Electronic Supplementary Information

Multicomponent reactions of phosphines, enynedioates and benzylidene malononitriles generated highly substituted cyclopentenes through an unexpected phosphine α-addition-δ-evolvement of an anion pathway

Shih-Ching Chuang,[a,]* Shih-Ping Sung,[a] Jie-Cheng Deng,[a] Mong-Feng Chiou,[a] Day-Shin Hsu[b]

[a]Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan, Republic of China 300

[b]Department of Chemistry and Biochemistry, National Chung-Cheng University, Chiayi, Taiwan, Republic of China 621

E-mail: jscchuang@faculty.nctu.edu.tw

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Fig. S1. ^{1}H NMR spectrum of compound **4a** (400 MHz, $CDCl_3$)

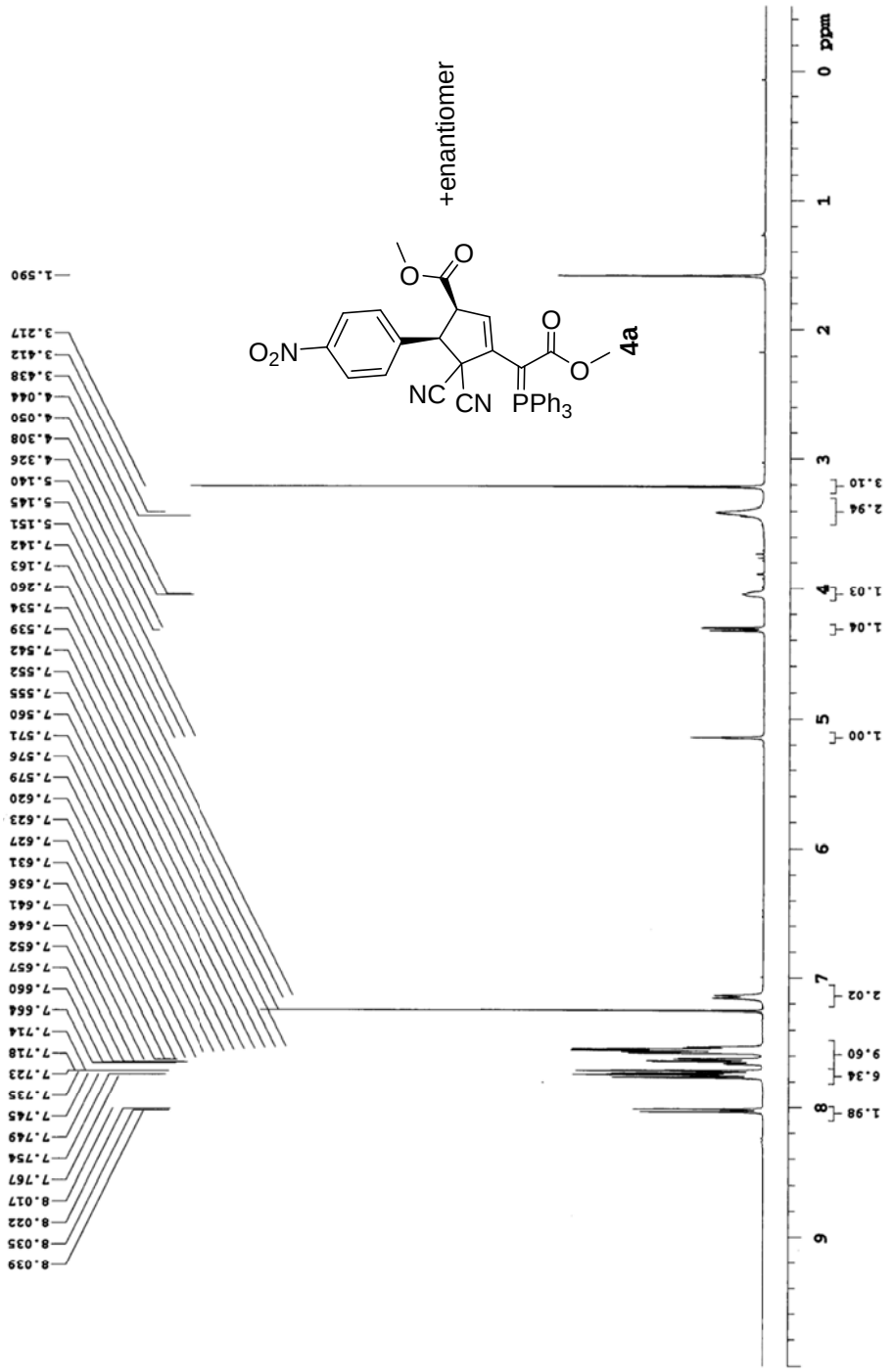

Fig. S2. ^{13}C NMR spectrum of compound **4a** (100 MHz, $CDCl_3$)

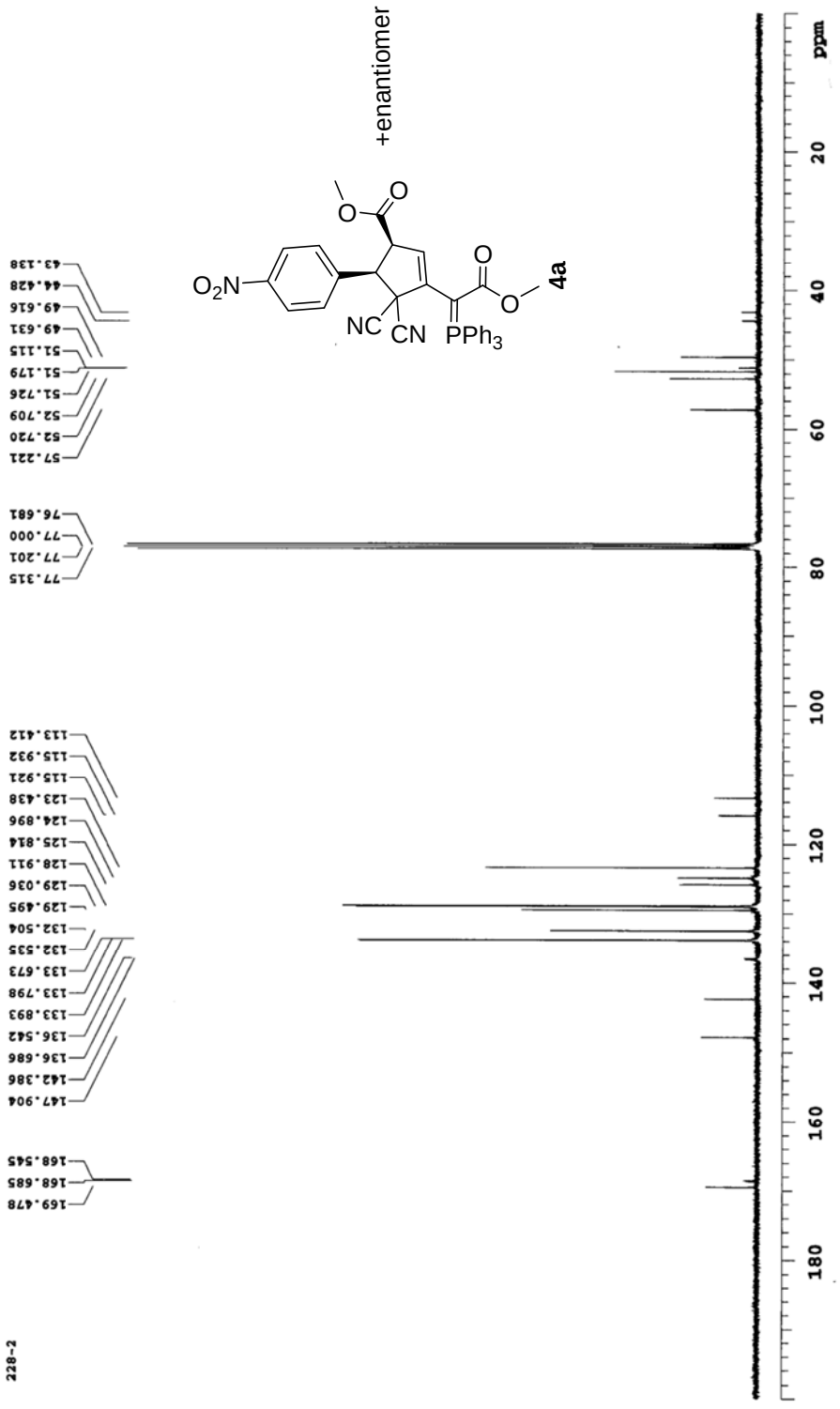

Fig. S3. ^{1}H NMR spectrum of compound **4a′** (400 MHz, $CDCl_3$)

