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MDPI

Diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate

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Supporting information

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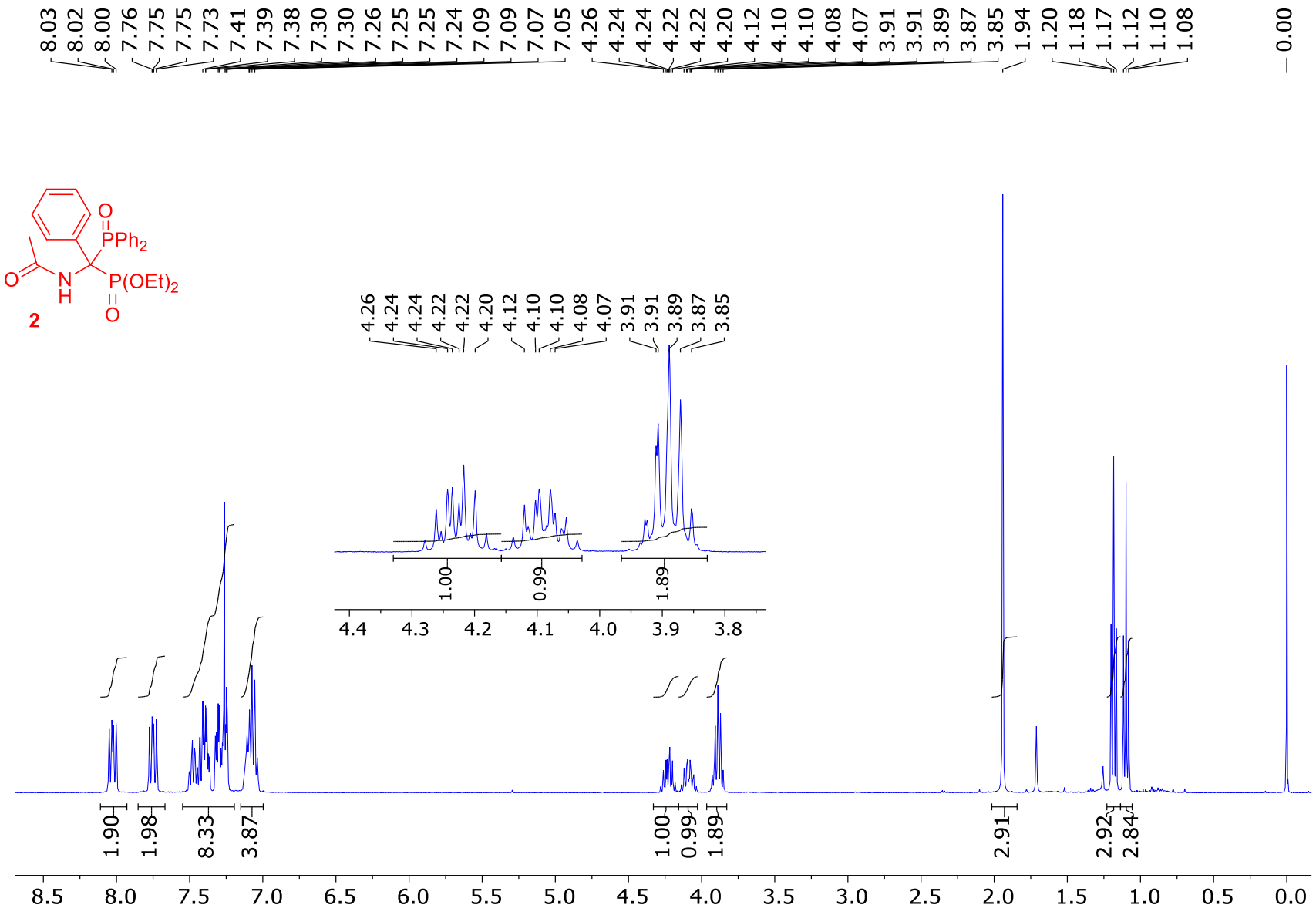
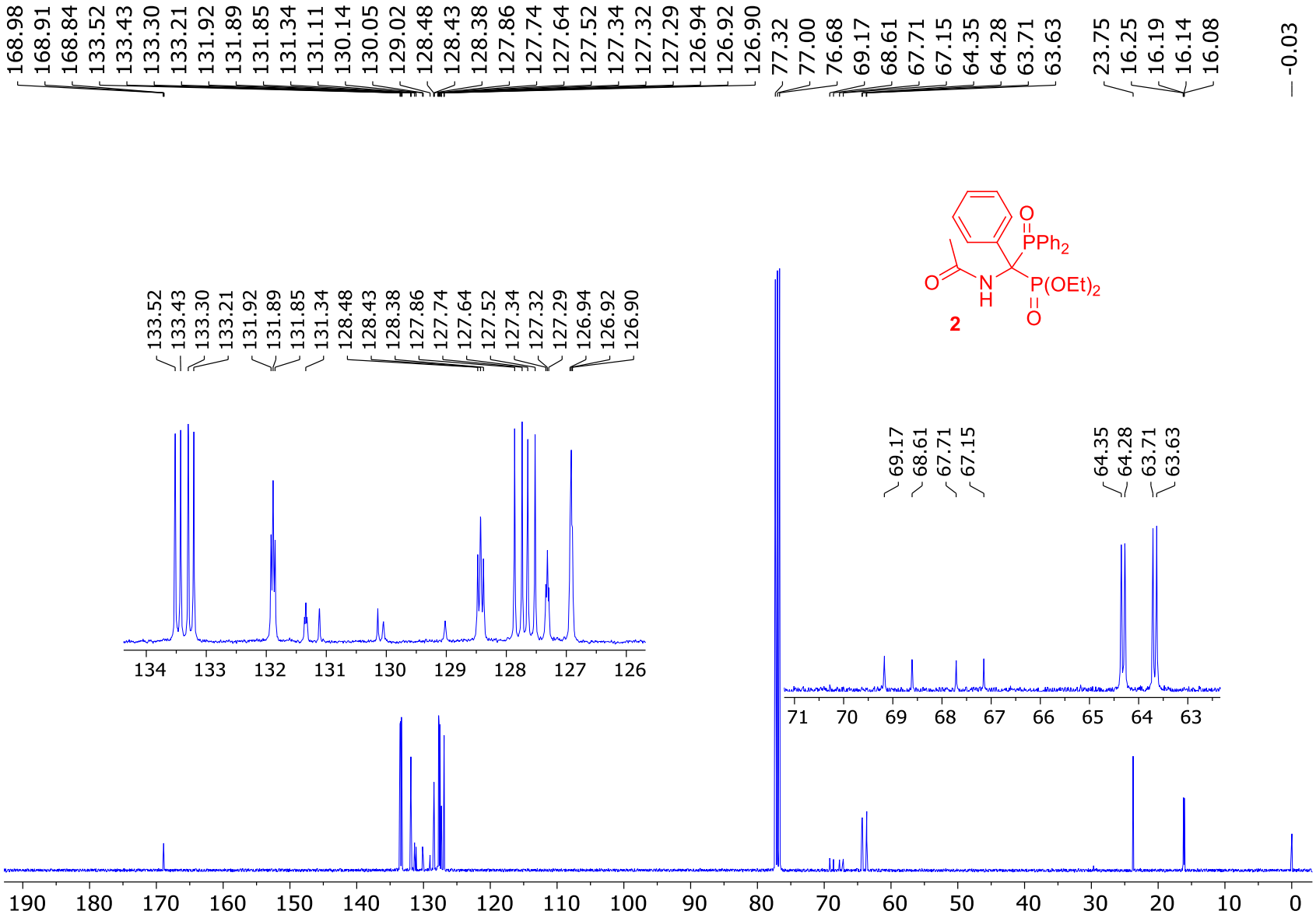
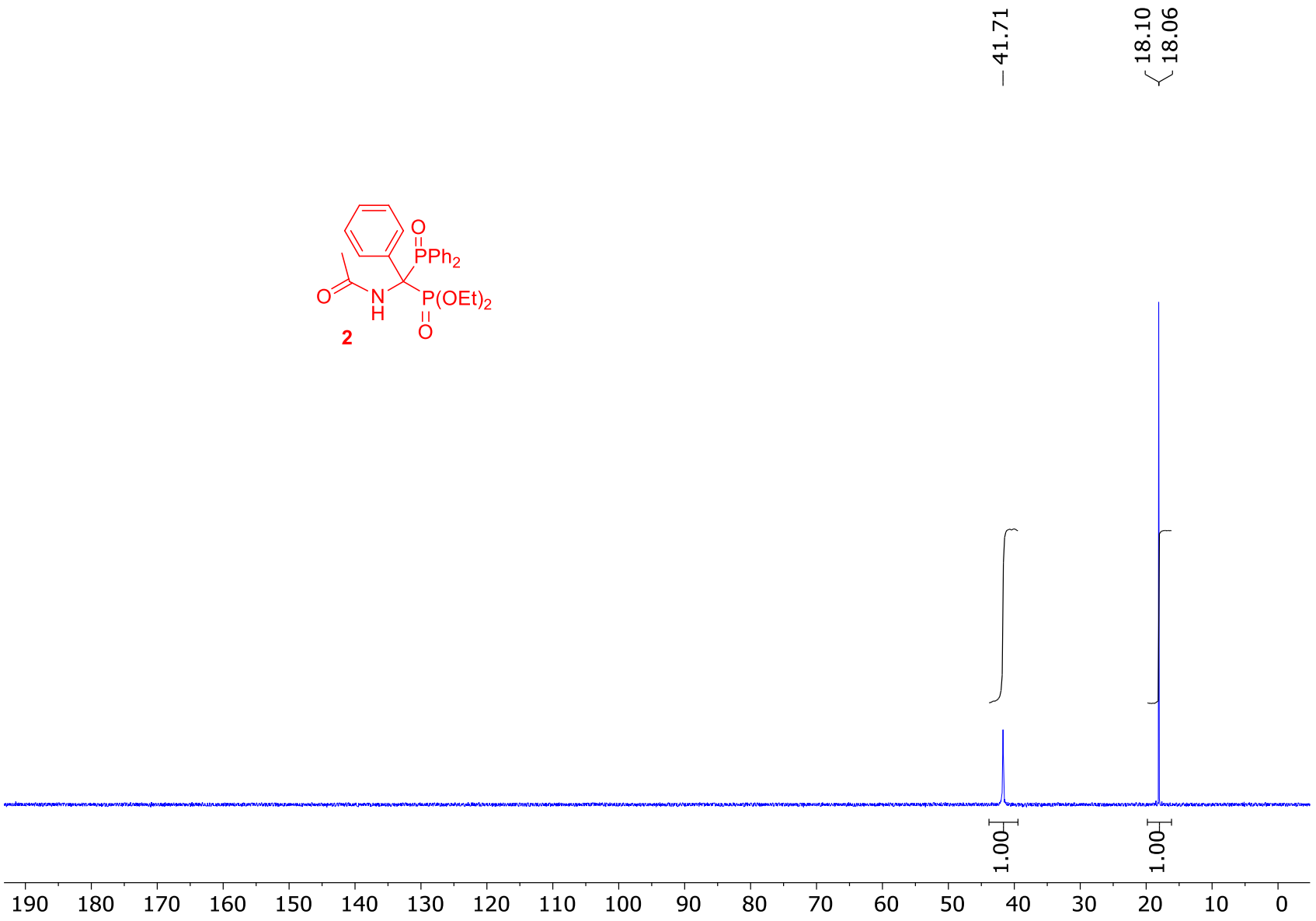


