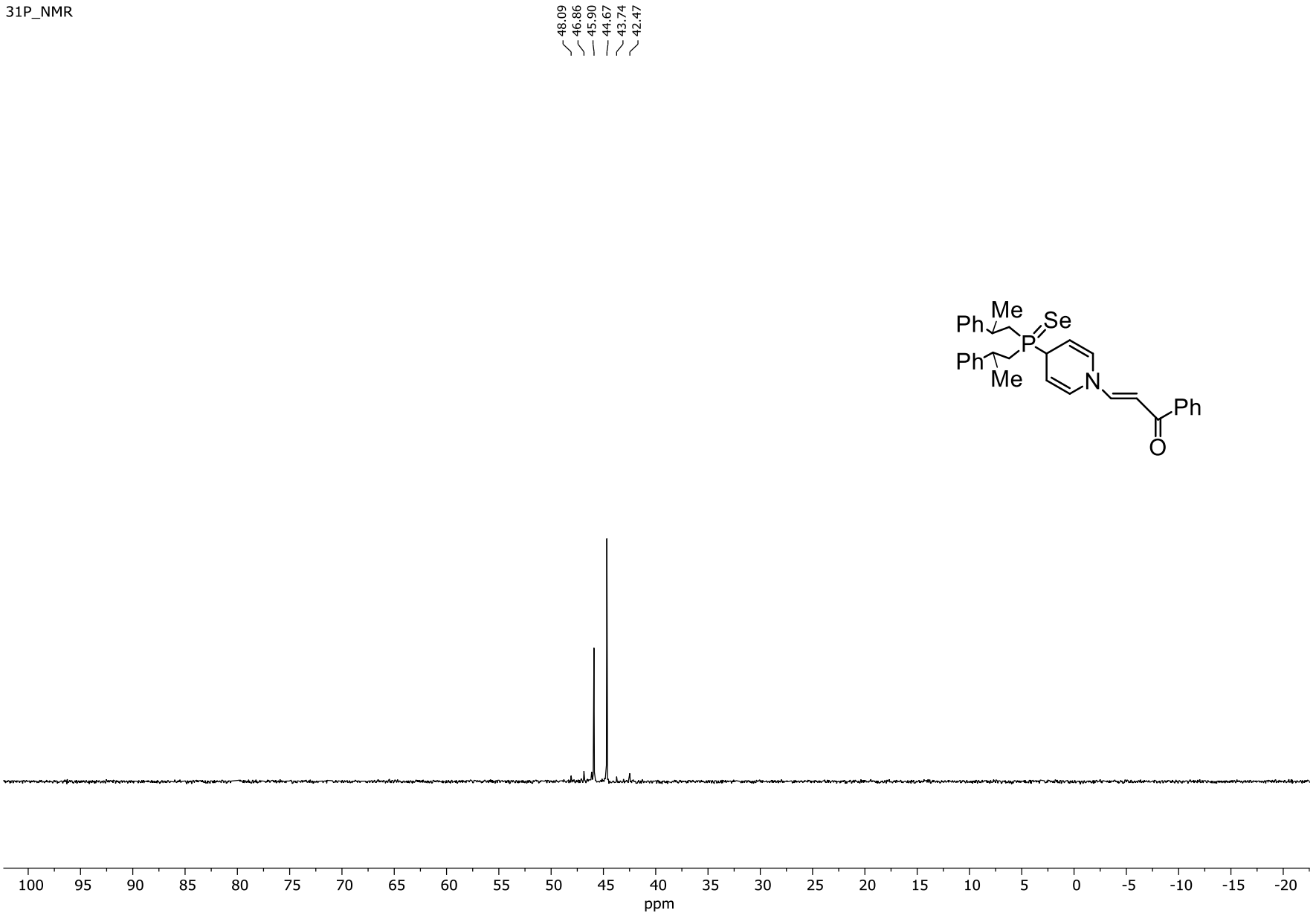
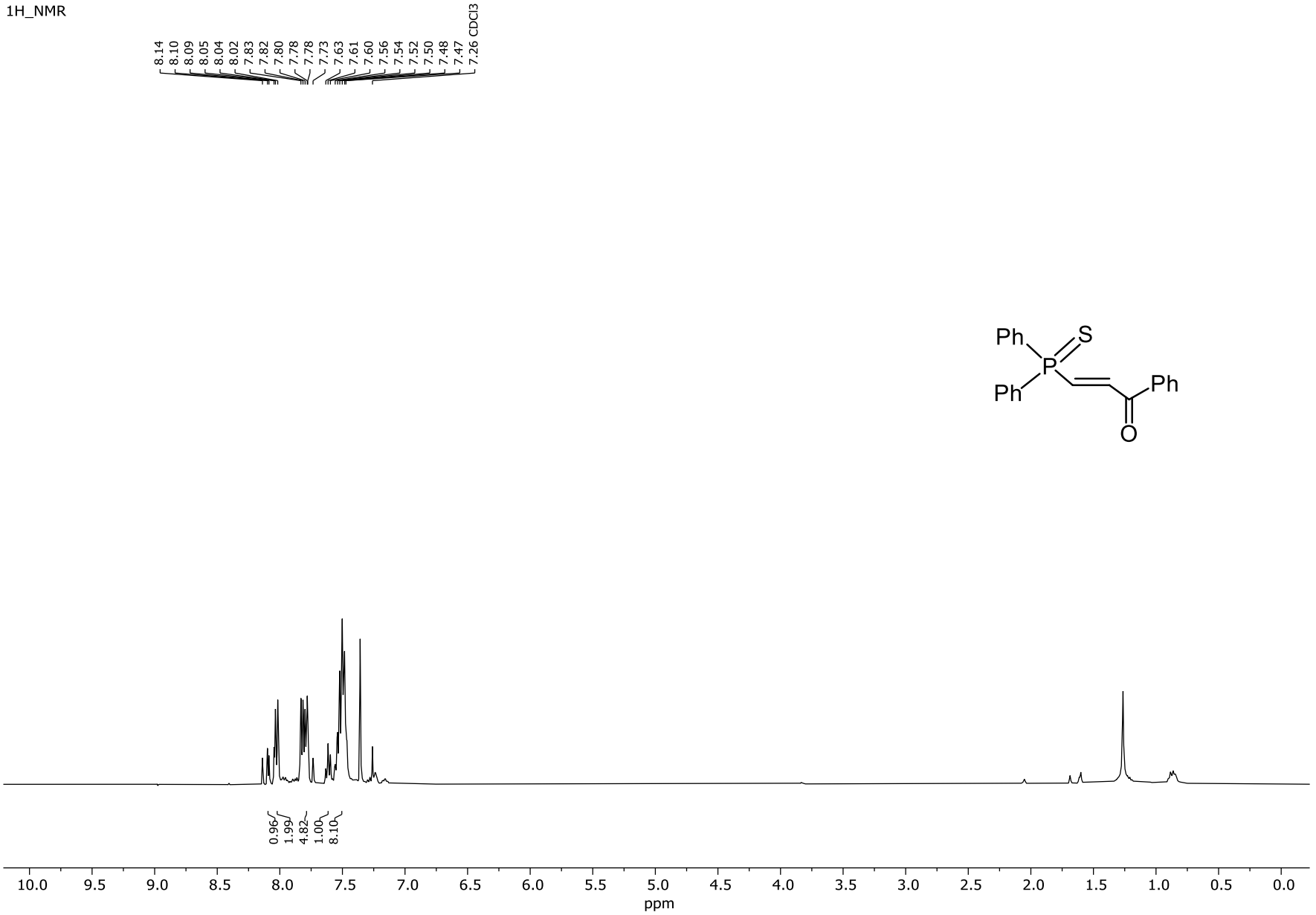


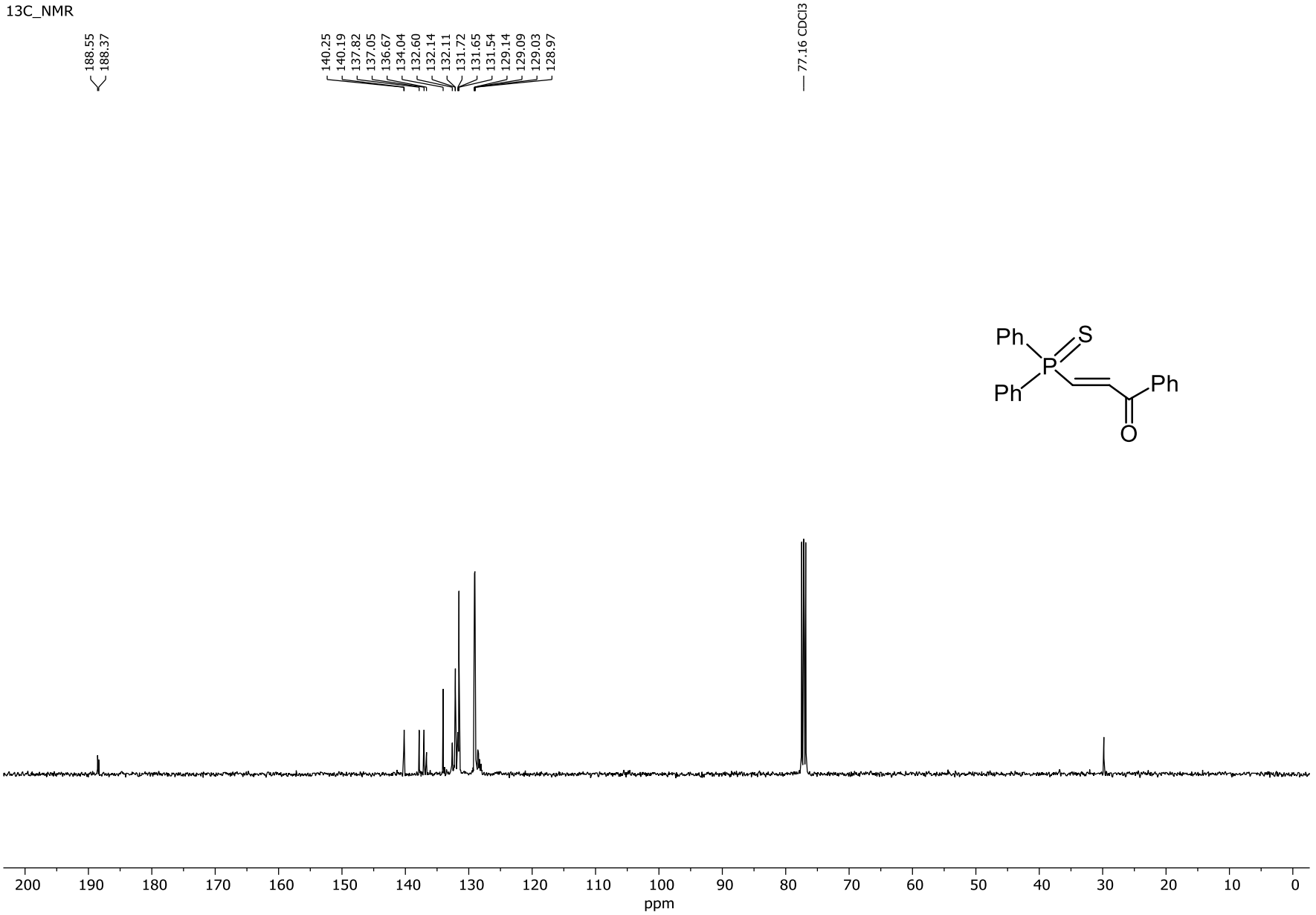
(2*E*)-3-{4-[Bis(2-phenylpropyl)selenophosphoryl]pyridin-1(4*H*)-yl}-1-phenylprop-2-en-1-one (7n)



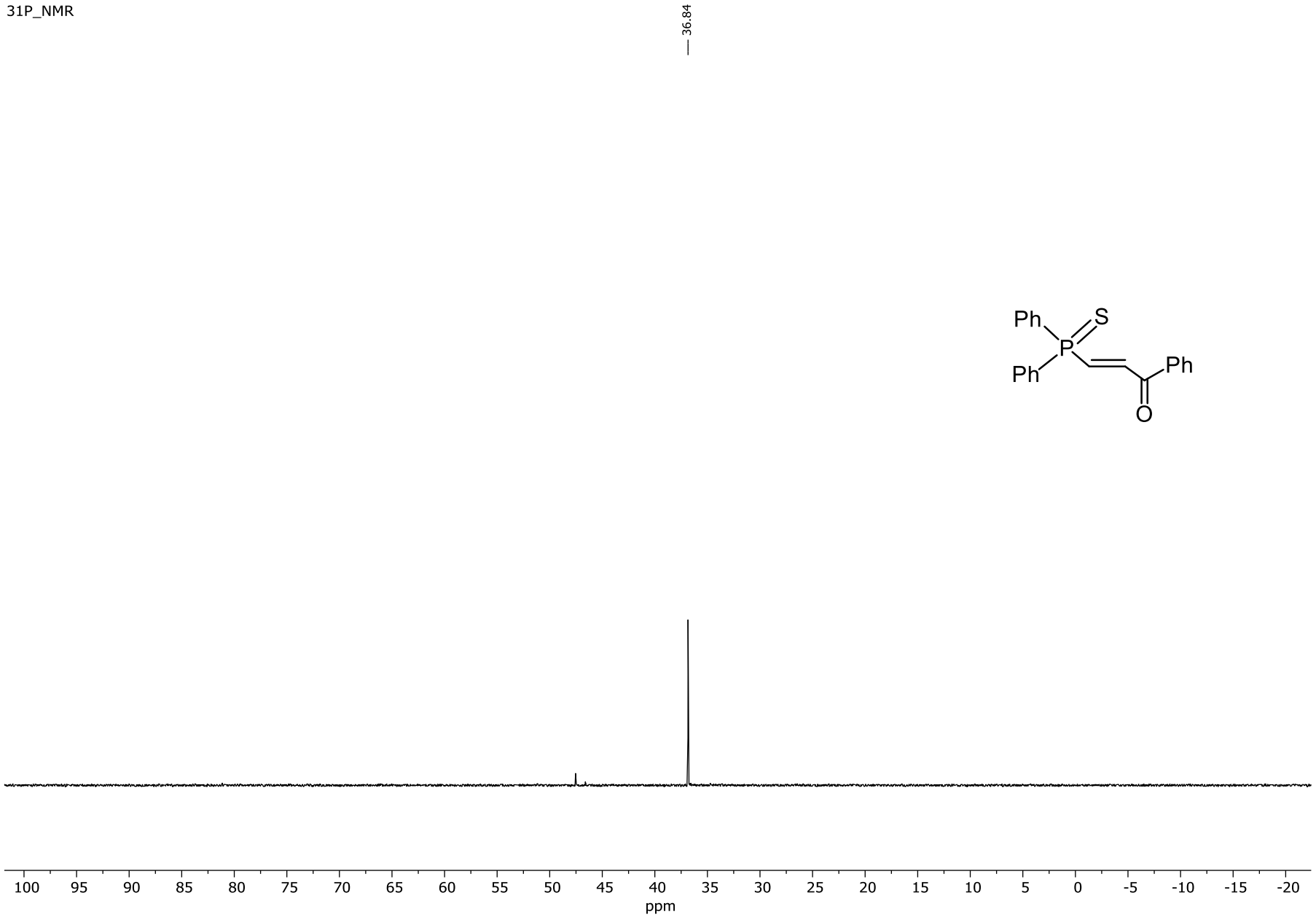
(2*E*)-3-(Diphenylthiophosphoryl)-1-phenylprop-2-en-1-one (8a)