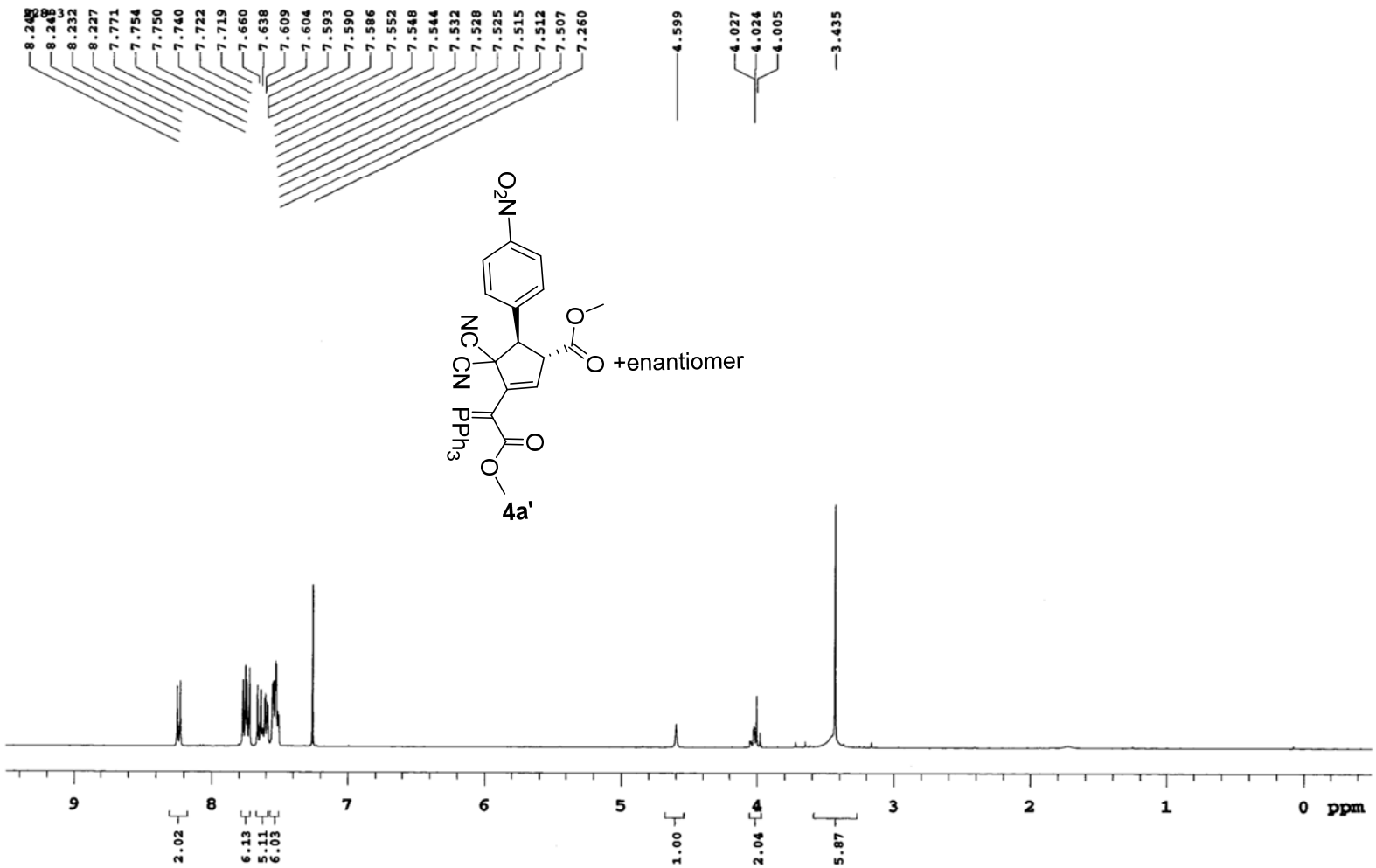

Fig. S4. ^{13}C NMR spectrum of compound **4a'** (100 MHz, $CDCl_3$)

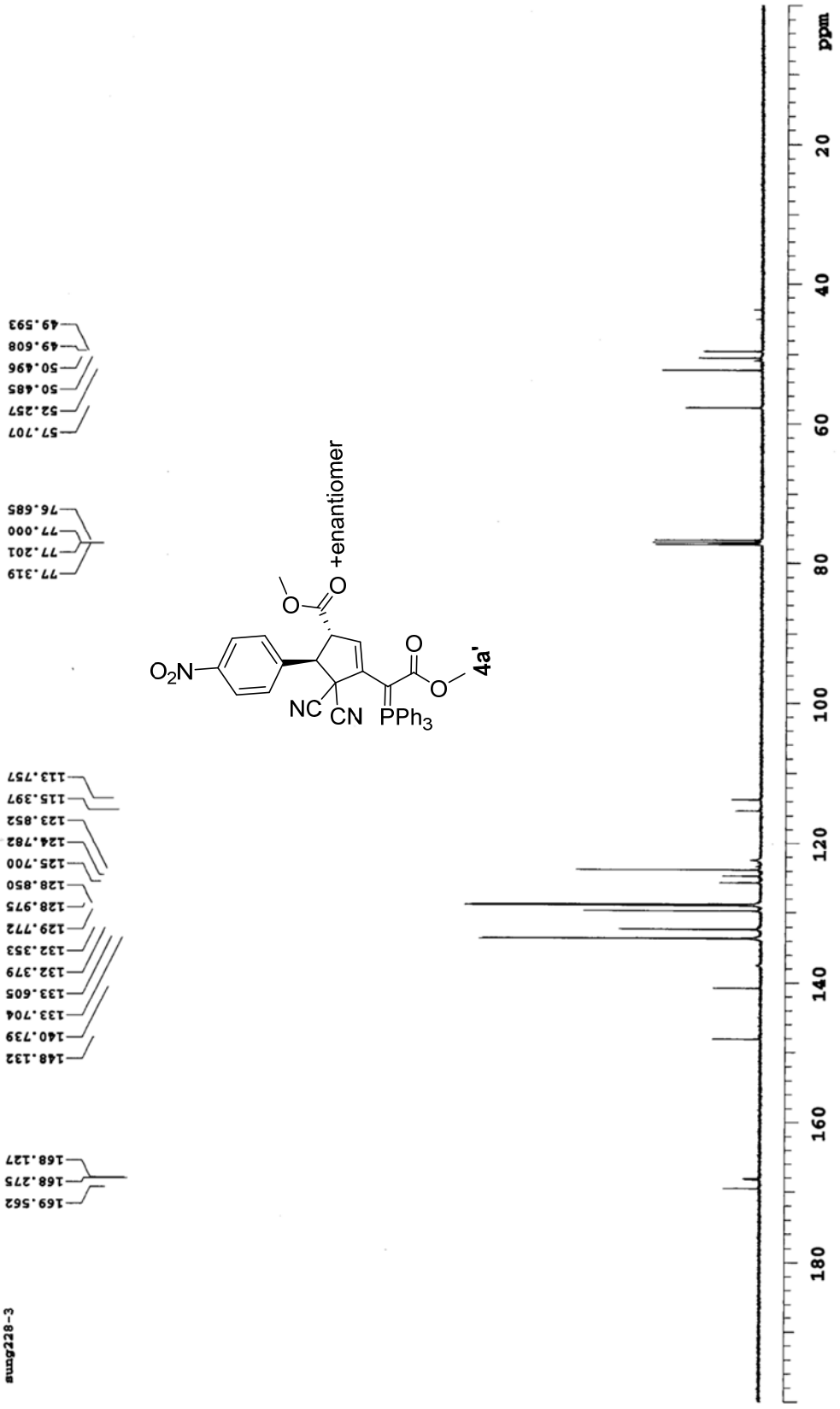

Fig. S5. ^{1}H NMR spectrum of compound **4b** (300 MHz, $CDCl_3$)