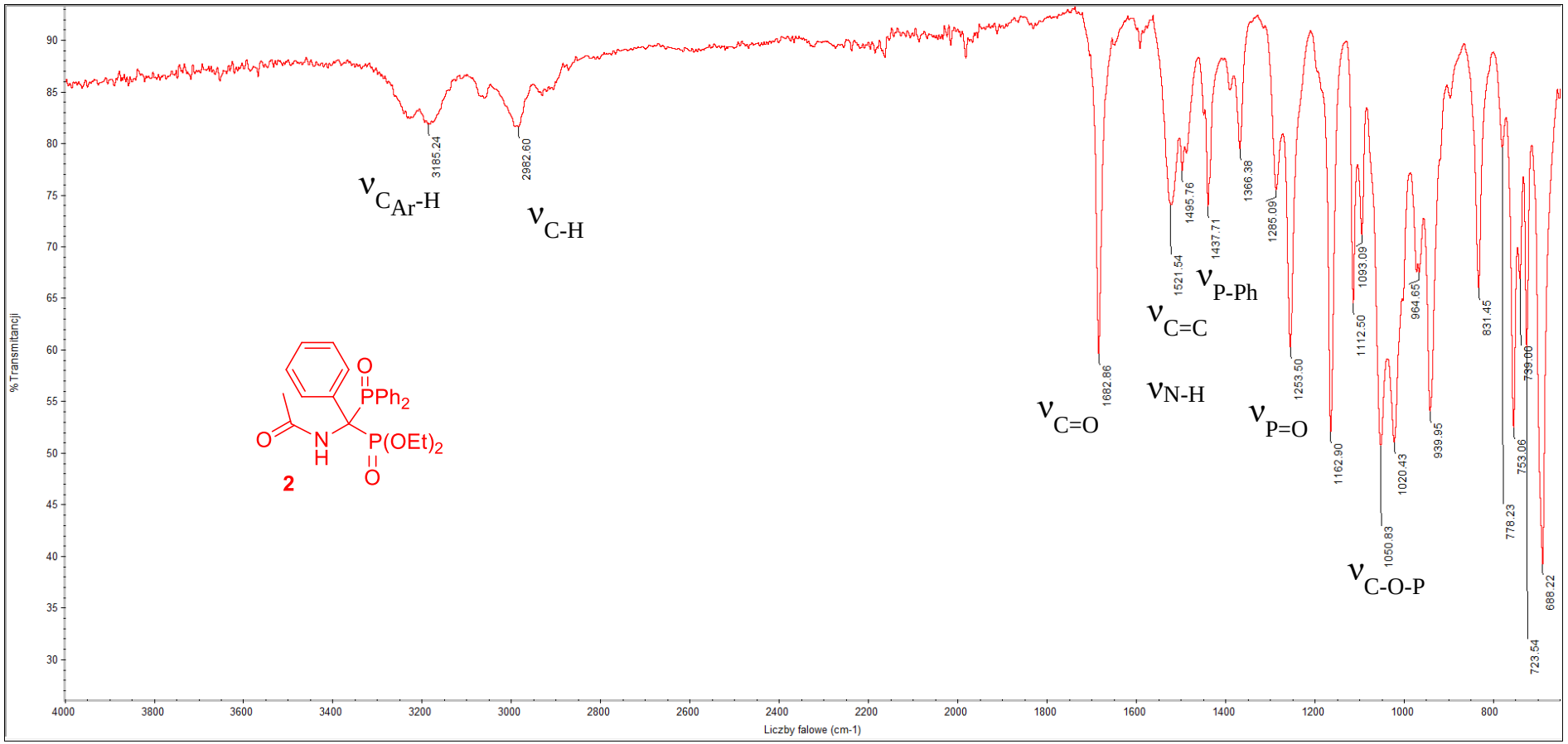
^{1}H NMR spectrum of diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate; 400 MHz/$CDCl_3$; δ (ppm).