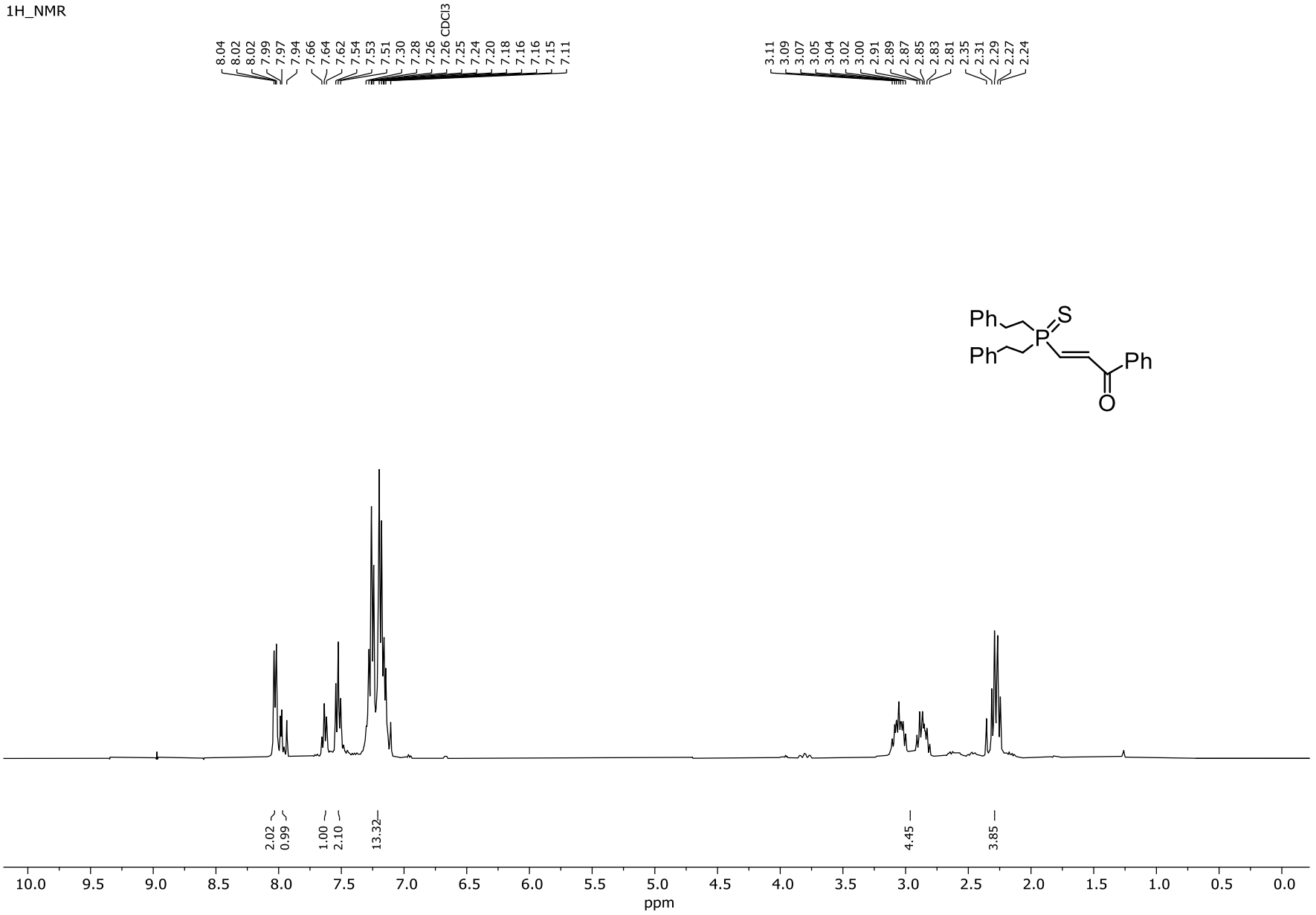
(2*E*)-3-(Diphenylthiophosphoryl)-1-phenylprop-2-en-1-one (8a)



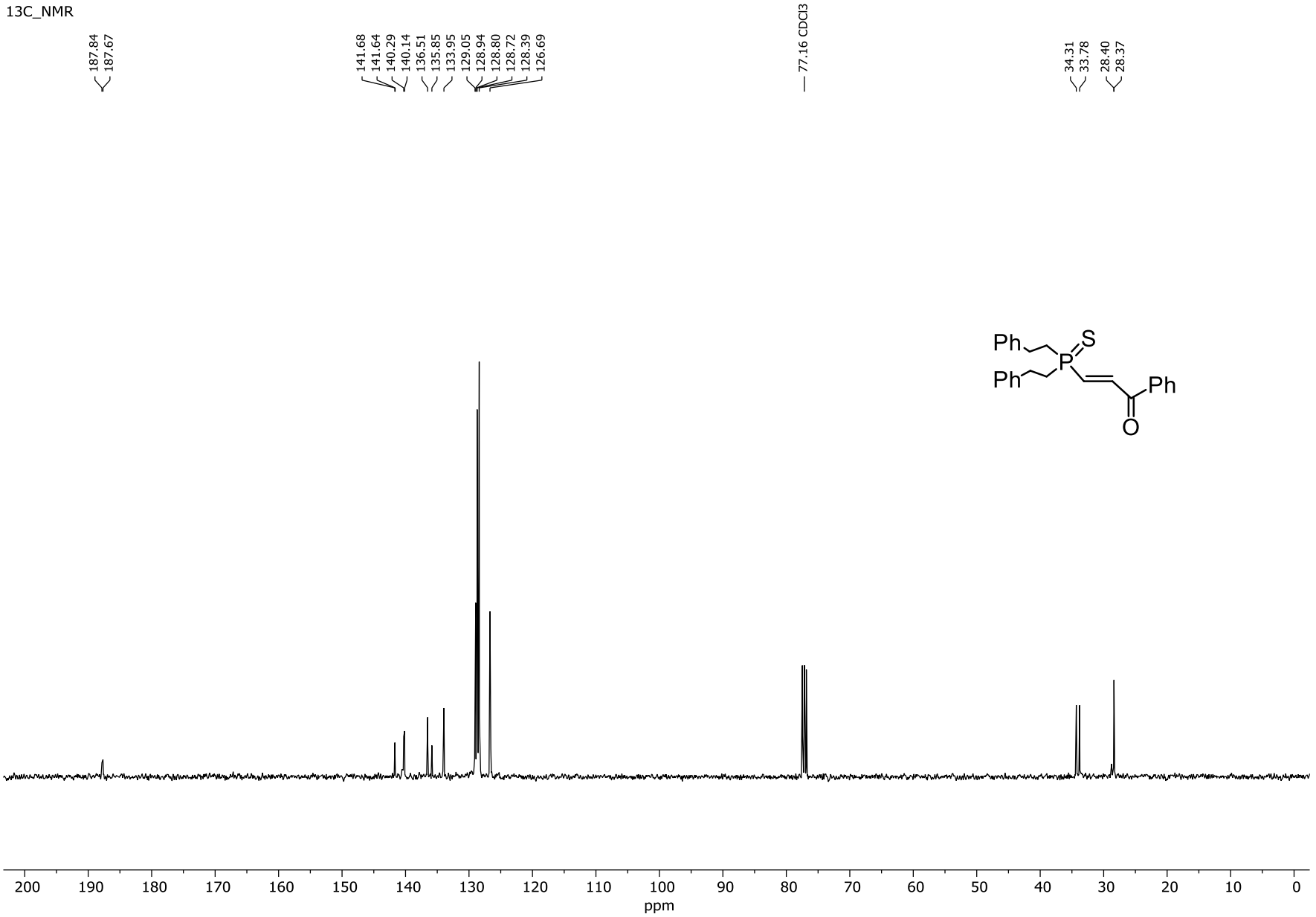
(2*E*)-3-(Diphenylthiophosphoryl)-1-phenylprop-2-en-1-one (8a)



(2*E*)-3-[Bis(2-phenylethyl)thiophosphoryl]-1-phenylprop-2-en-1-one (8b)



(2*E*)-3-[Bis(2-phenylethyl)thiophosphoryl]-1-phenylprop-2-en-1-one (8b)



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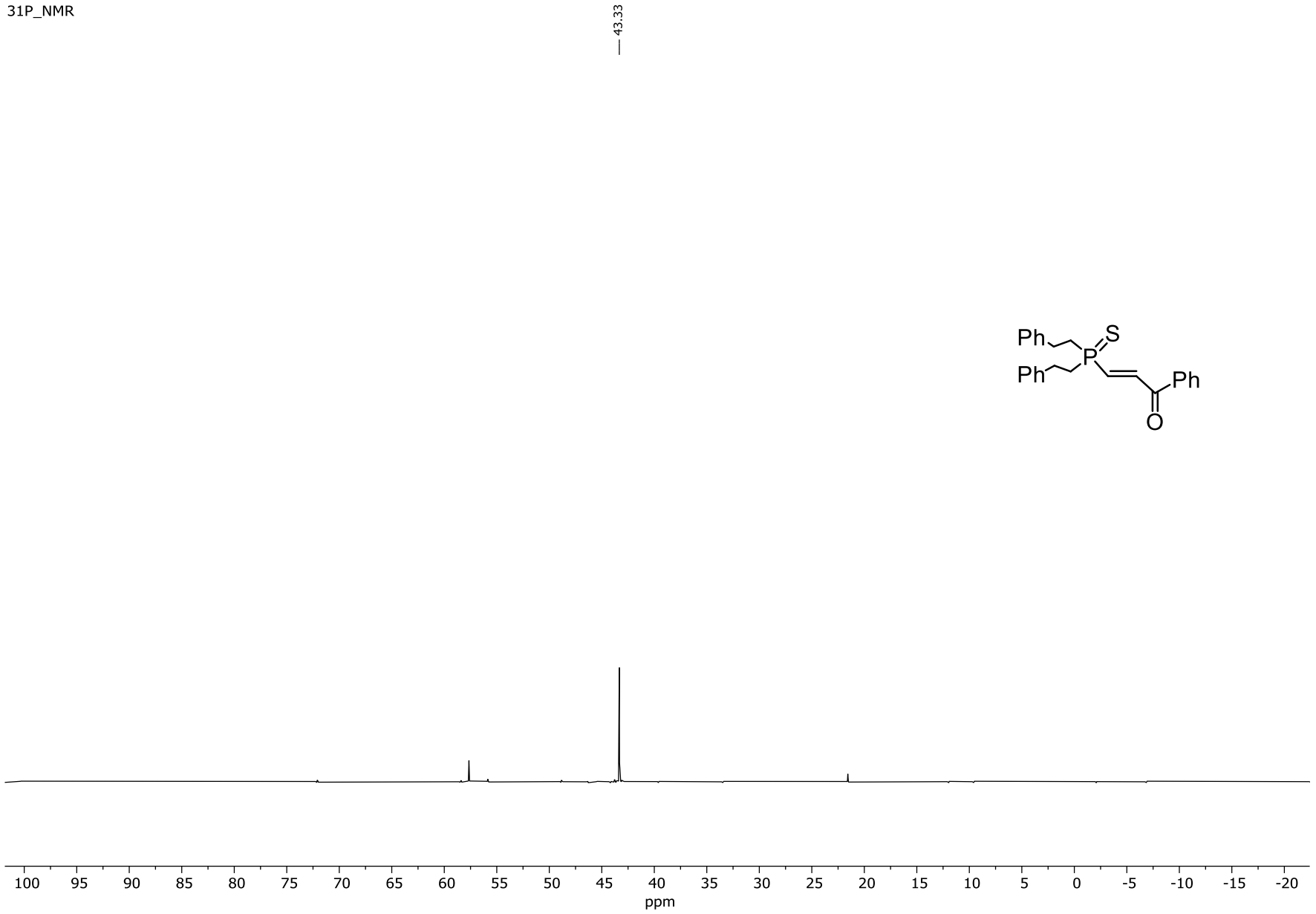
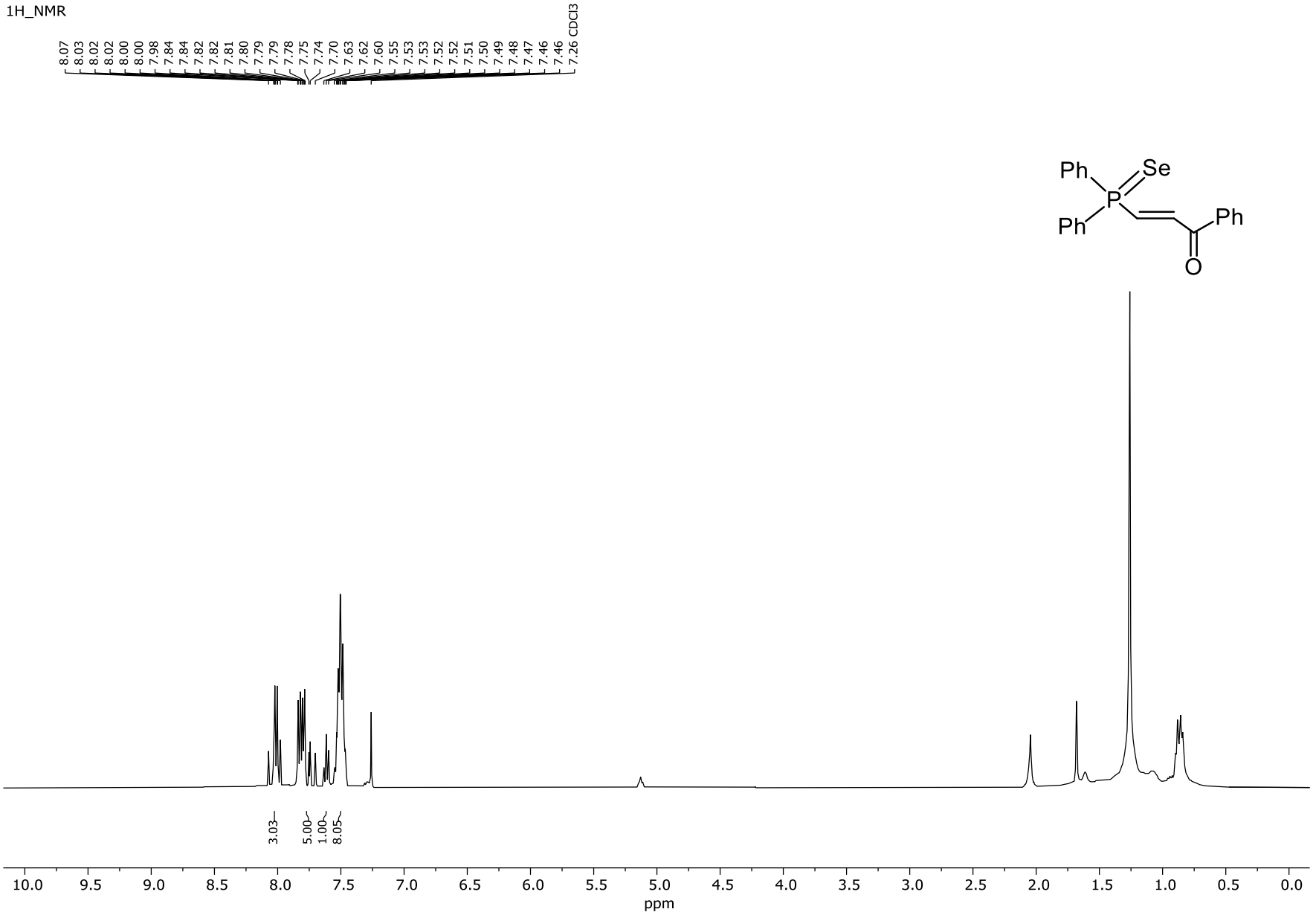
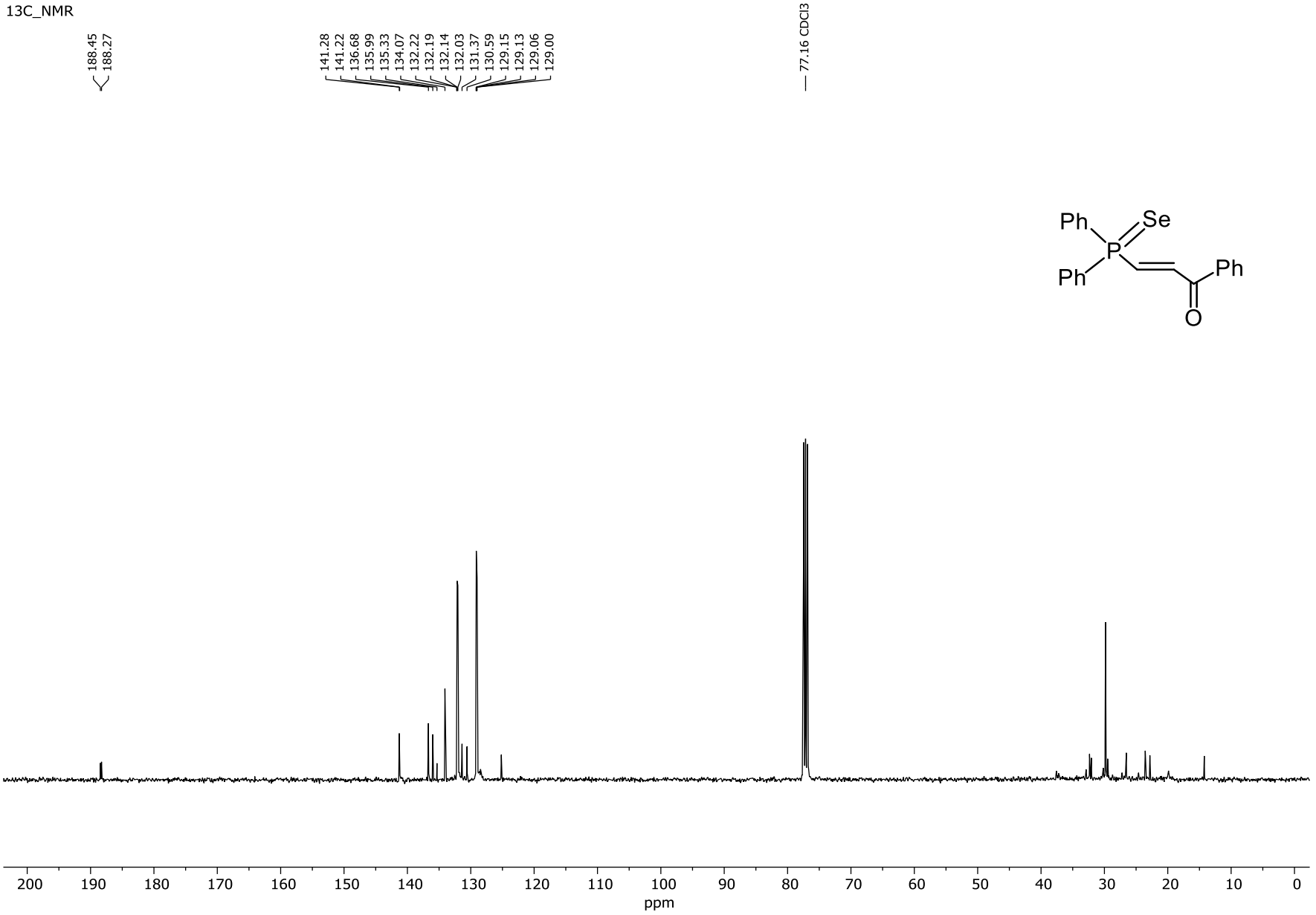