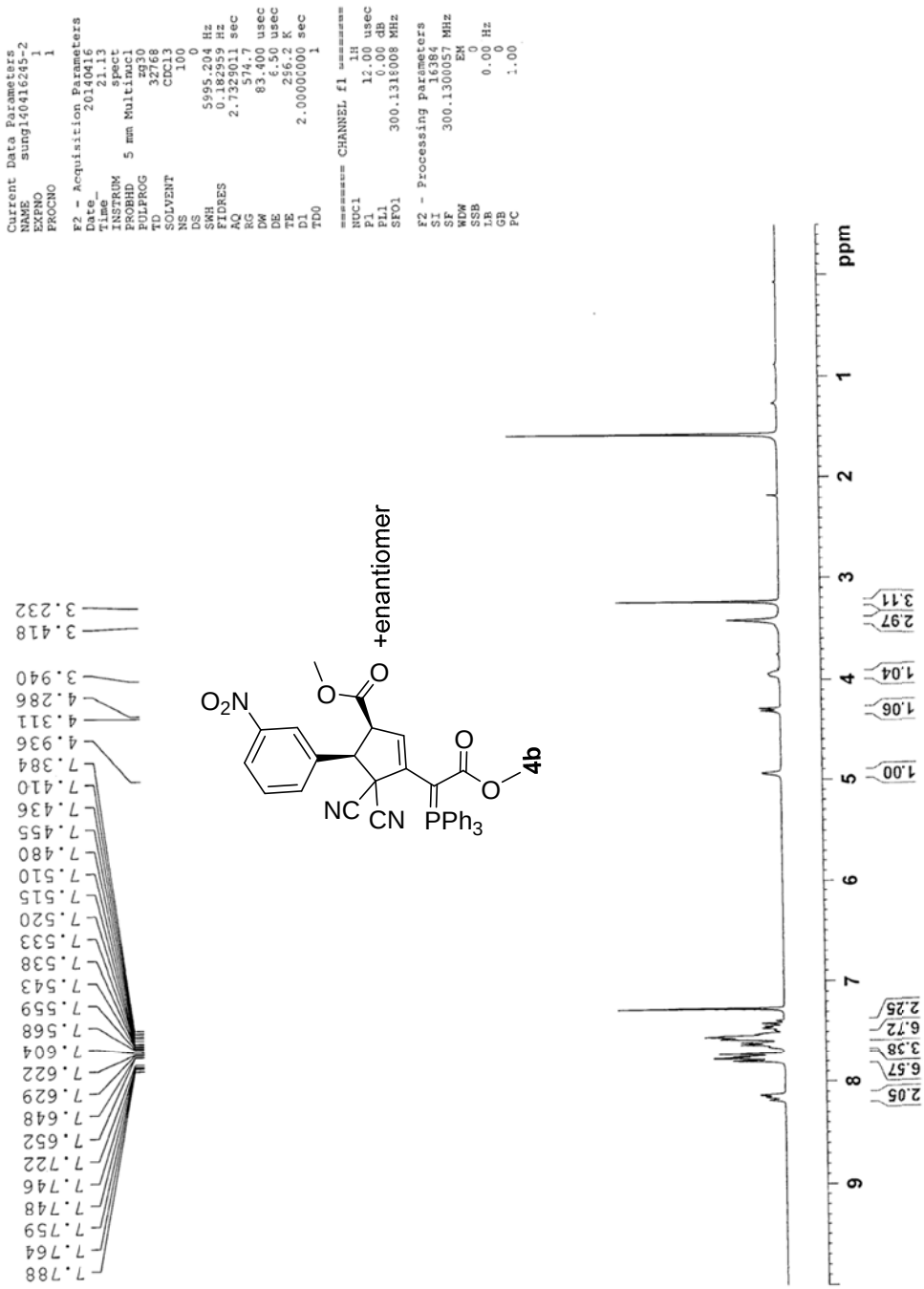

Fig. S6. ^{13}C NMR spectrum of compound **4b** (100 MHz, $CDCl_3$)

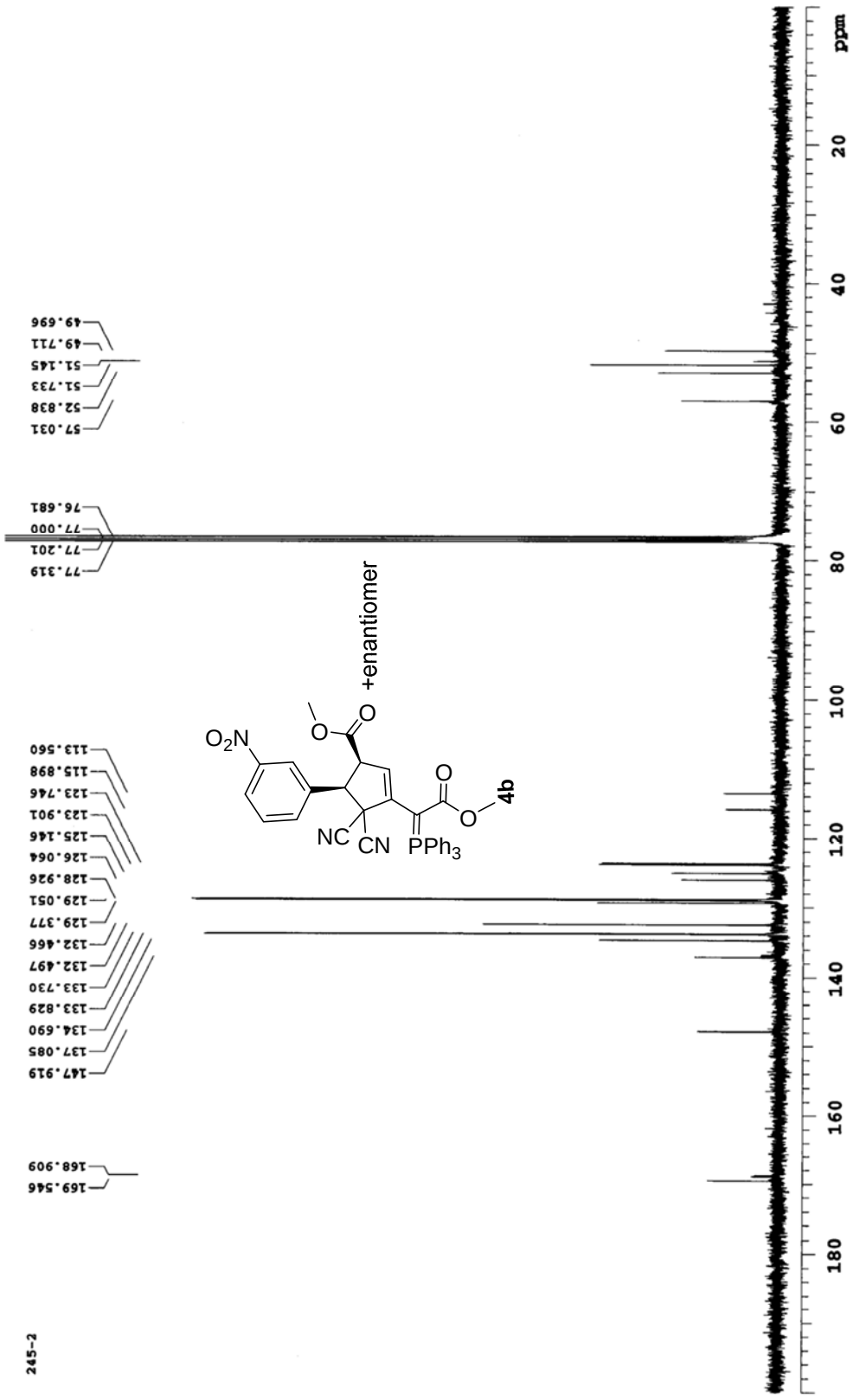

Fig. S7. ^{1}H NMR spectrum of compound **4b′** (300 MHz, $CDCl_3$)