^{13}C NMR spectrum of diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate; 100 MHz/$CDCl_3$; δ (ppm).



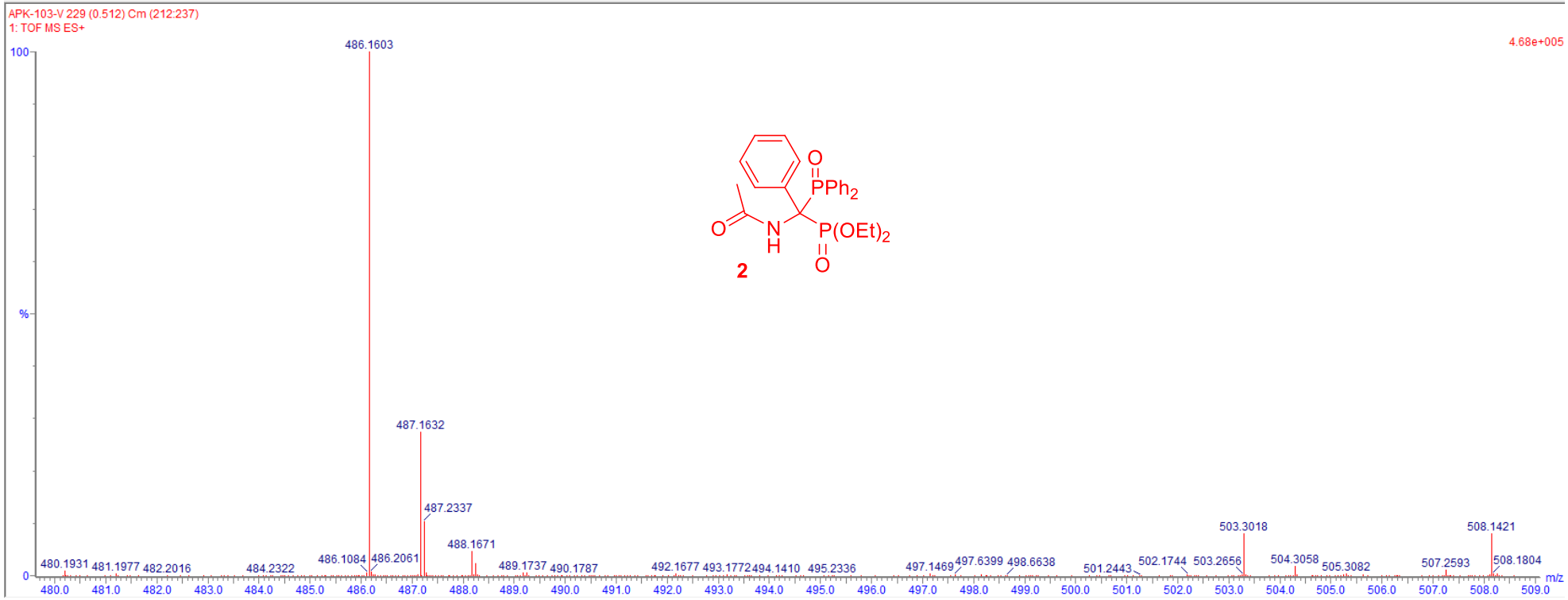
^{31}P NMR spectrum of diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate; 162 MHz/$CDCl_3$; δ (ppm).



IR spectrum of diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate; ATR; cm^{-1}.

Tolerance = 100.0 mDa / DBE: min = -10.0, max = 200.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
49 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)
Elements Used:

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	P
486.1603	100.00	486.1599	0.4	0.8	12.5	C25 H30 N O5 P2	483.0	1.058	34.70	25	30	1	5	2
		486.1682	-7.9	-16.2	12.5	C25 H29 N O7 P	486.9	4.966	0.70	25	29	1	7	1
		486.1470	13.3	27.4	17.5	C28 H25 N O5 P	489.9	7.926	0.04	28	25	1	5	1
		486.1447	15.6	32.1	8.5	C21 H30 N O8 P2	490.4	8.510	0.02	21	30	1	8	2
		486.1811	-20.8	-42.8	7.5	C22 H34 N O7 P2	489.0	7.065	0.09	22	34	1	7	2
		486.1318	28.5	58.6	13.5	C24 H25 N O8 P	486.9	4.959	0.70	24	25	1	8	1
		486.1235	36.8	75.7	13.5	C24 H26 N O6 P2	483.2	1.265	28.22	24	26	1	6	2
		486.2045	-44.2	-90.9	11.5	C26 H33 N O6 P	488.7	6.764	0.12	26	33	1	6	1



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MS spectrum of diethyl 1-(*N*-acetylamino)-1-(diphenylphosphinoyl)-1-phenylmethylphosphonate.