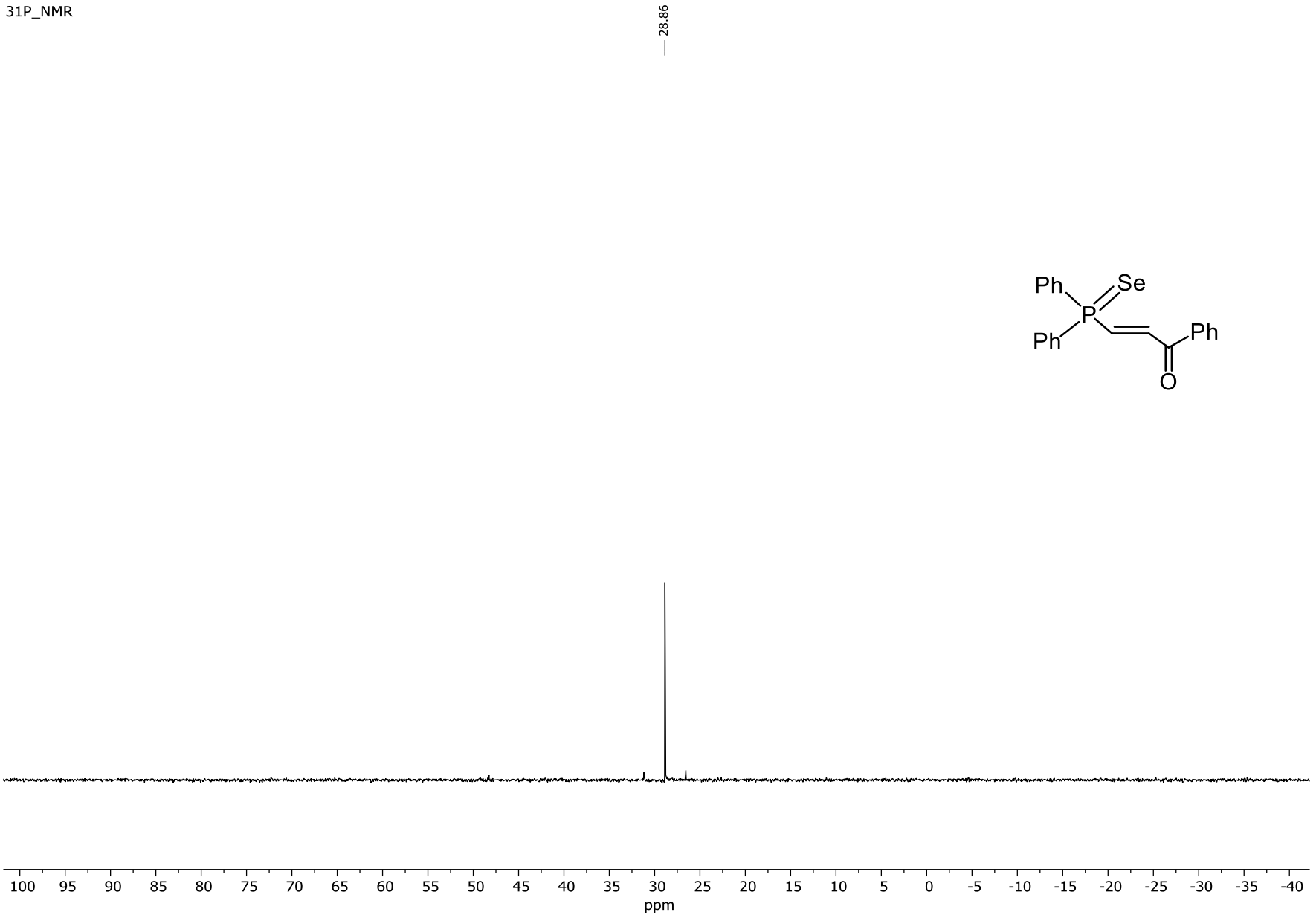
(2*E*)-3-(Diphenylselenophosphoryl)-1-phenylprop-2-en-1-one (8c)



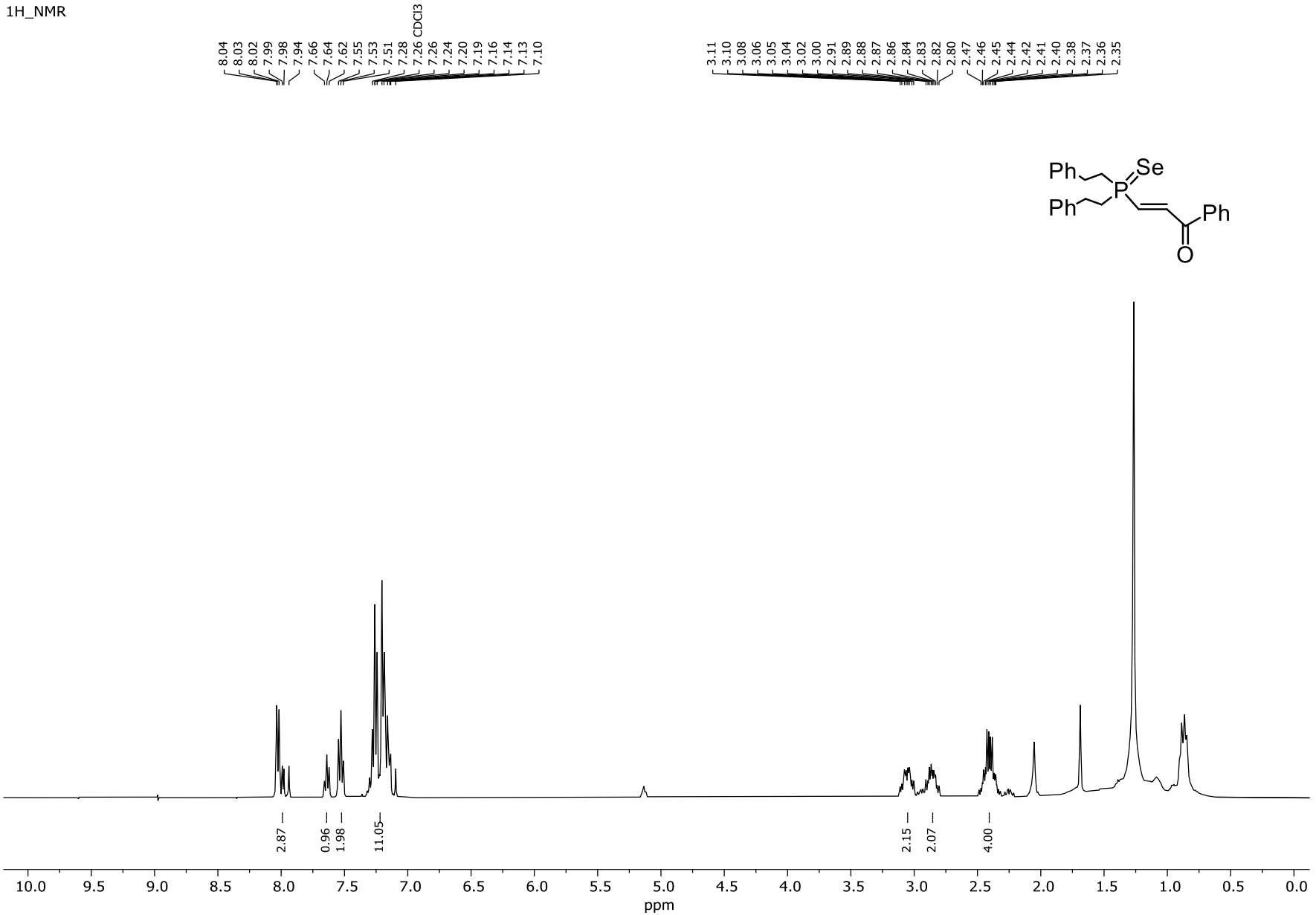
(2*E*)-3-(Diphenylselenophosphoryl)-1-phenylprop-2-en-1-one (8c)



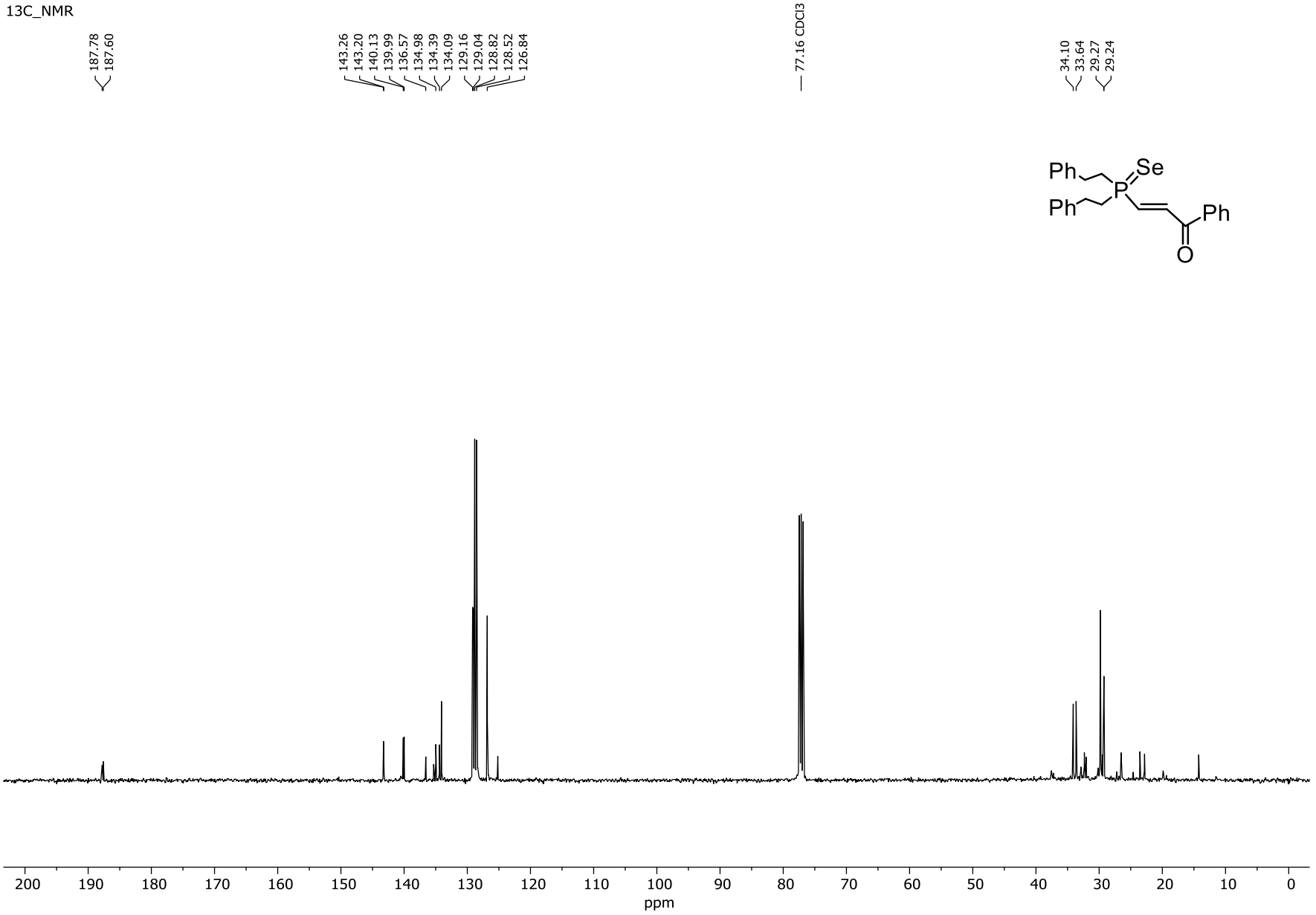
(2*E*)-3-(Diphenylselenophosphoryl)-1-phenylprop-2-en-1-one (8c)