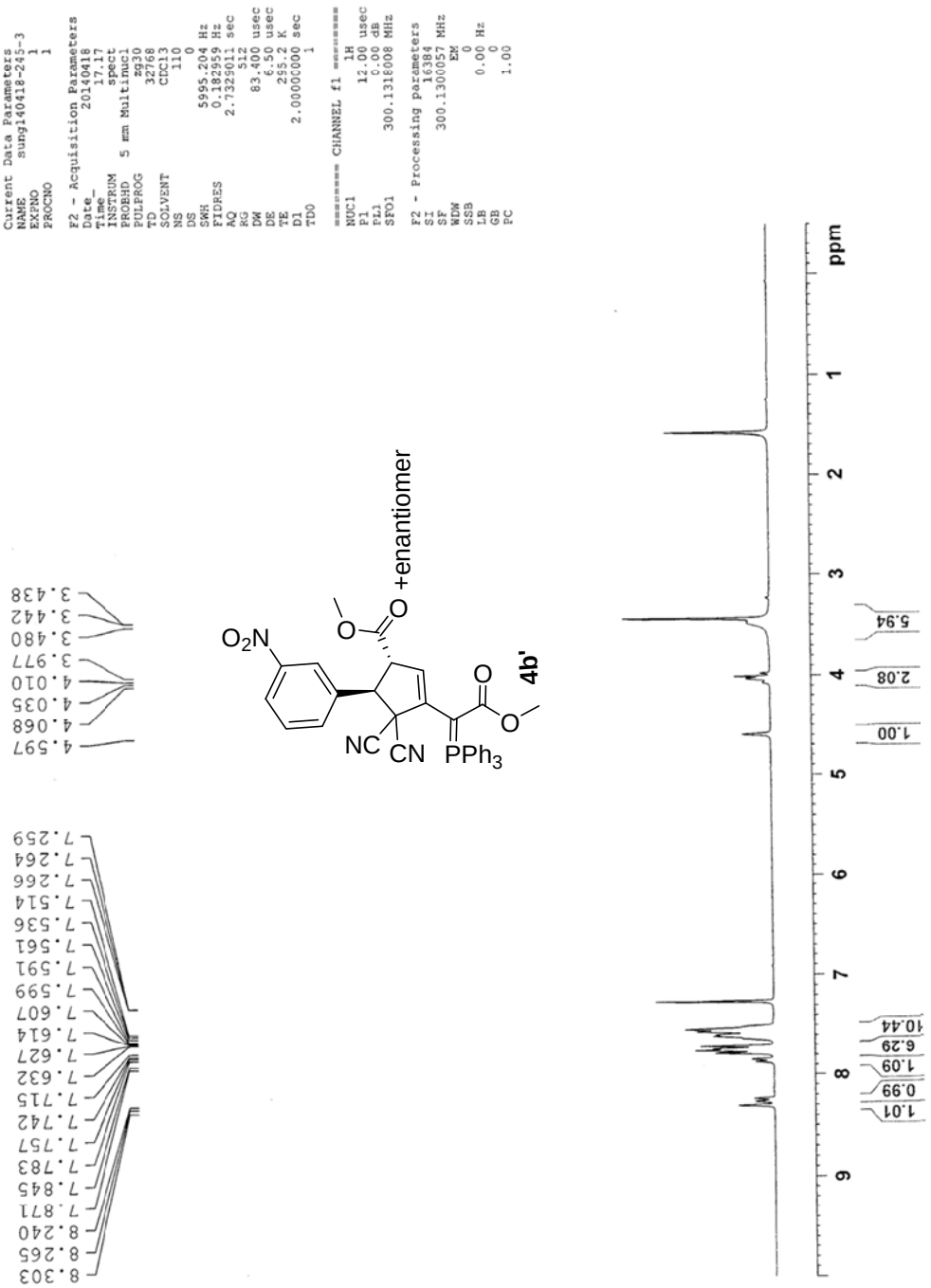

Fig. S8. ^{13}C NMR spectrum of compound **4b'** (100 MHz, $CDCl_3$)

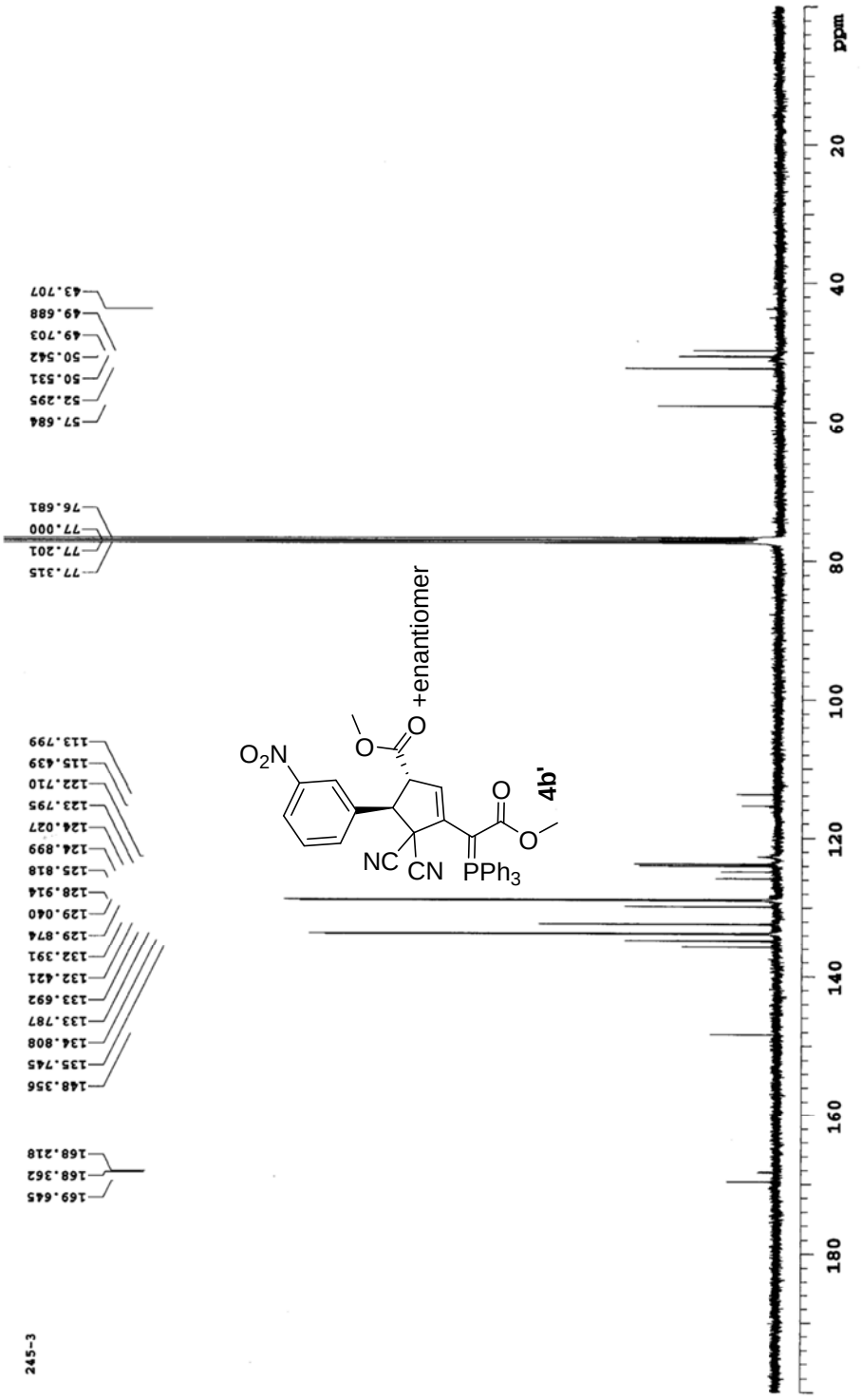

Fig. S9. ^{1}H NMR spectrum of compound **4c** (300 MHz, $CDCl_3$)

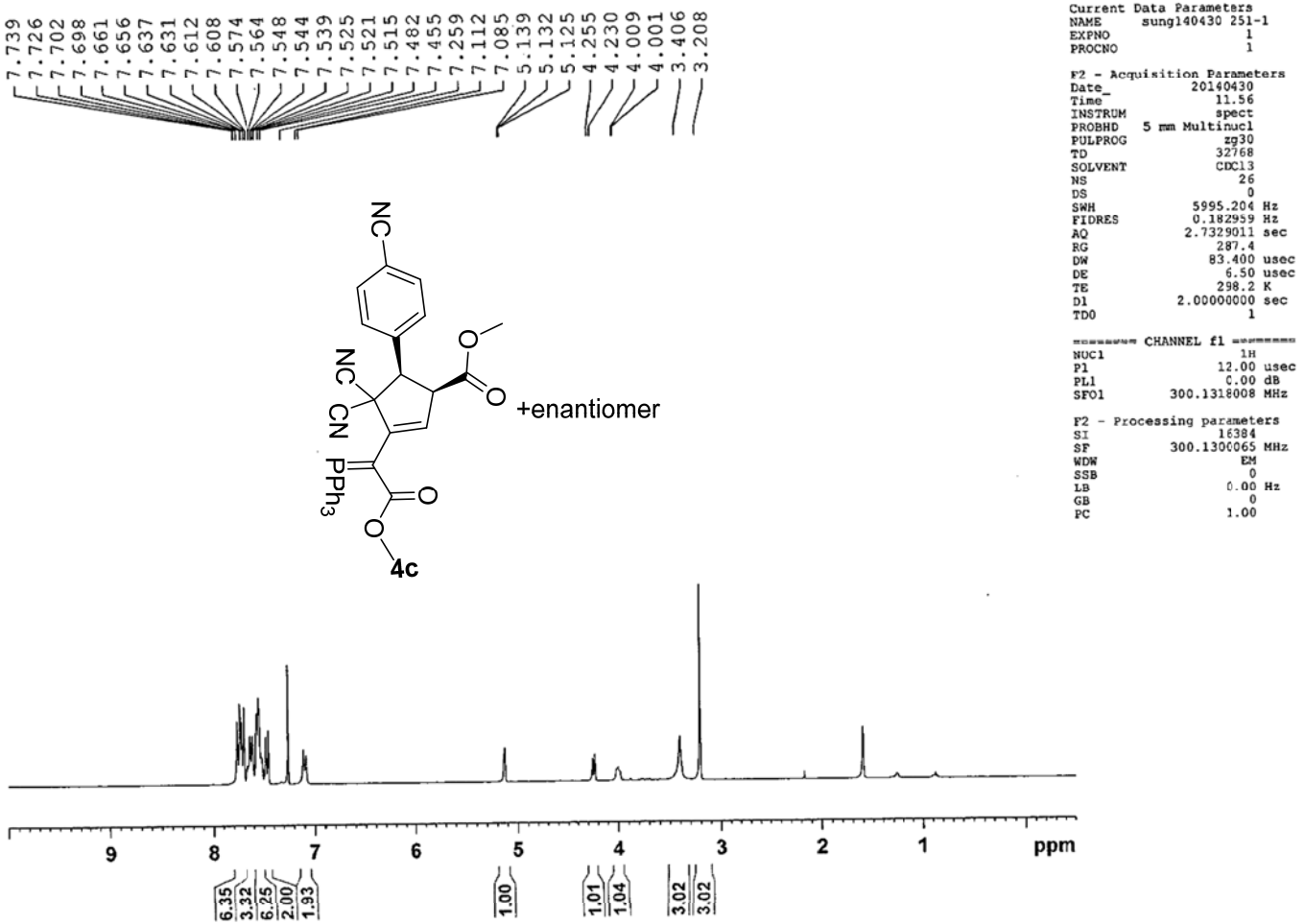

Fig. S10. ^{13}C NMR spectrum of compound **4c** (100 MHz, $CDCl_3$)