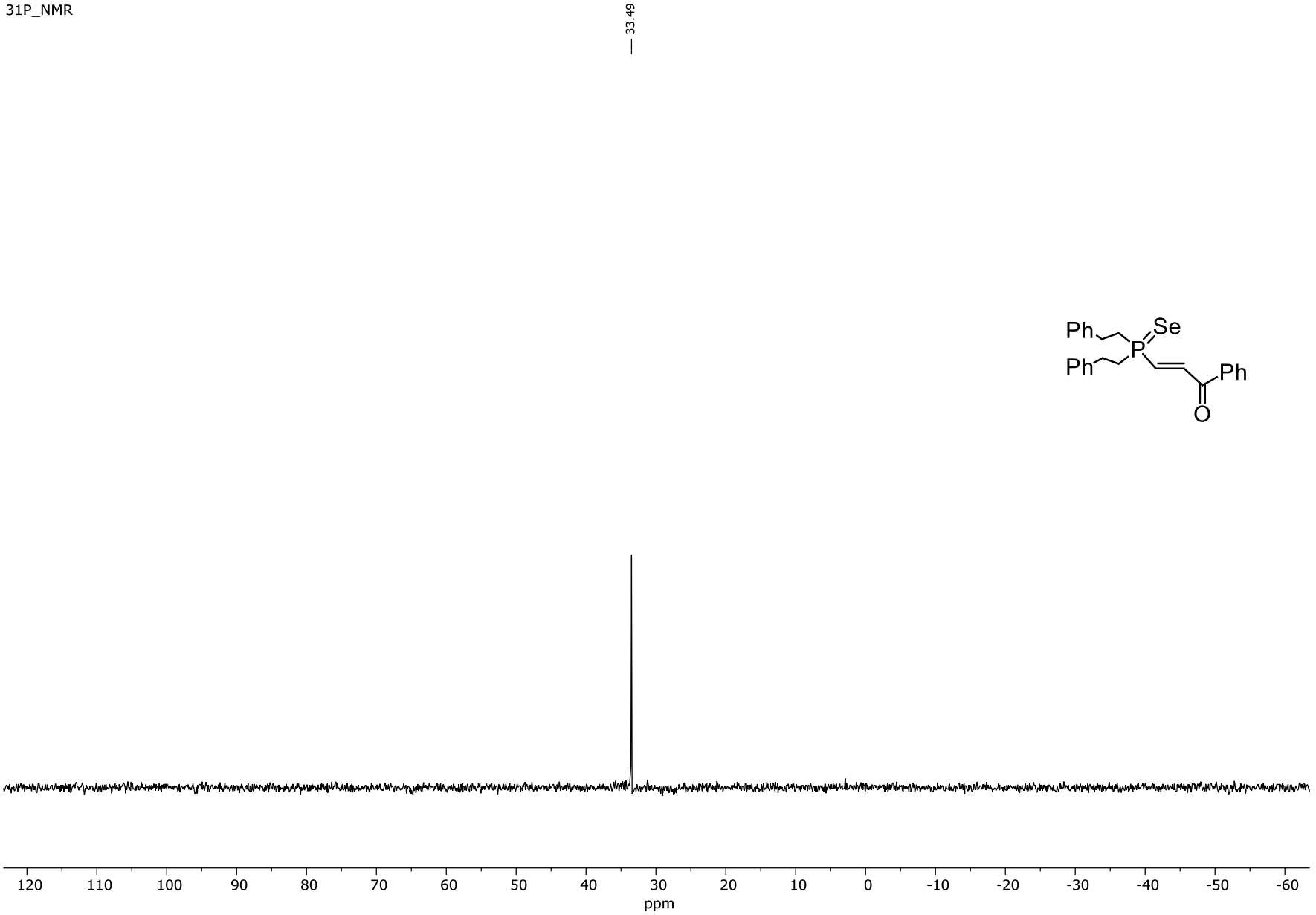
(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-phenylprop-2-en-1-one (8d)



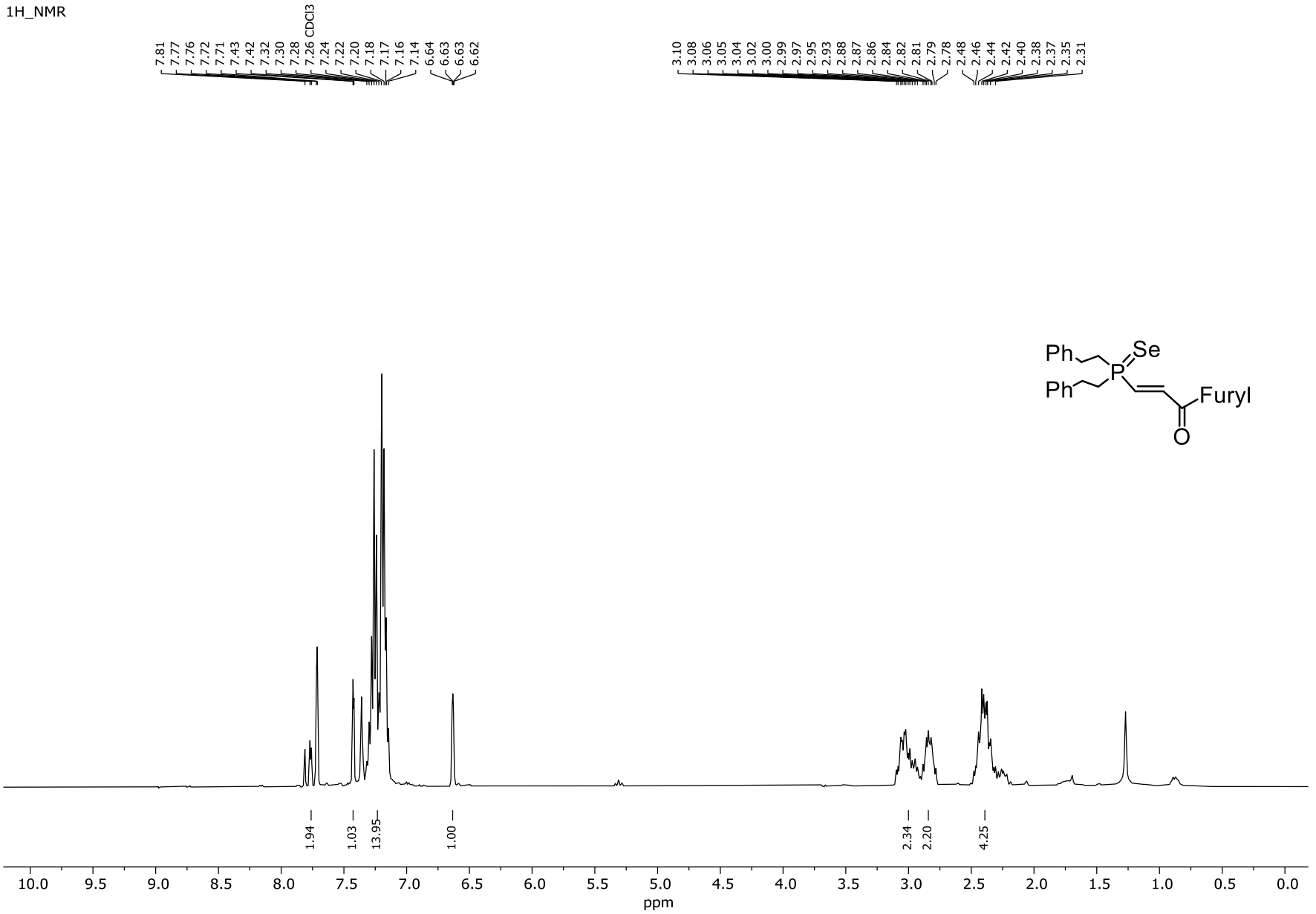
(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-phenylprop-2-en-1-one (8d)



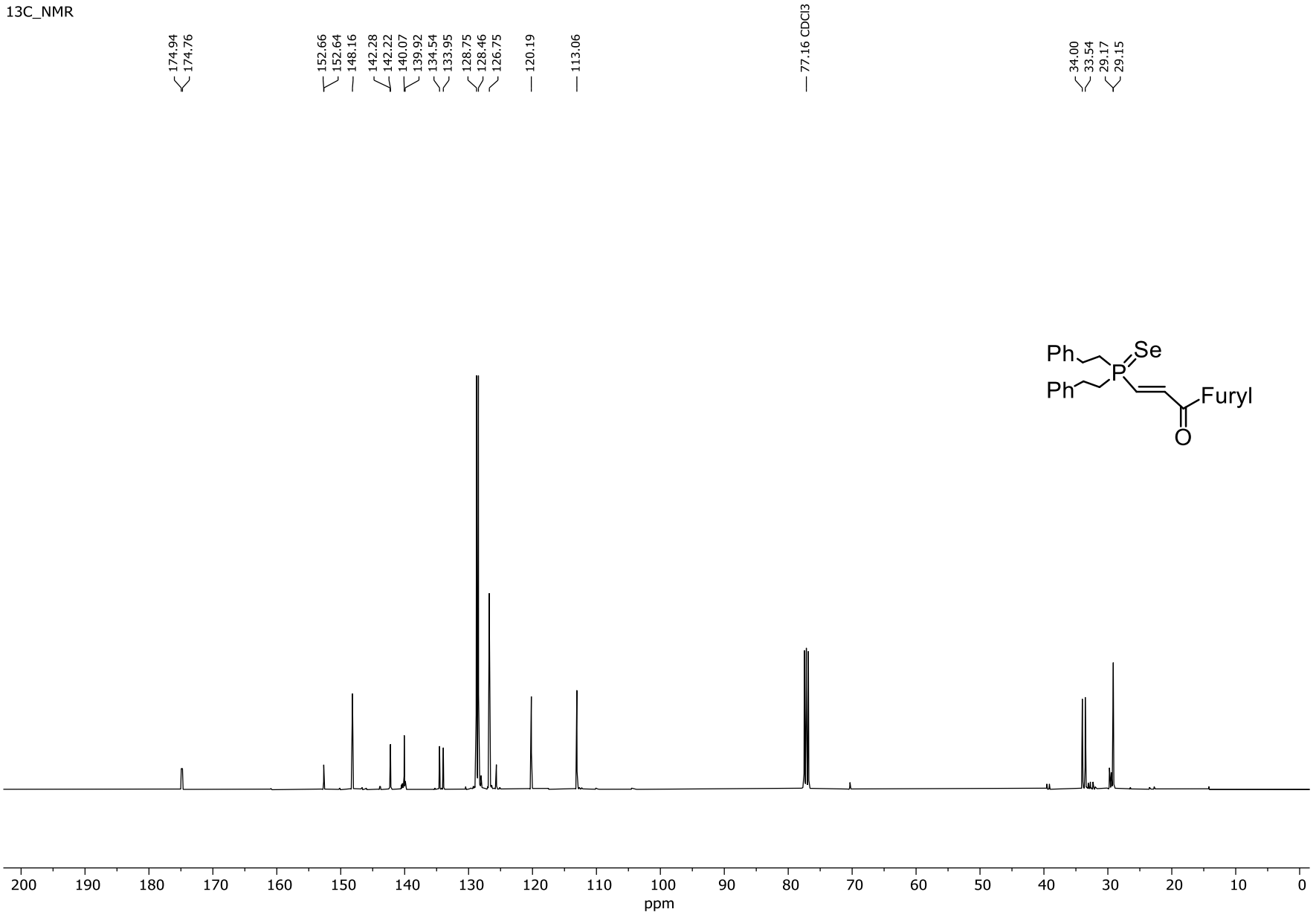
(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-phenylprop-2-en-1-one (8d)



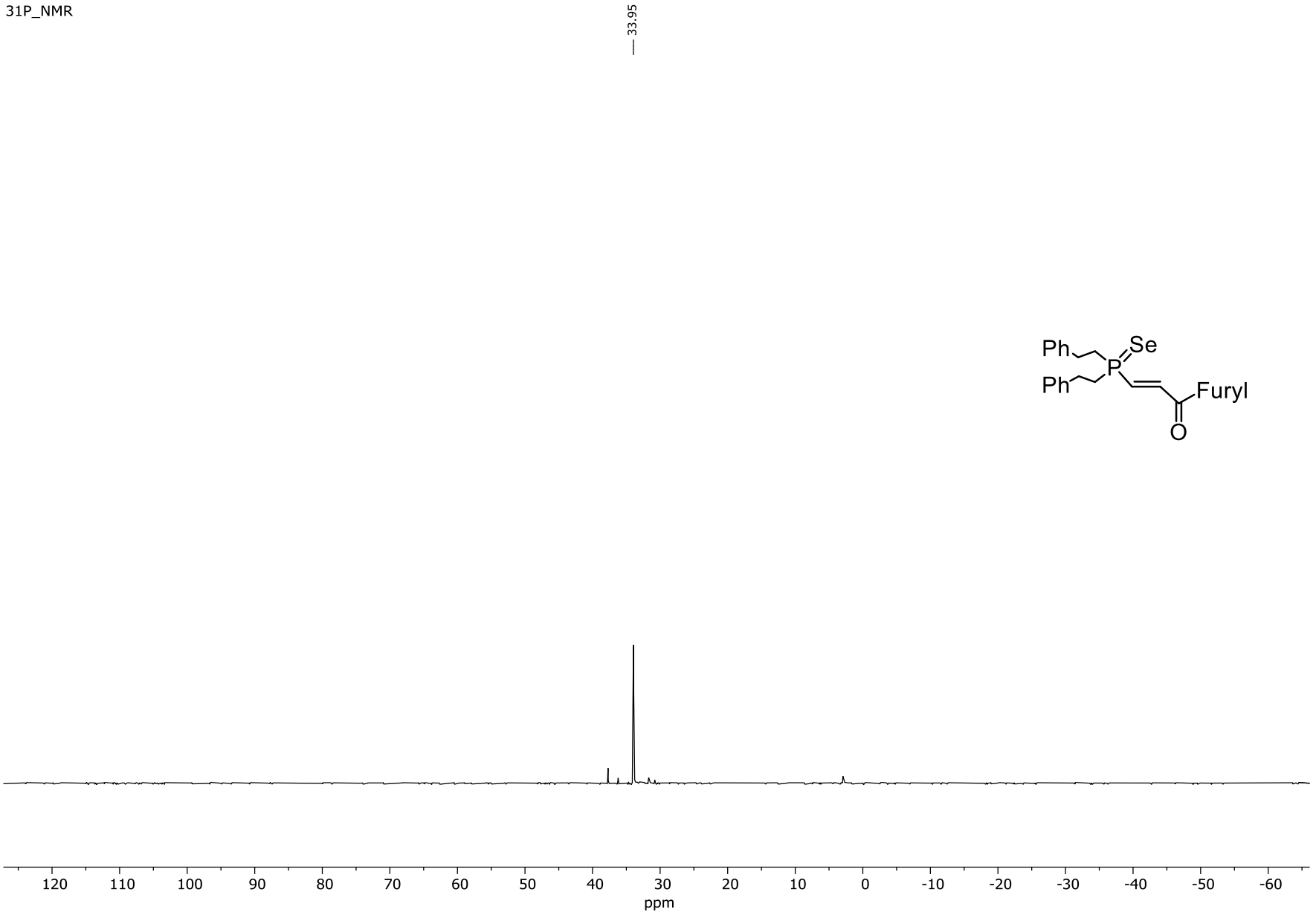
(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-(furan-2-yl)prop-2-en-1-one (8e)



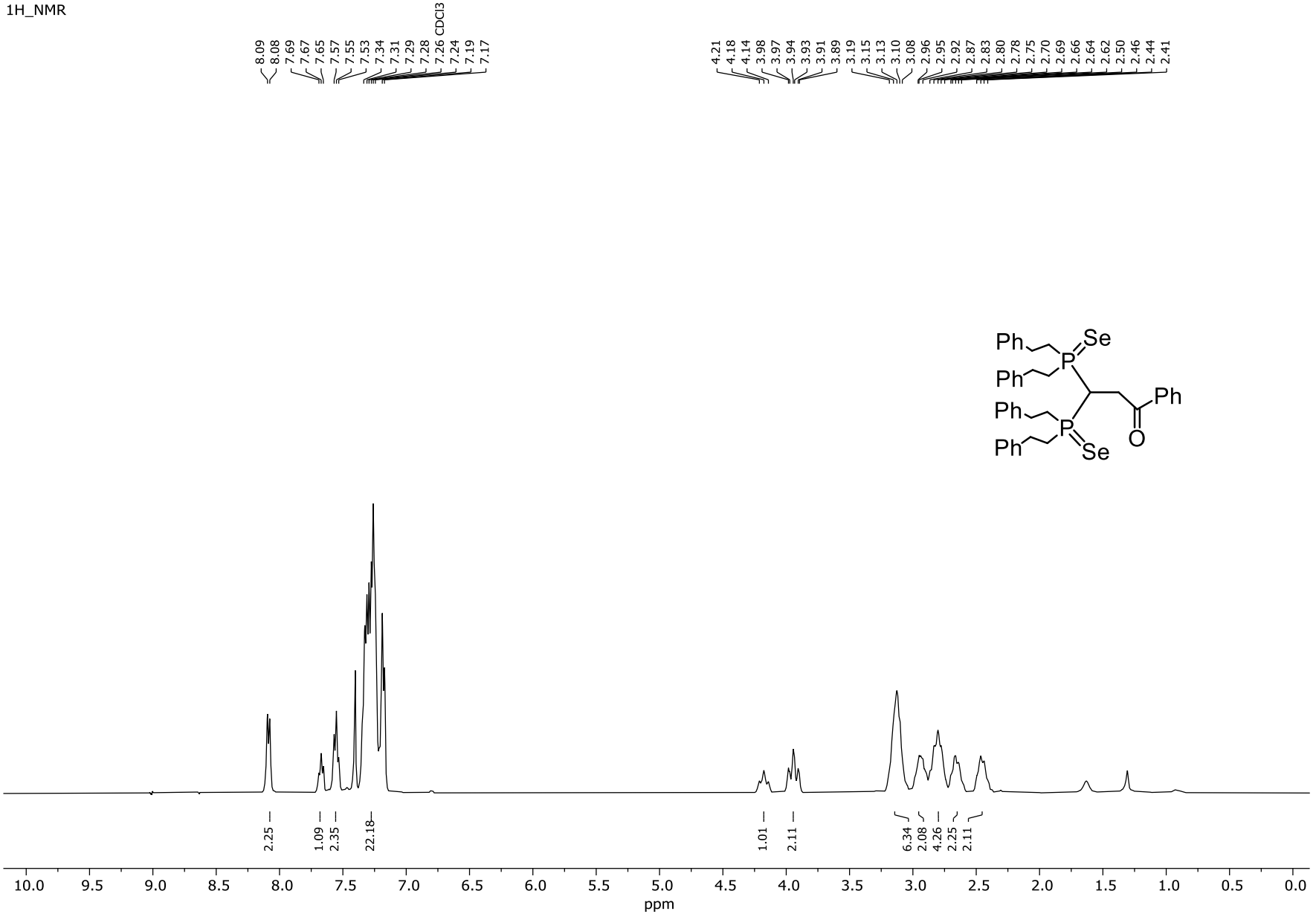
(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-(furan-2-yl)prop-2-en-1-one (8e)



(2*E*)-3-[Bis(2-phenylethyl)selenophosphoryl]-1-(furan-2-yl)prop-2-en-1-one (8e)



3,3-Bis[bis(2-phenylethyl)selenophosphoryl]-1-phenylpropan-1-one (9)



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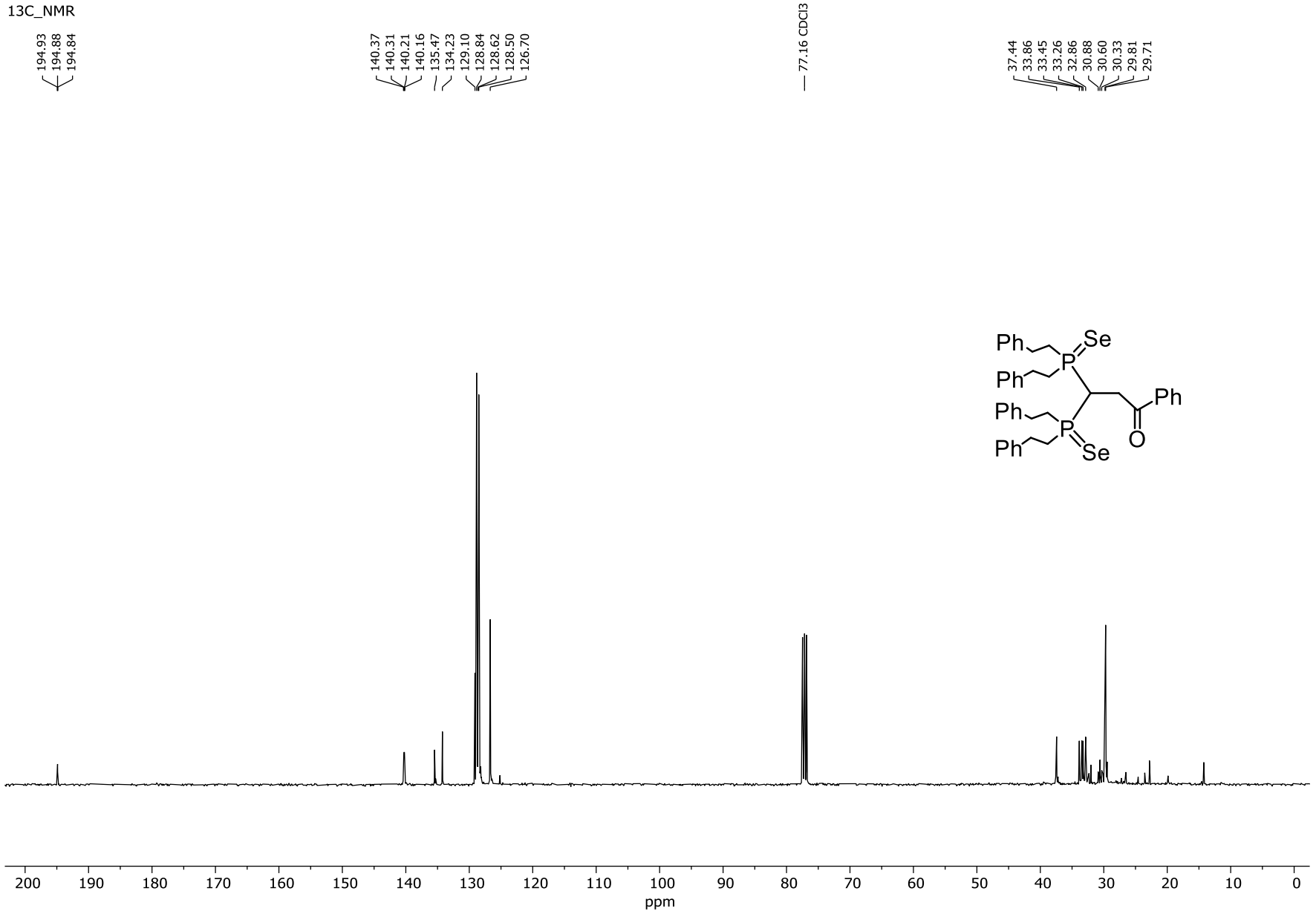
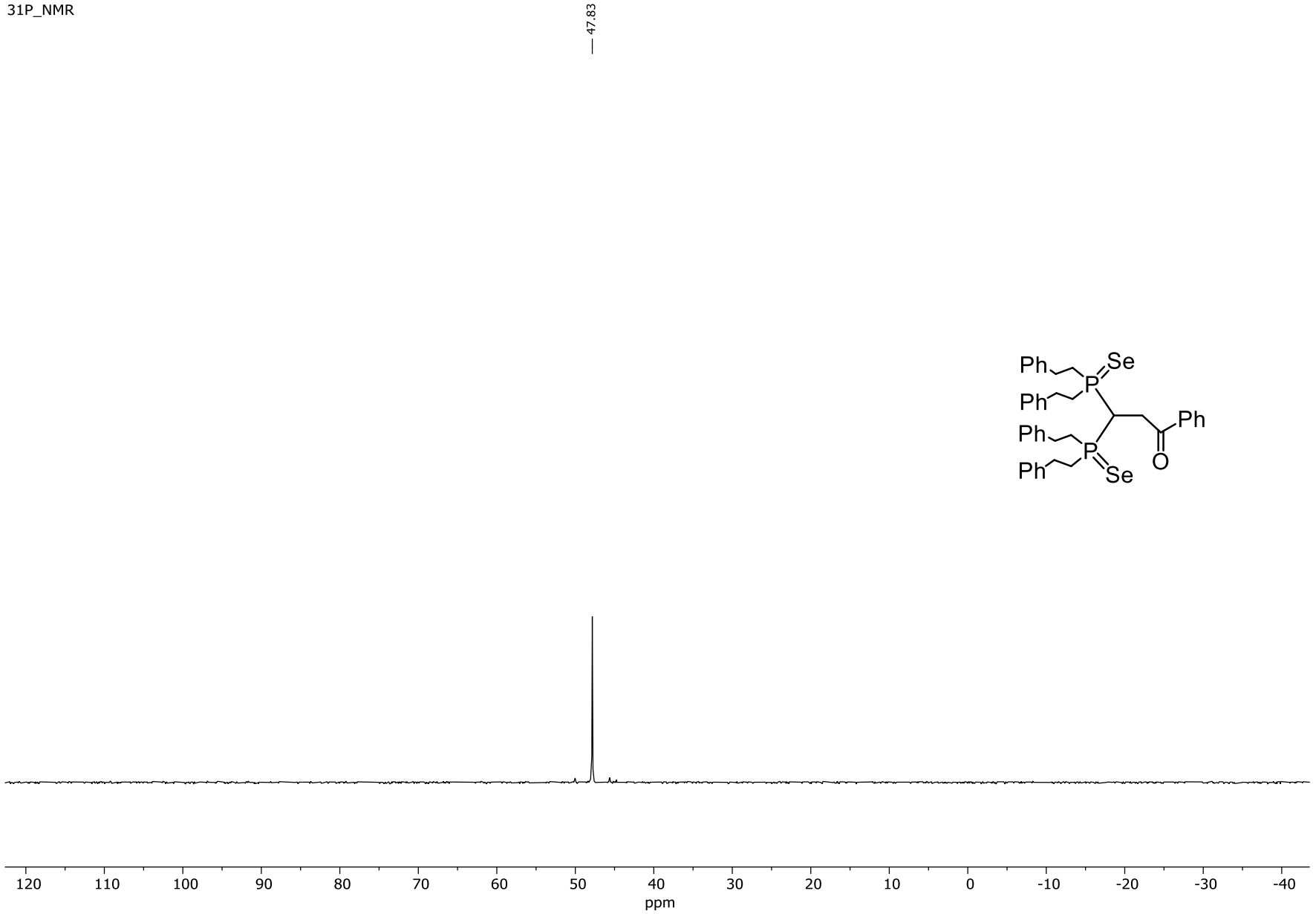
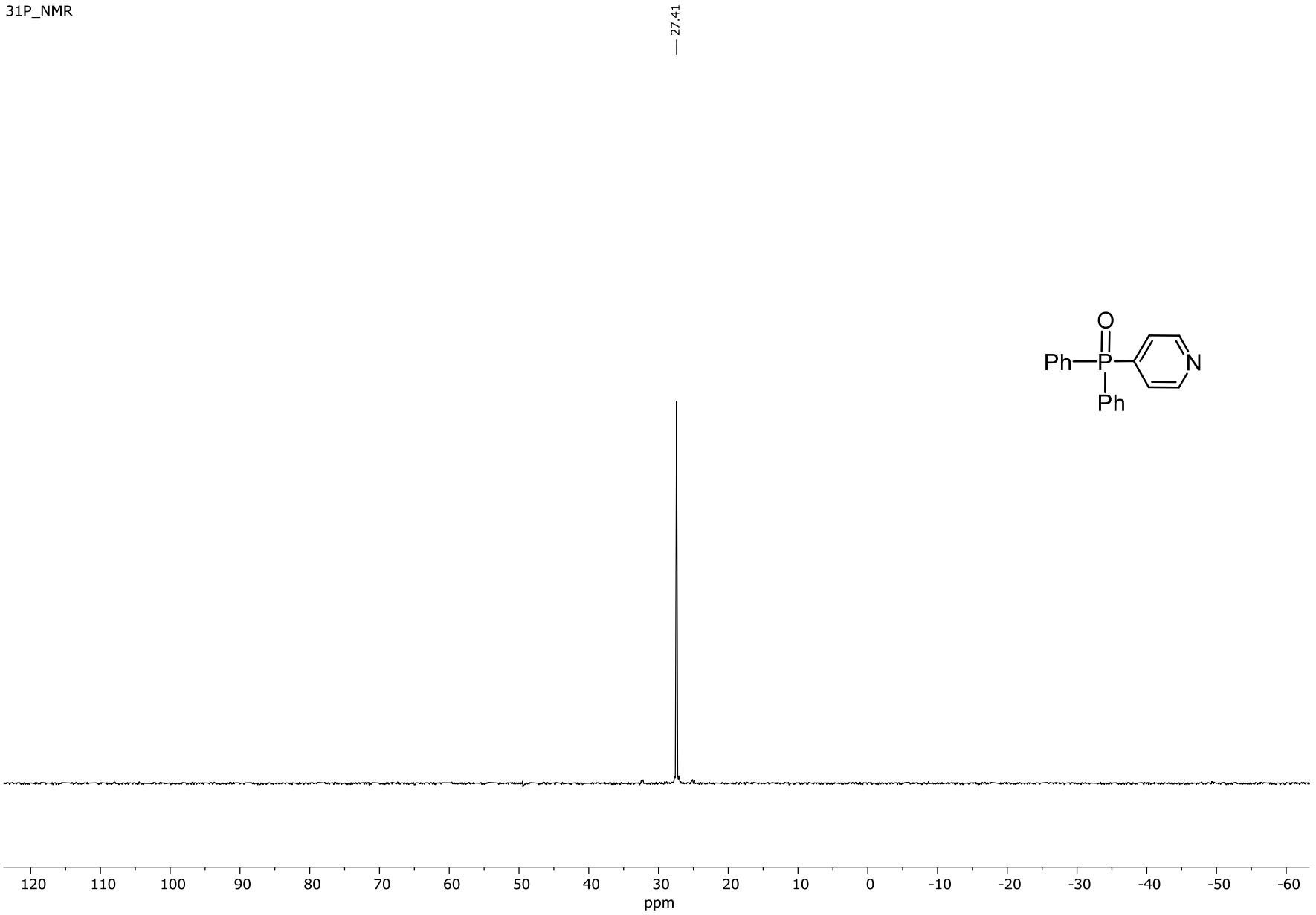


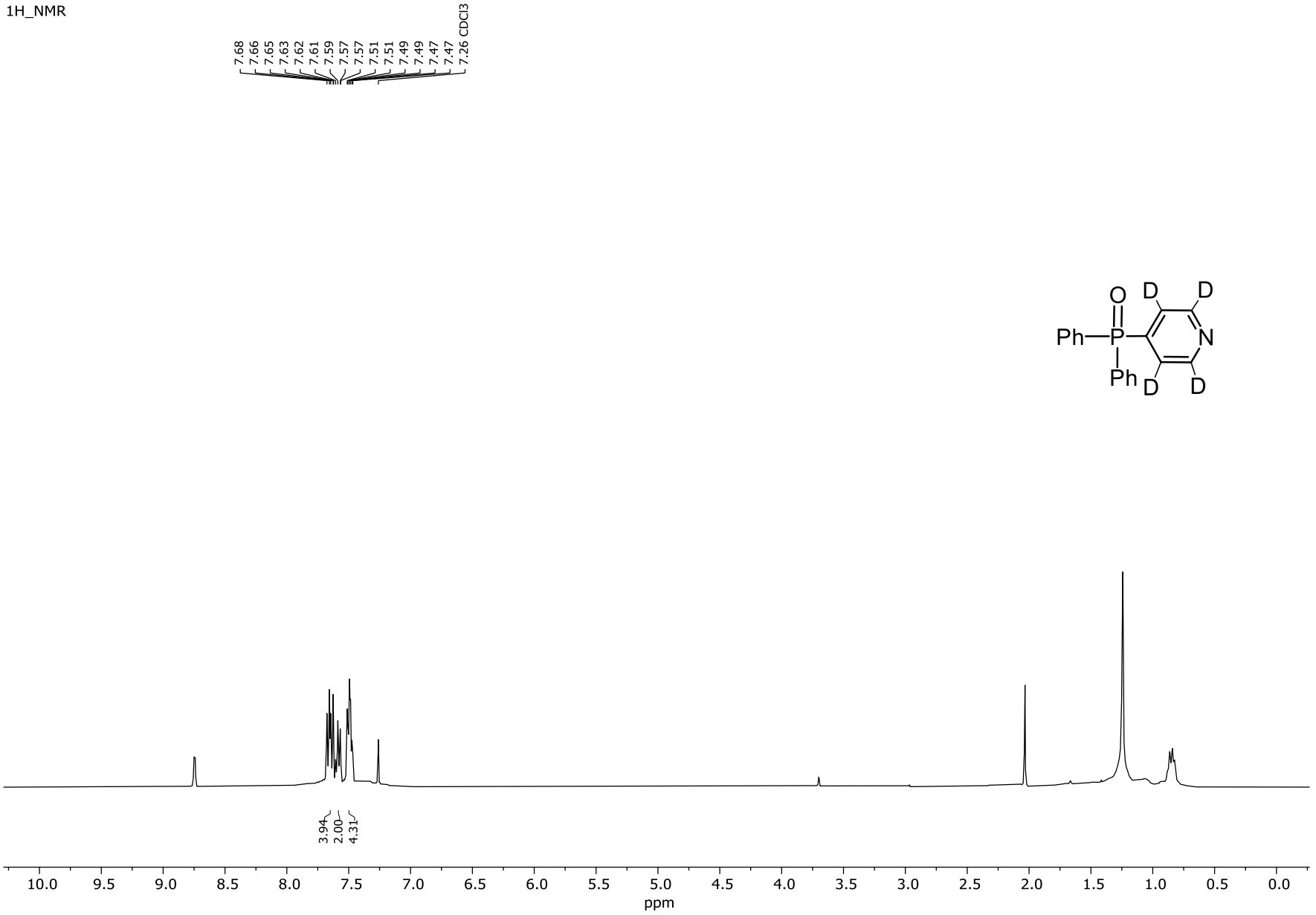
3,3-Bis[bis(2-phenylethyl)selenophosphoryl]-1-phenylpropan-1-one (9)