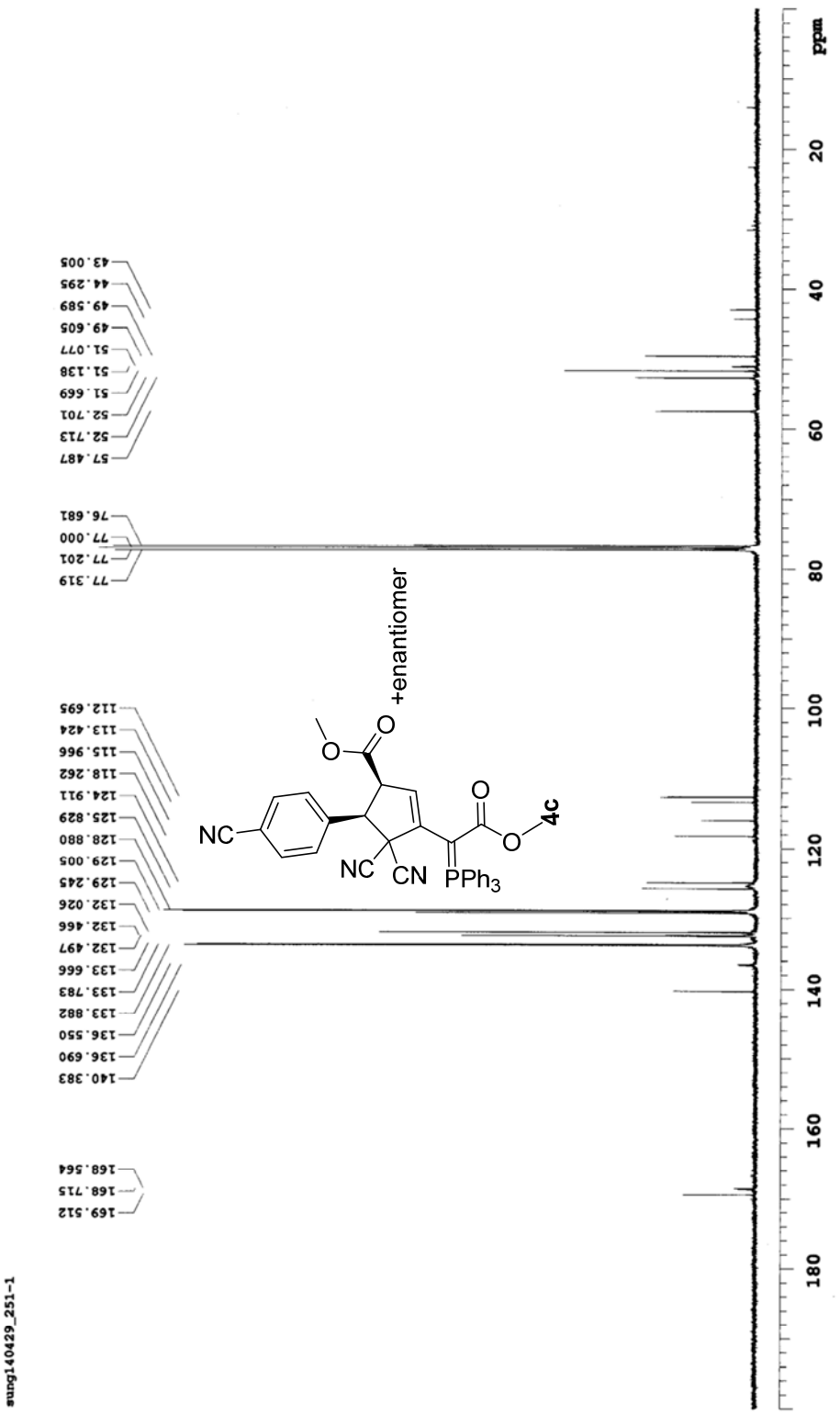

Fig. S11. ^{1}H NMR spectrum of compound **4c'** (300 MHz, $CDCl_3$)

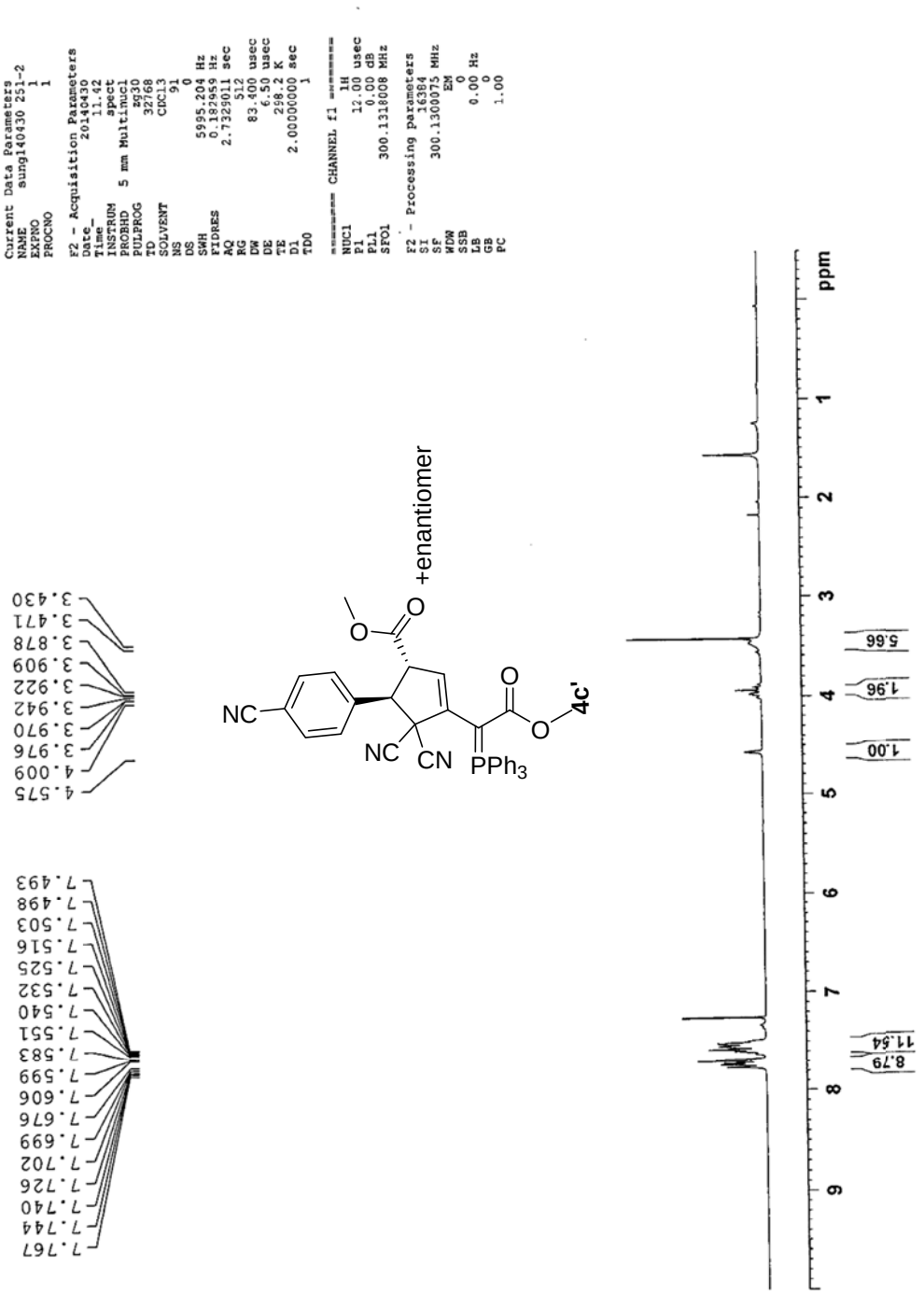

Fig. S12. ^{13}C NMR spectrum of compound **4c'** (100 MHz, $CDCl_3$)