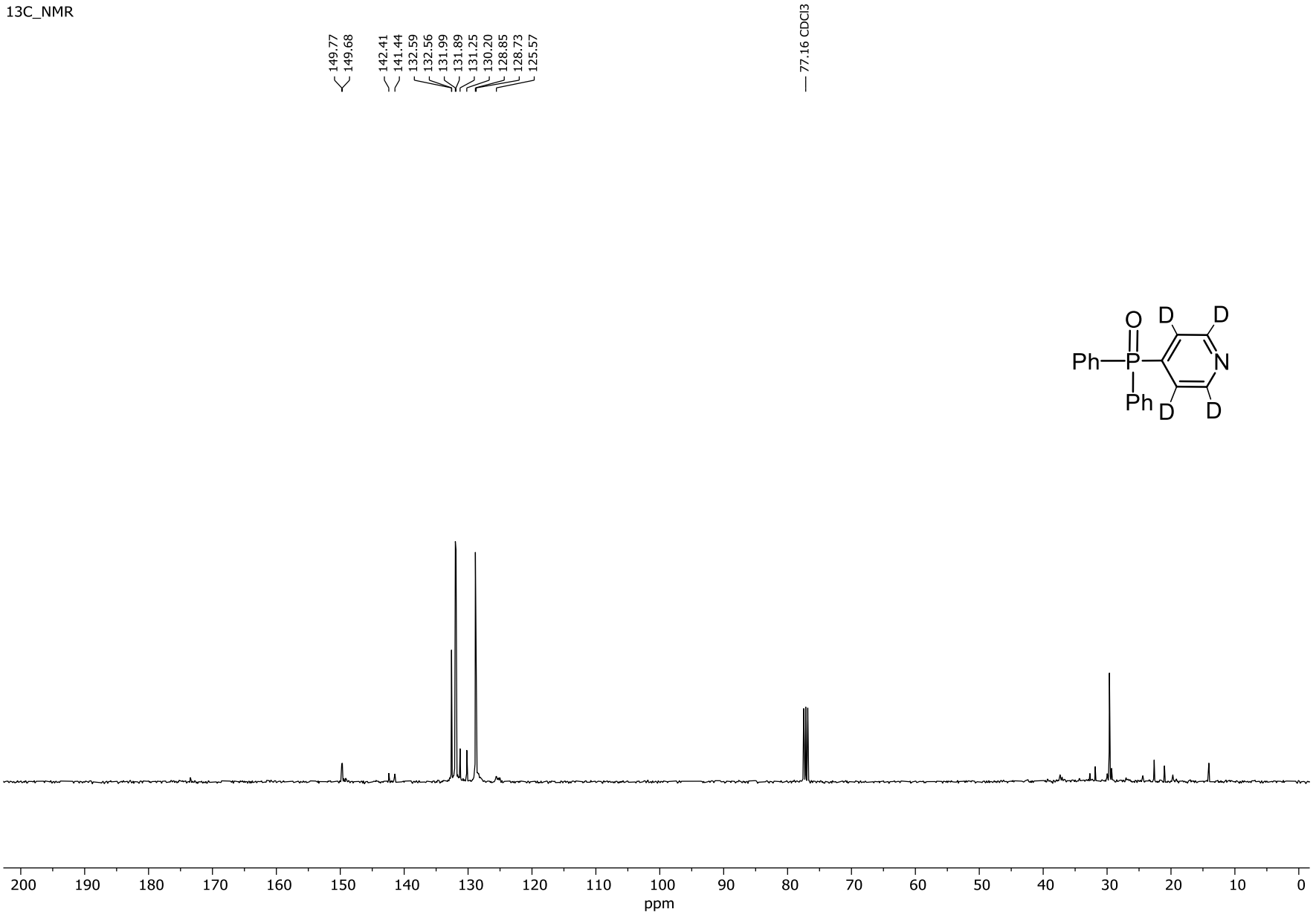
4-(Diphenylphosphoryl)pyridine (11a)



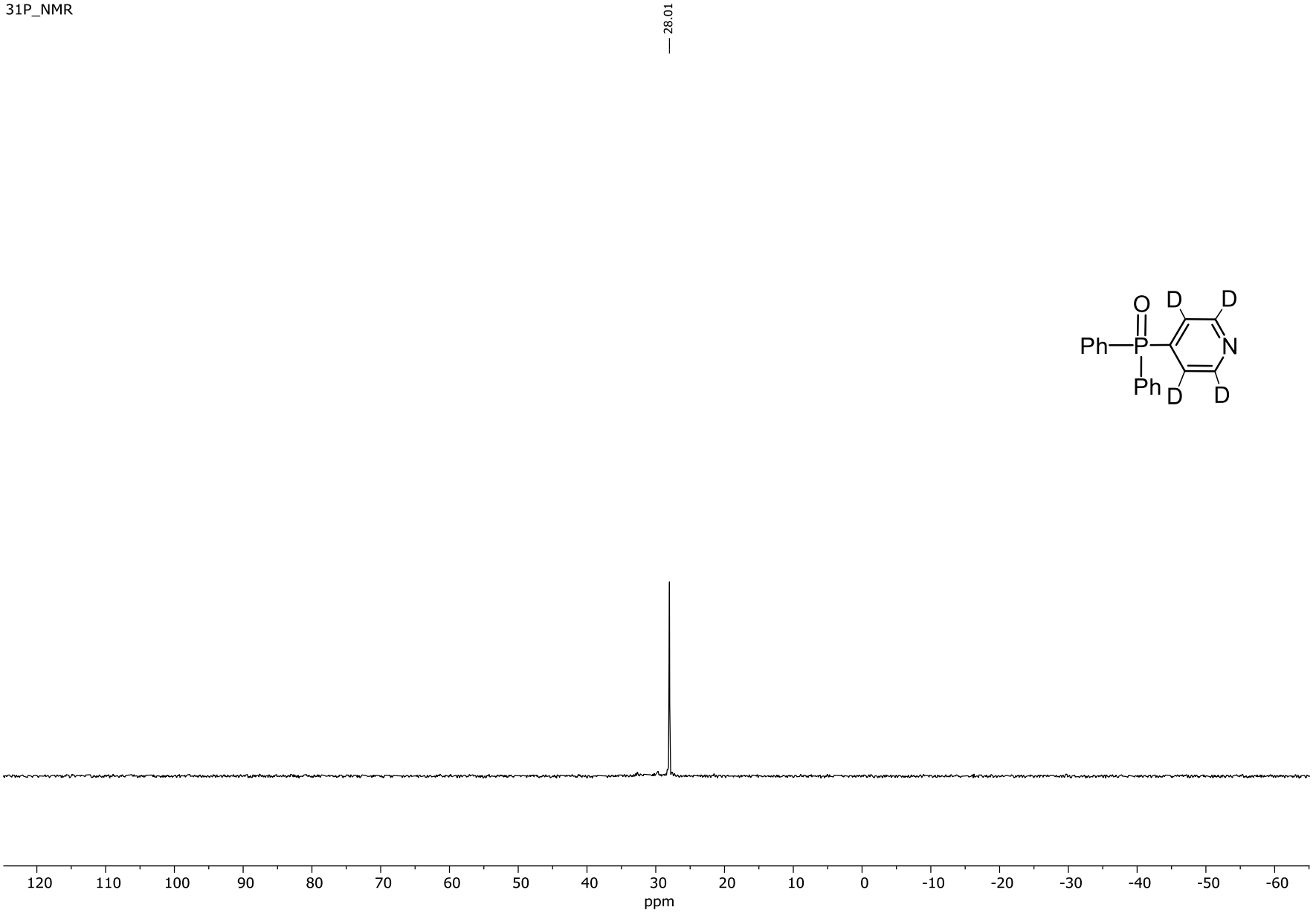
4-(Diphenylphosphoryl)pyridine-2,3,5,6-*d*$_4$ (11b)



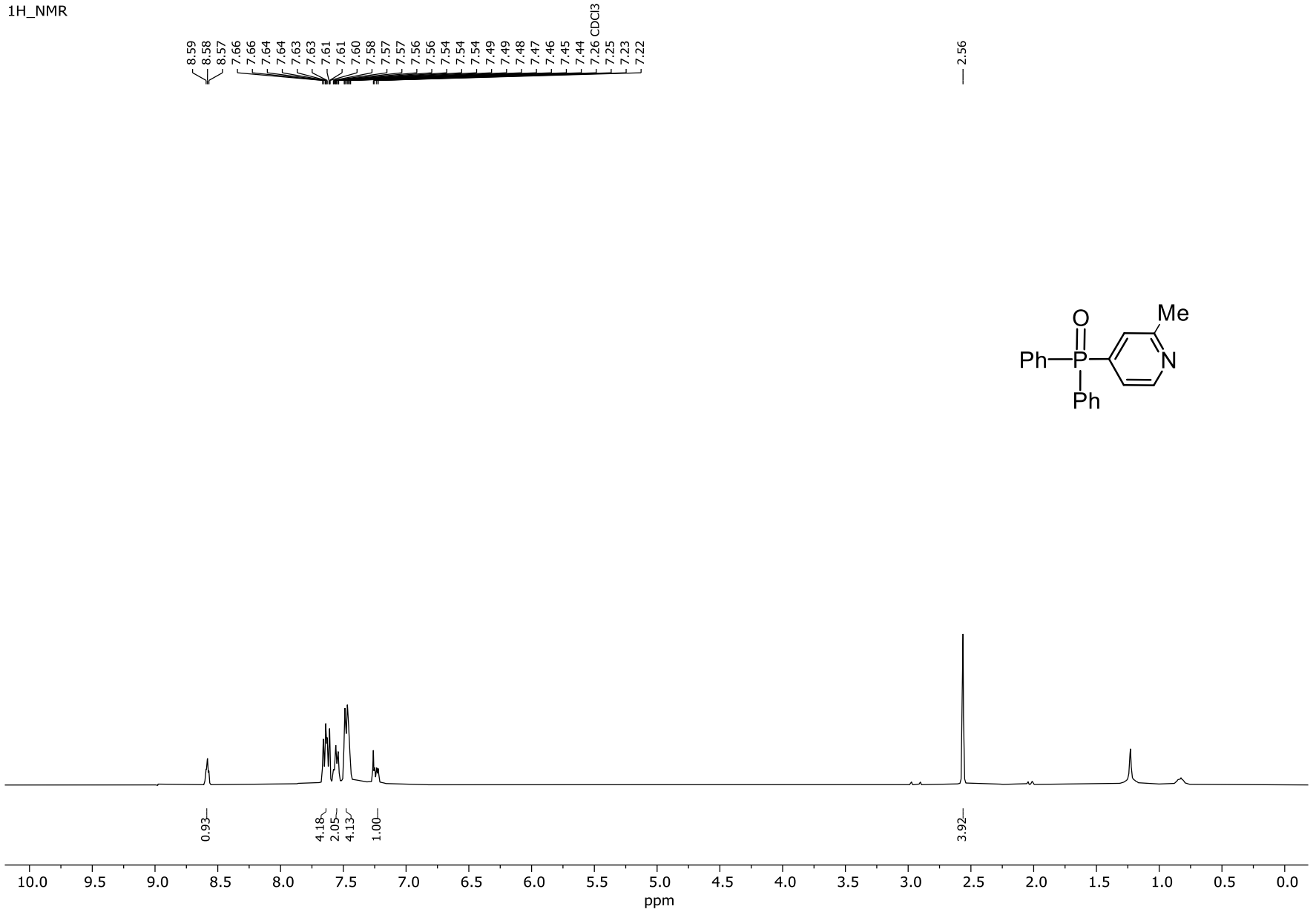
4-(Diphenylphosphoryl)pyridine-2,3,5,6-*d*$_4$ (11b)



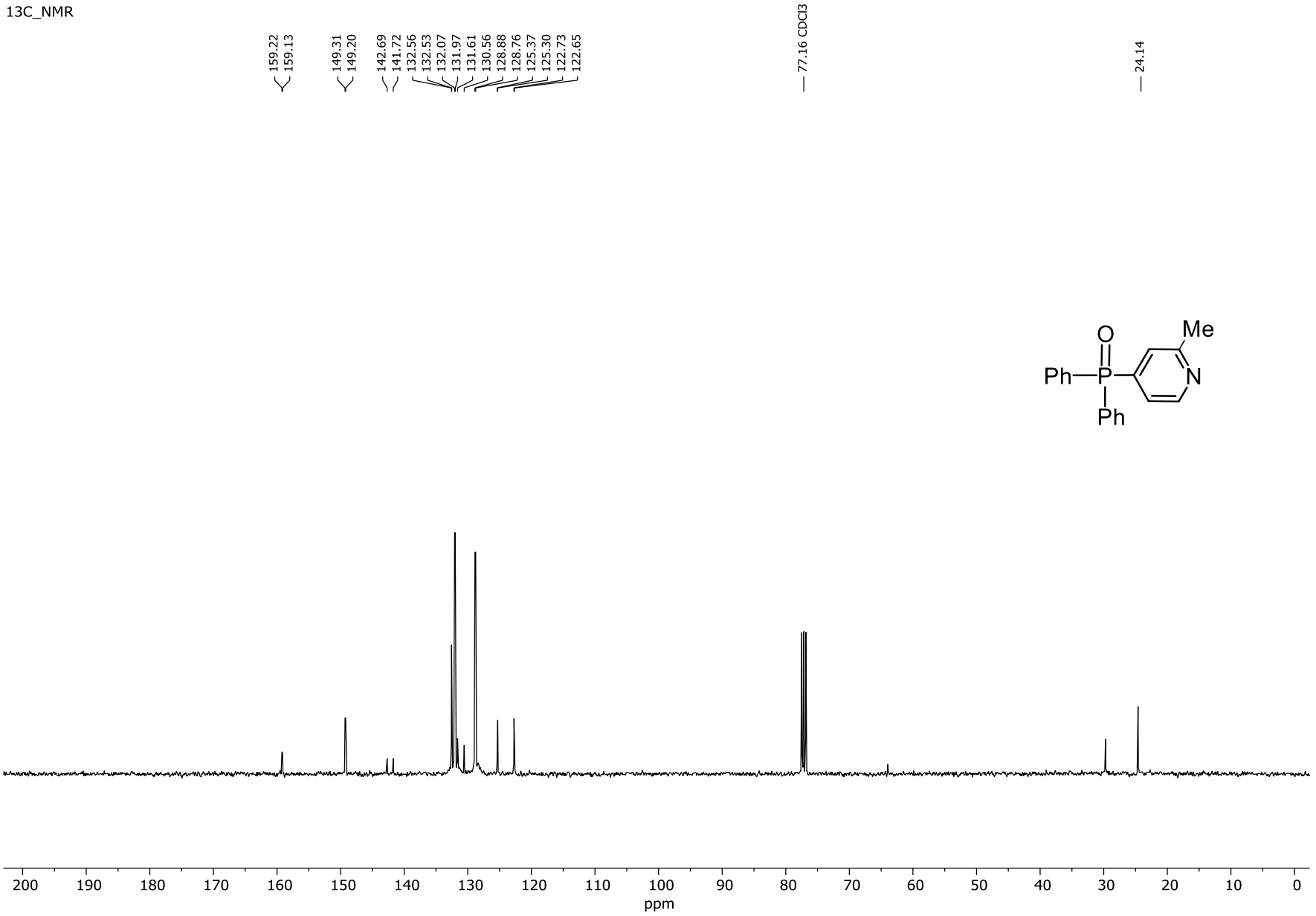
4-(Diphenylphosphoryl)pyridine-2,3,5,6-*d*$_4$ (11b)



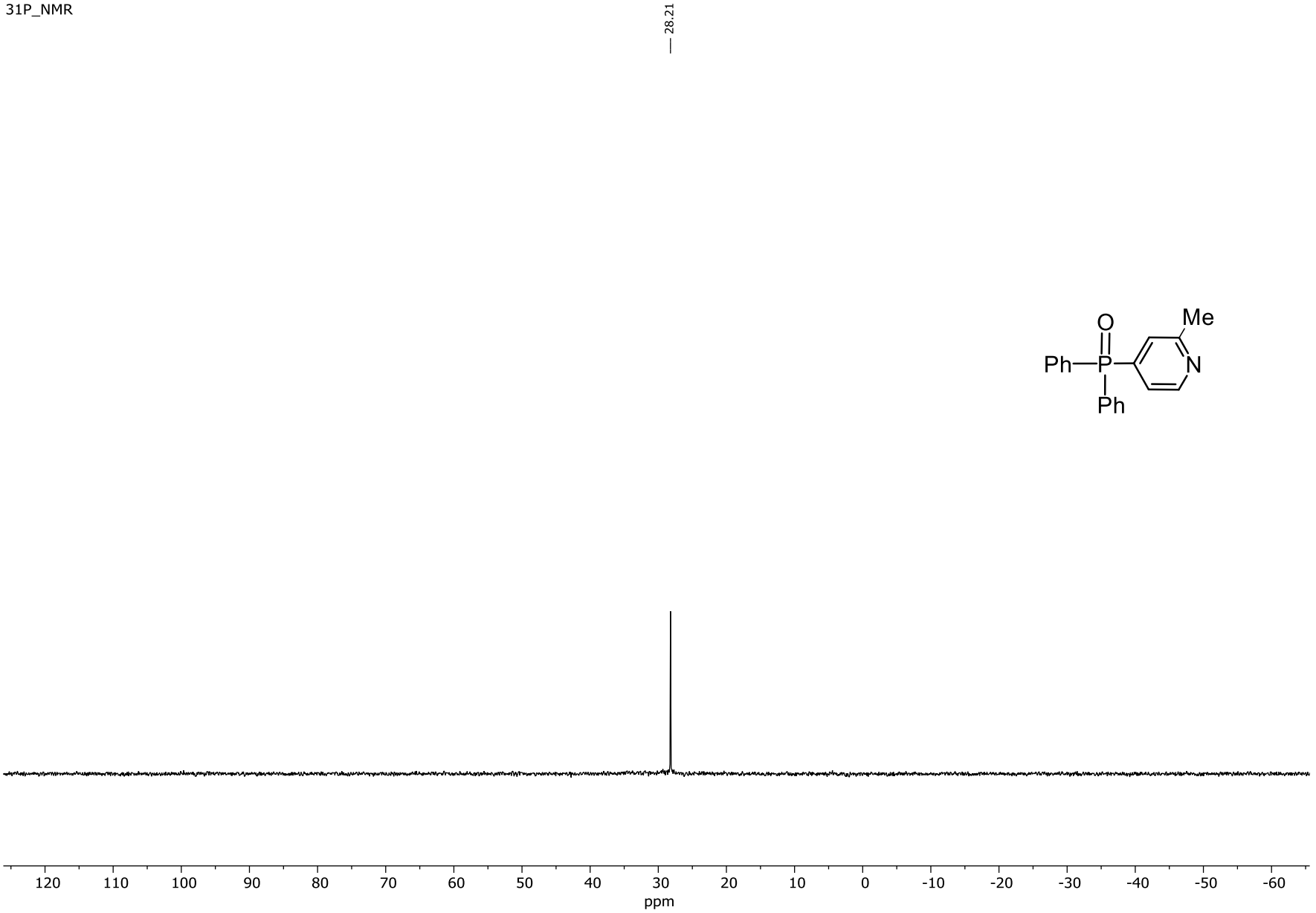
4-(Diphenylphosphoryl)-2-methylpyridine (11c)



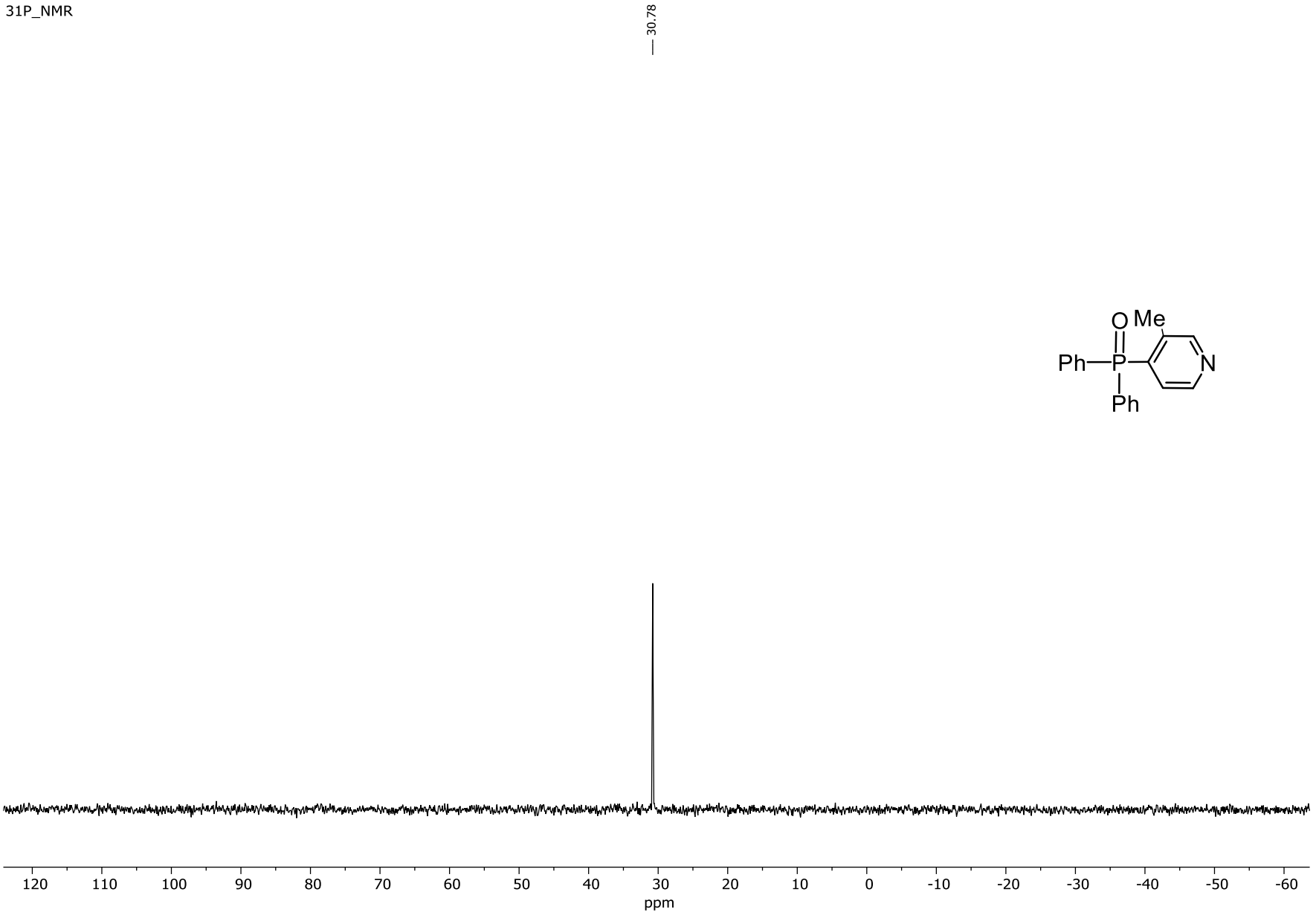
4-(Diphenylphosphoryl)-2-methylpyridine (11c)



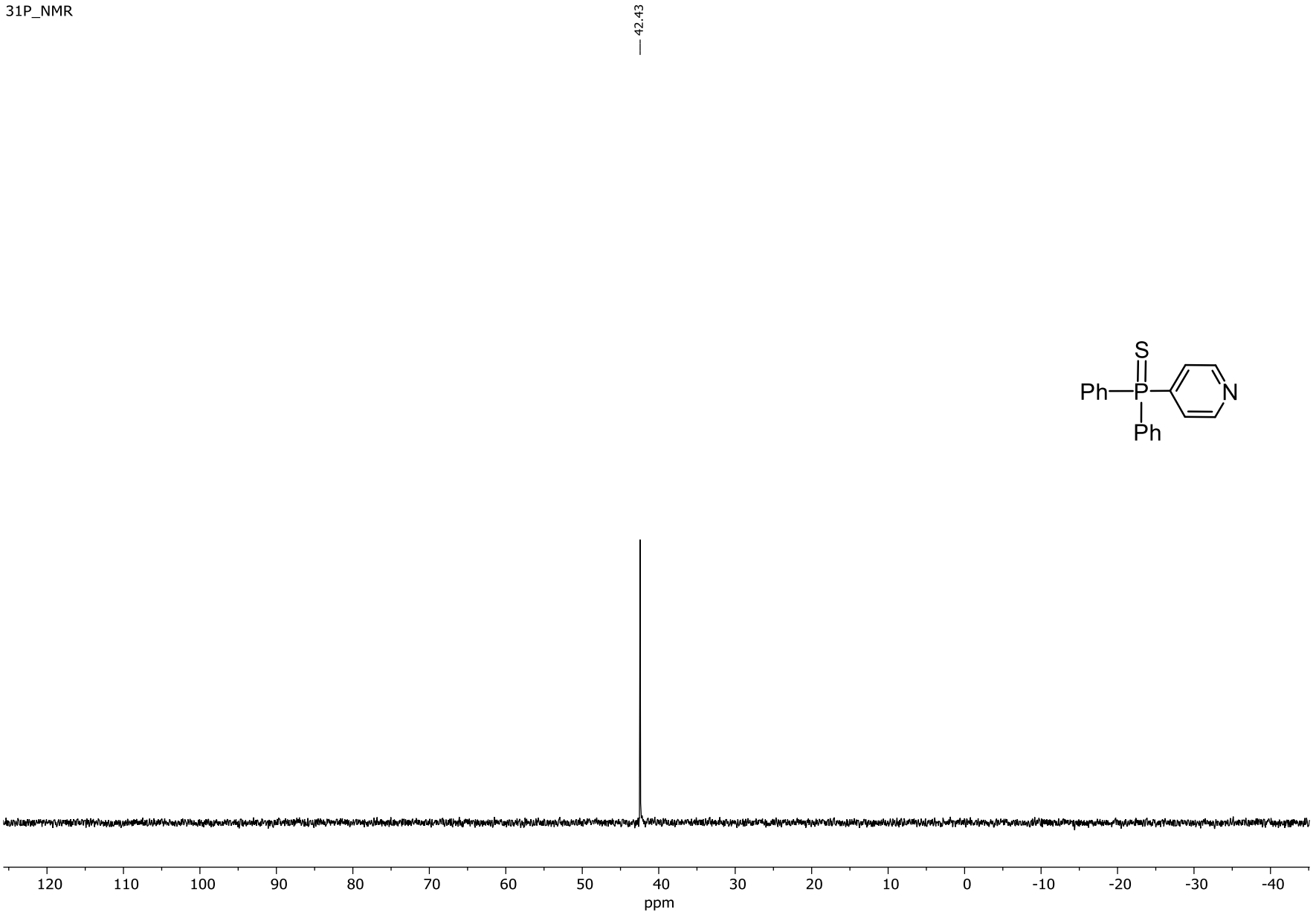
4-(Diphenylphosphoryl)-2-methylpyridine (11c)



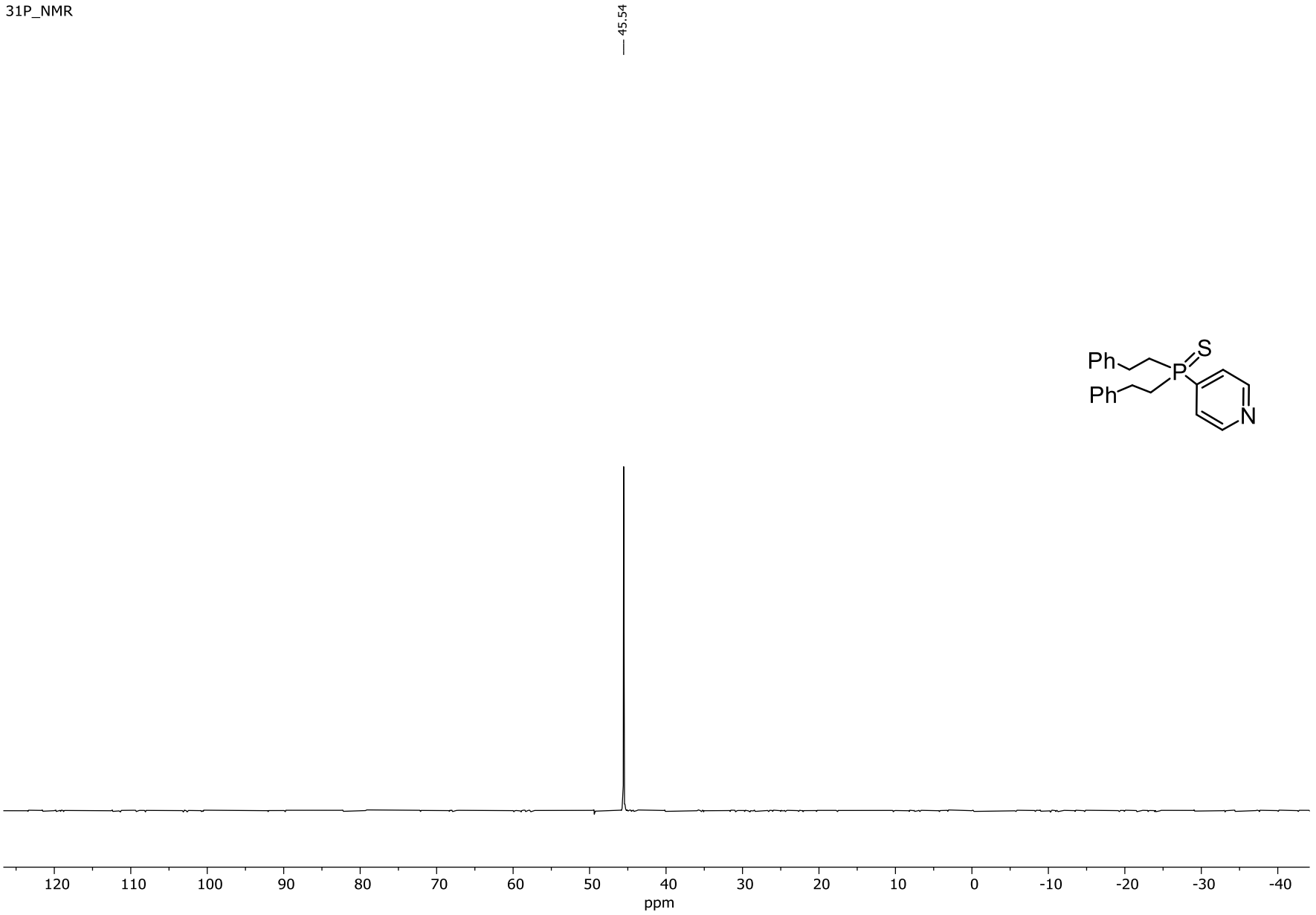
4-(Diphenylphosphoryl)-3-methylpyridine (11d)