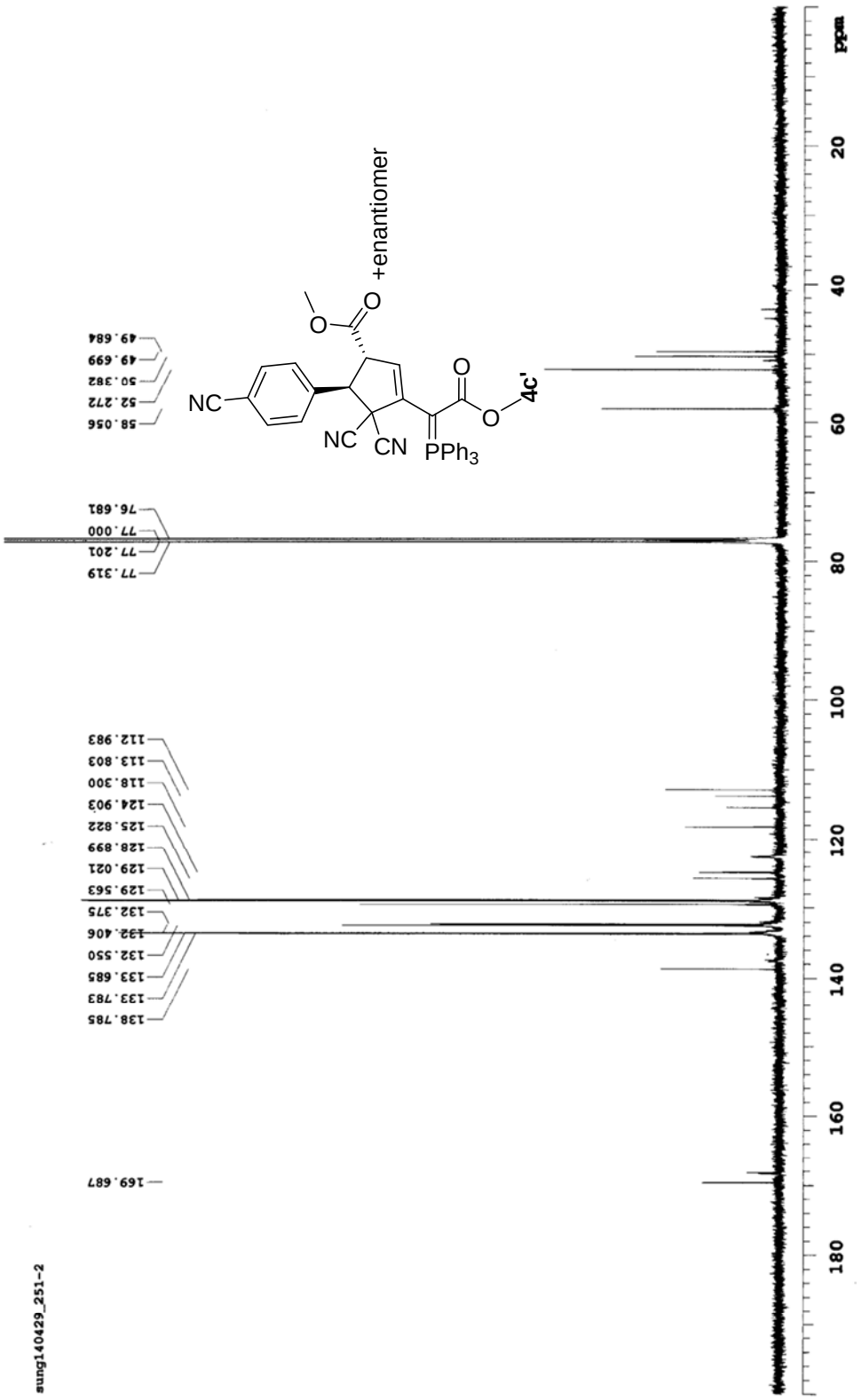

Fig. S13. ^{1}H NMR spectrum of compound **4d** (300 MHz, $CDCl_3$)

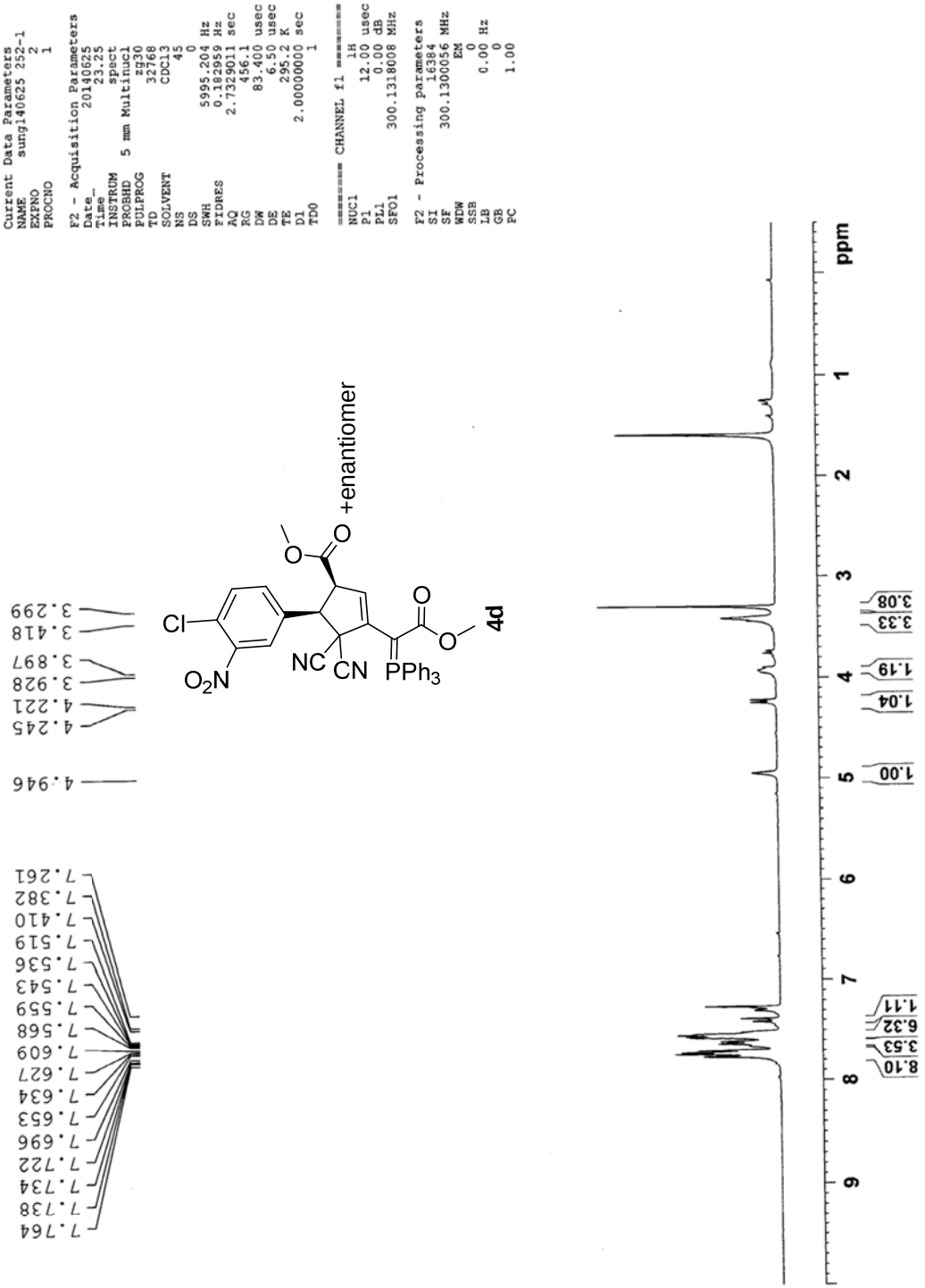

Fig. S14. ^{13}C NMR spectrum of compound **4d** (100 MHz, $CDCl_3$)