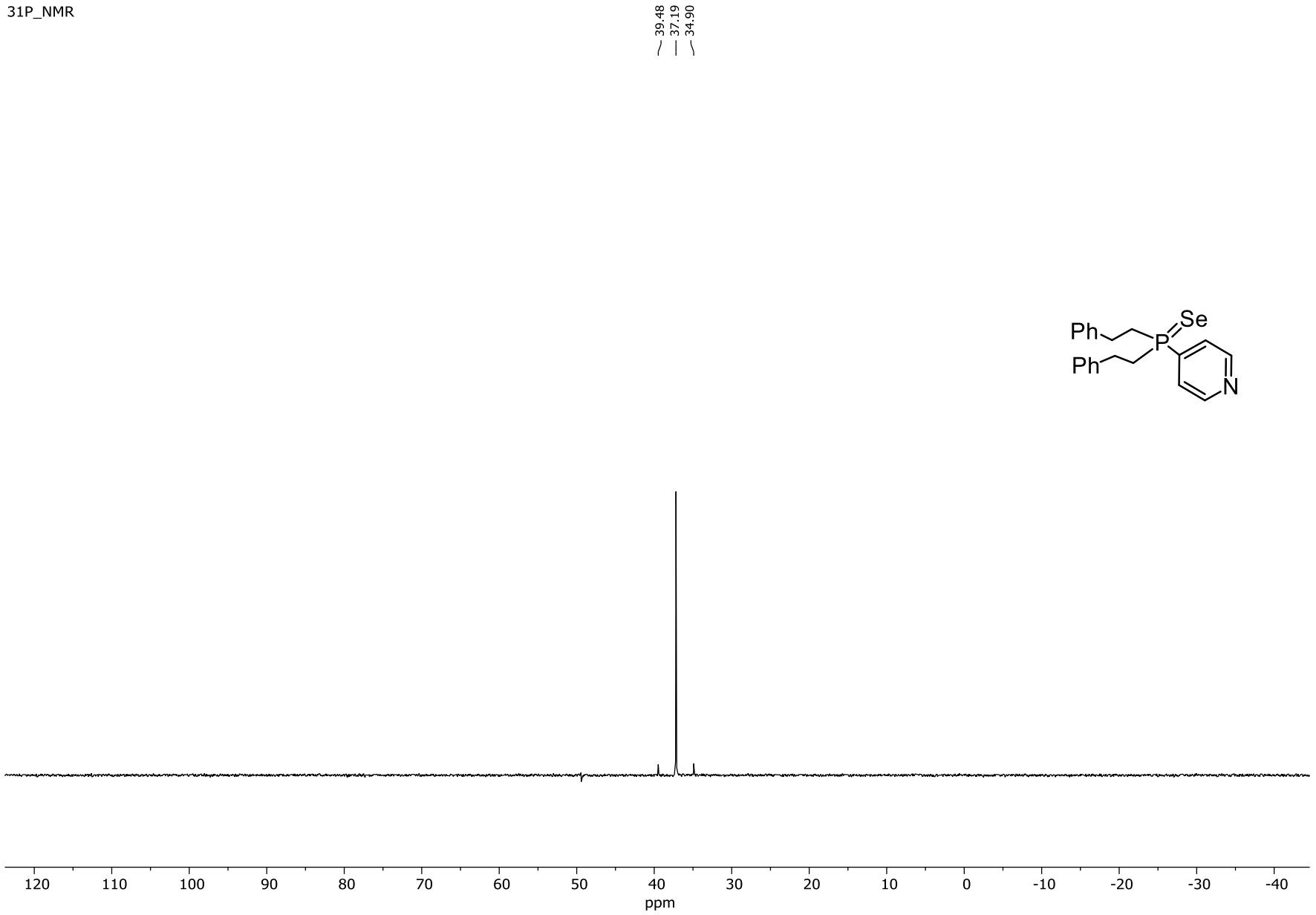
4-(Diphenylthiophosphoryl)pyridine (11e)



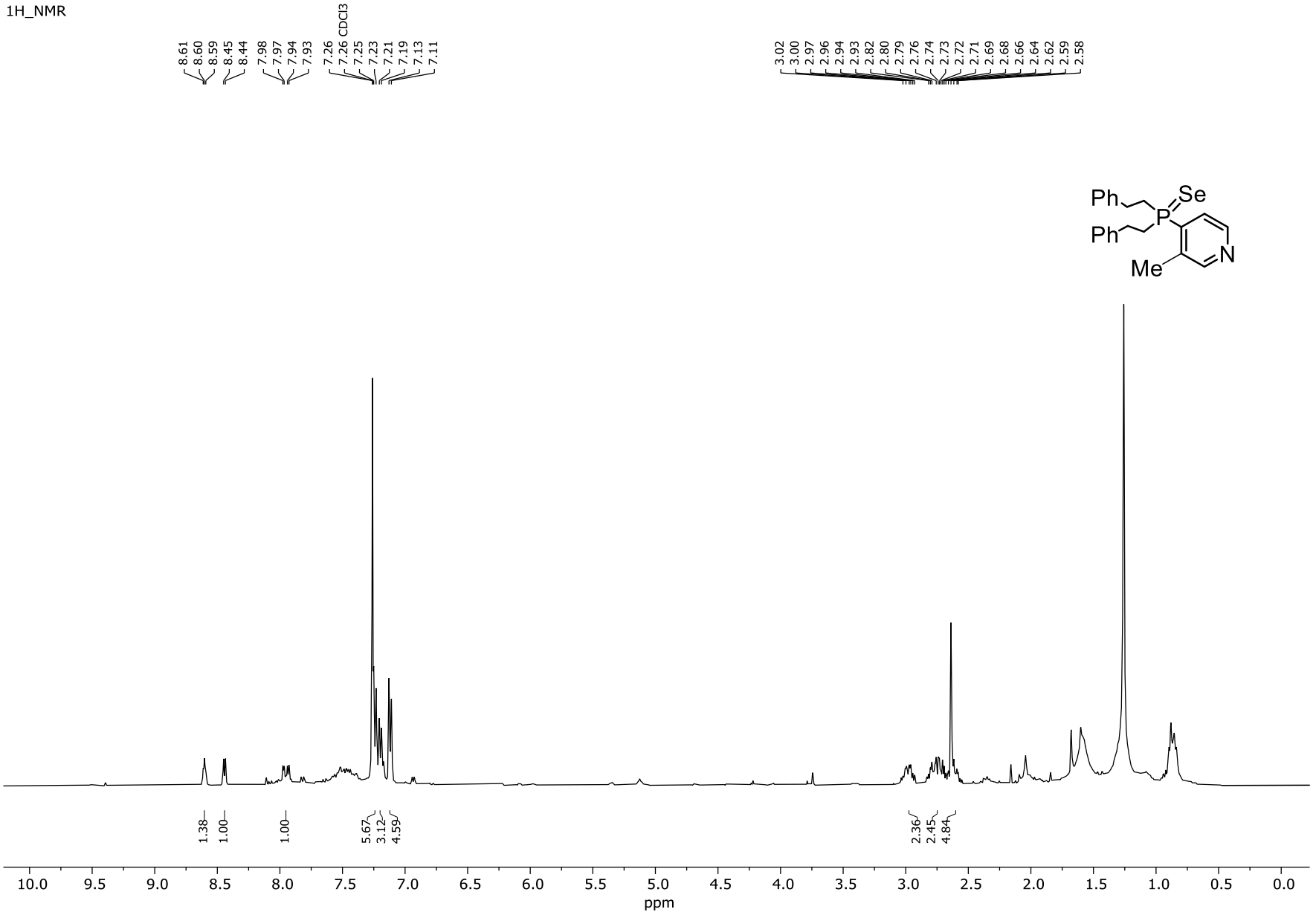
4-[Bis(2-phenylethyl)thiophosphoryl]pyridine (11f)



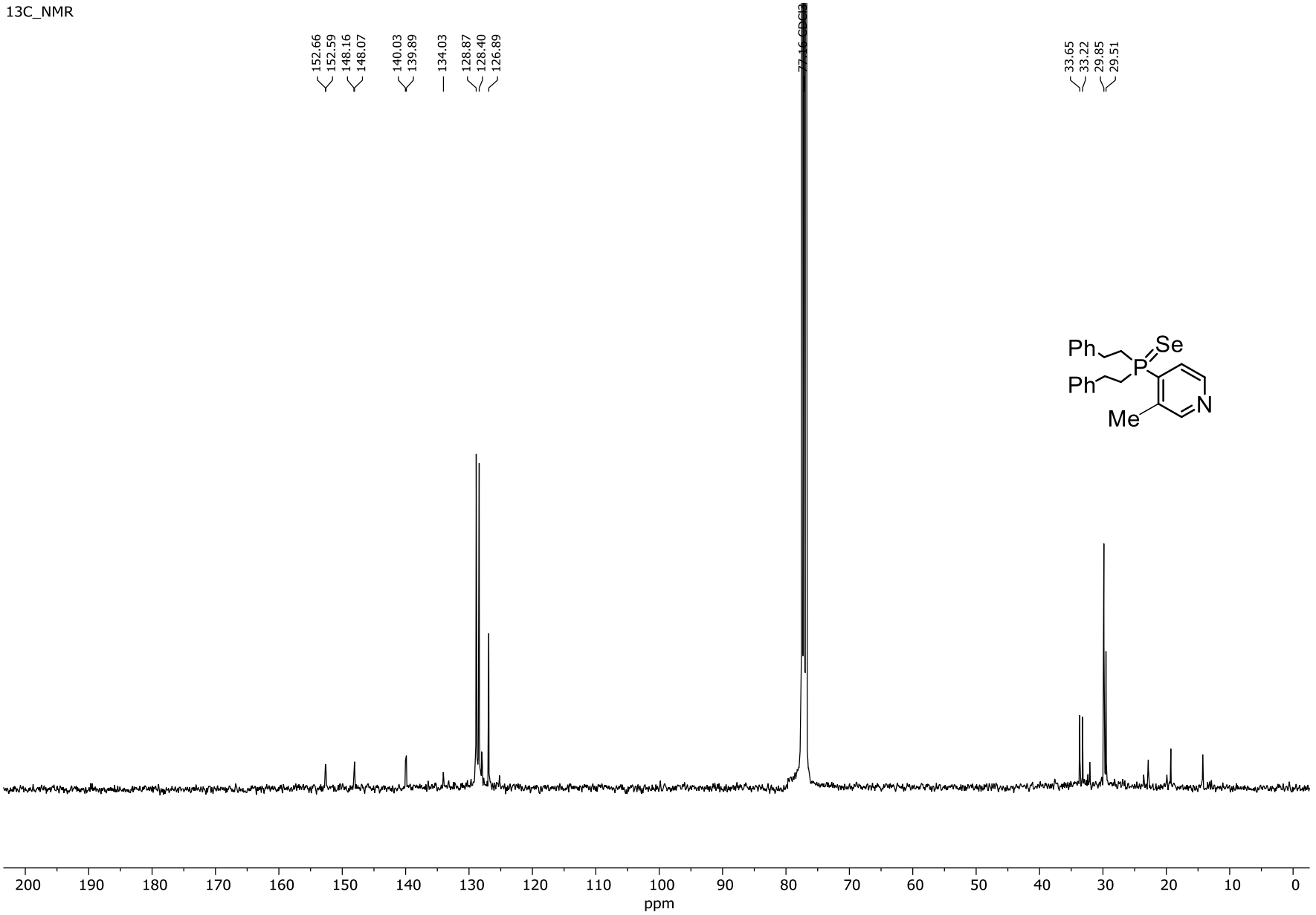
4-[Bis(2-phenylethyl)selenophosphoryl]pyridine (11g)



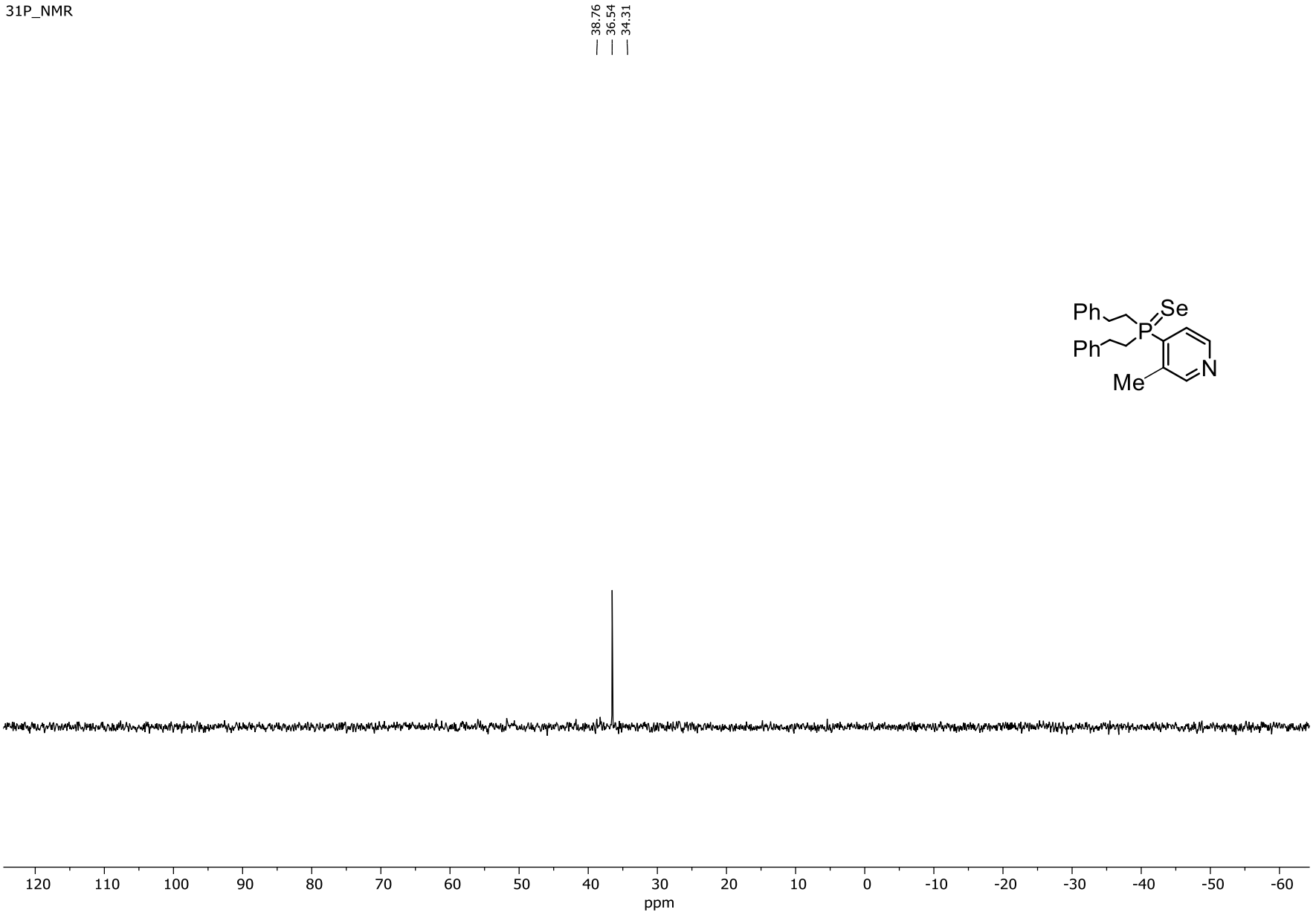
4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridine (11h)



4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridine (11h)



4-[Bis(2-phenylethyl)selenophosphoryl]-3-methylpyridine (11h)



4-[Bis(2-phenylpropyl)selenophosphoryl]pyridine (11i)