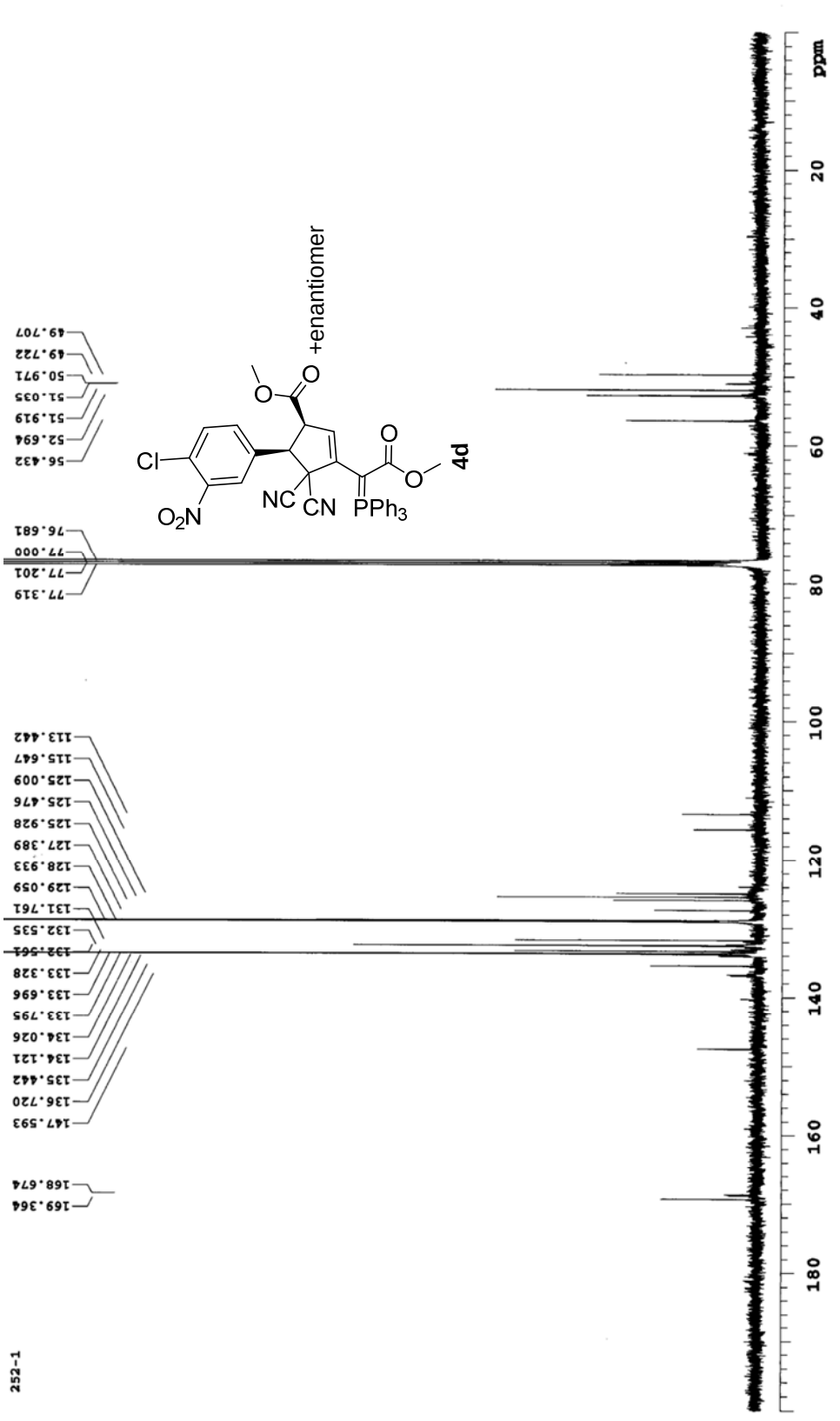

Fig. S15. ^{1}H NMR spectrum of compound **4d'** (300 MHz, $CDCl_3$)

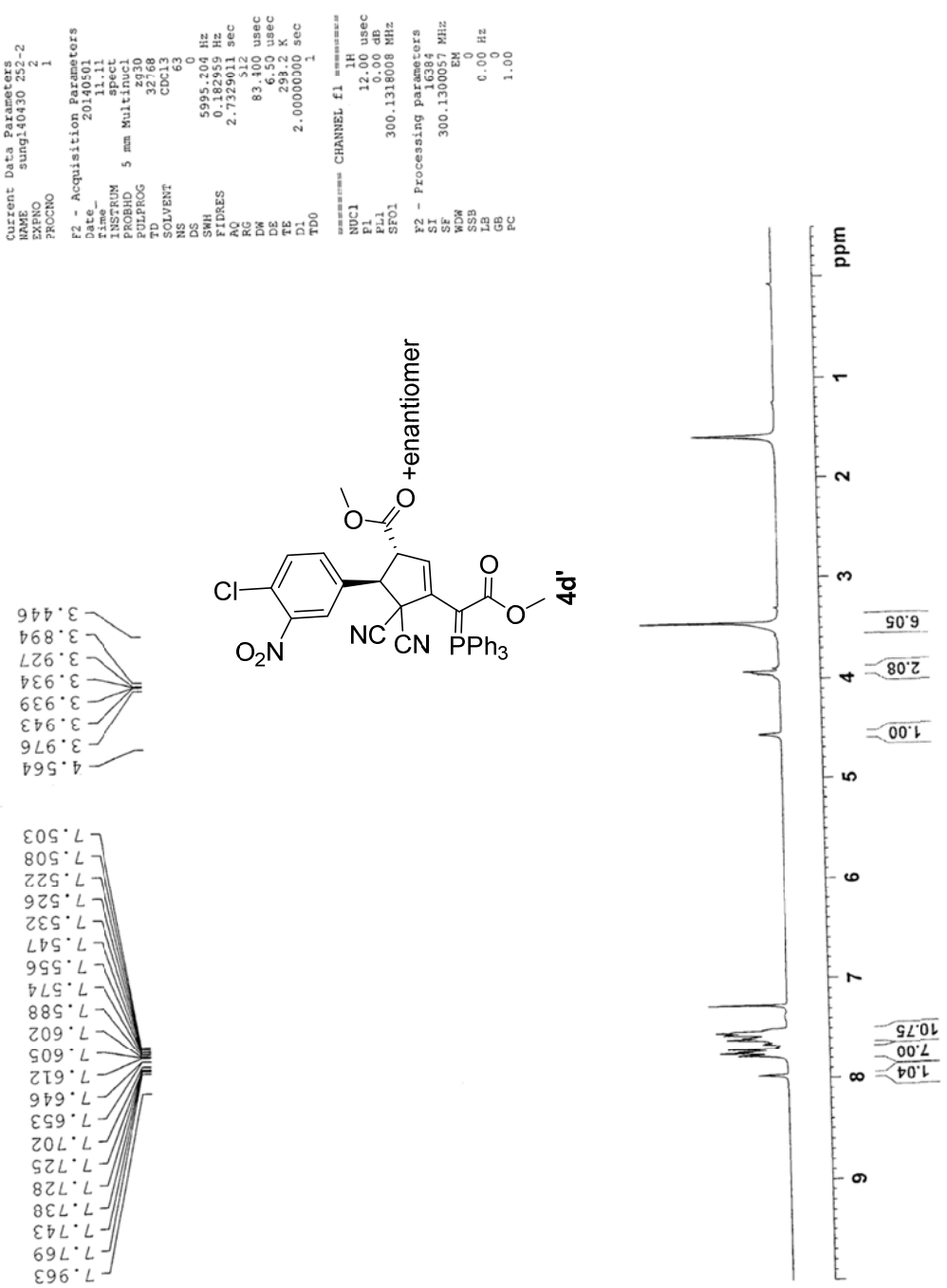

Fig. S16. ^{13}C NMR spectrum of compound **4d′** (175.9 MHz, $CDCl_3$)

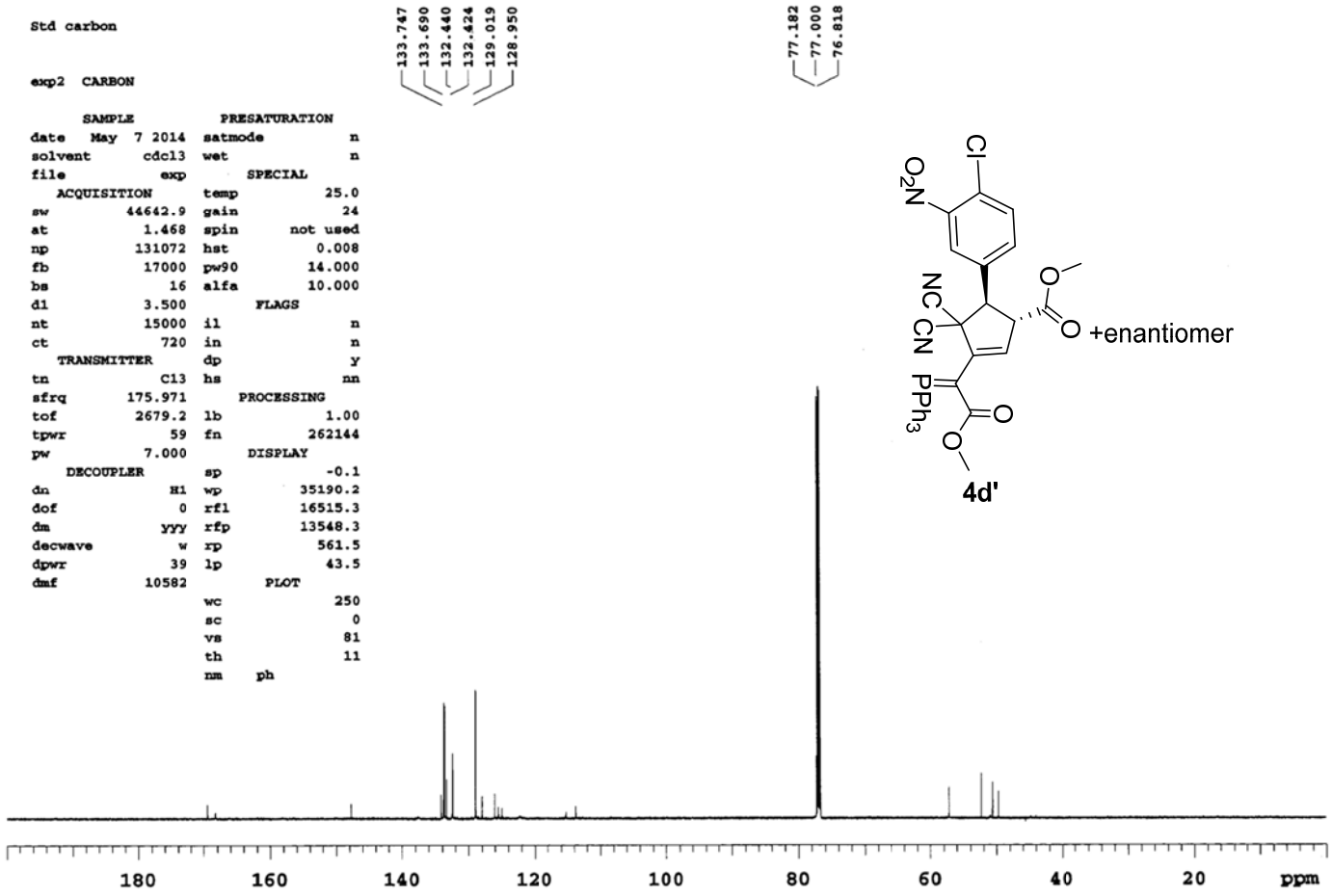

Fig. S17. ^{1}H NMR spectrum of compound **4e** (400 MHz, $CDCl_3$)

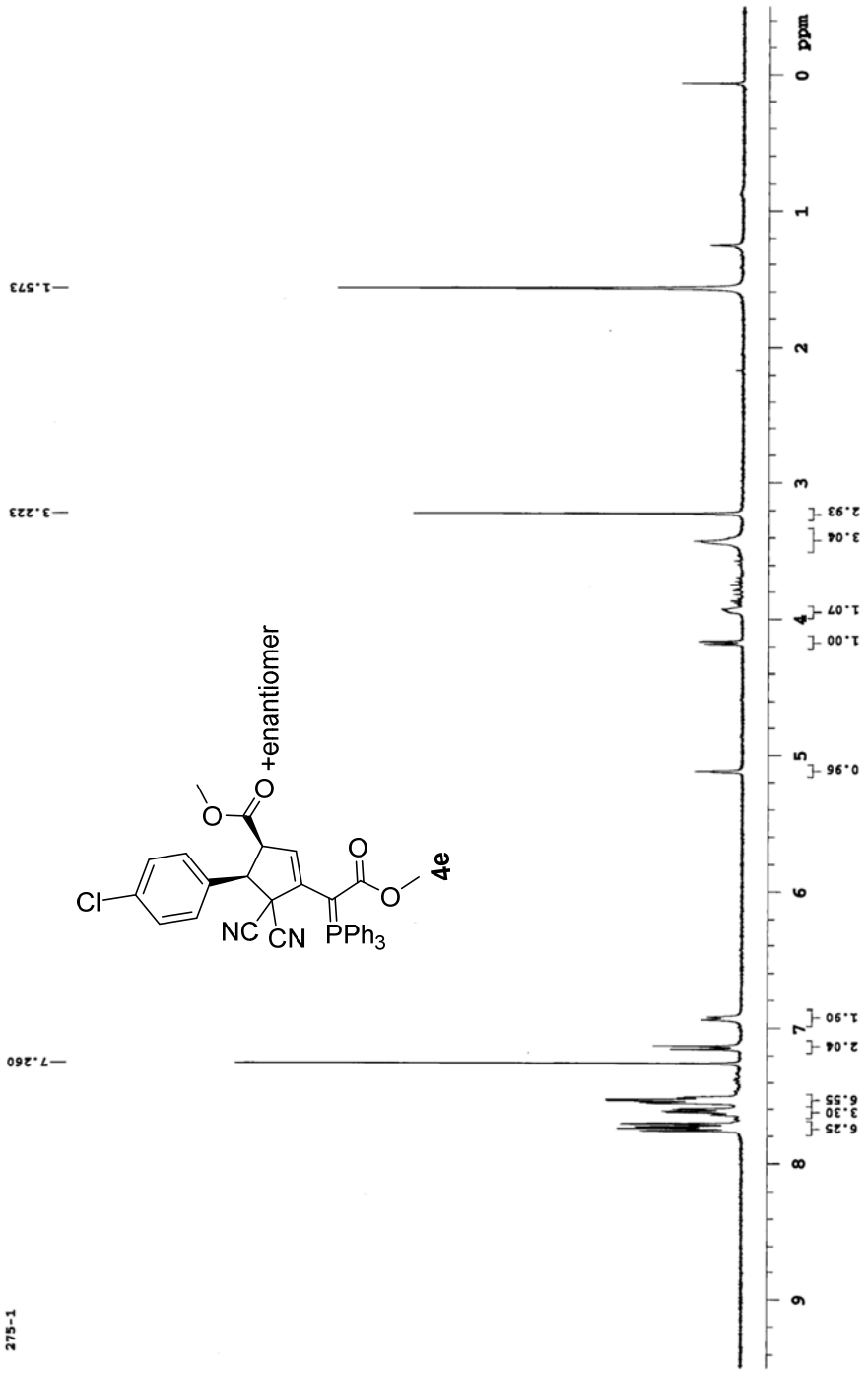

Fig. S18. ^{13}C NMR spectrum of compound **4e** (100 MHz, $CDCl_3$)

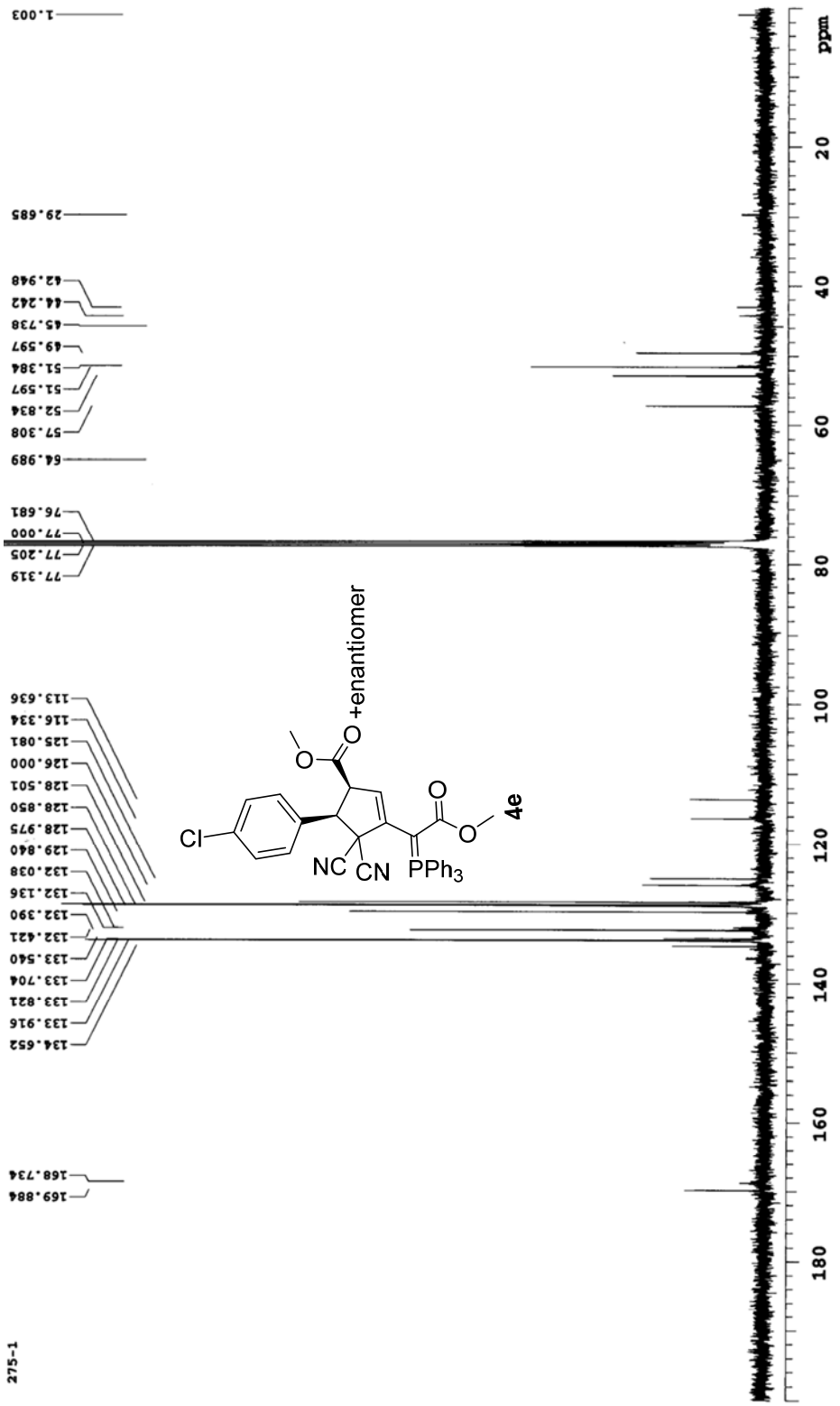

Fig. S19. ^{1}H NMR spectrum of compound **4e'** (400 MHz, $CDCl_3$)

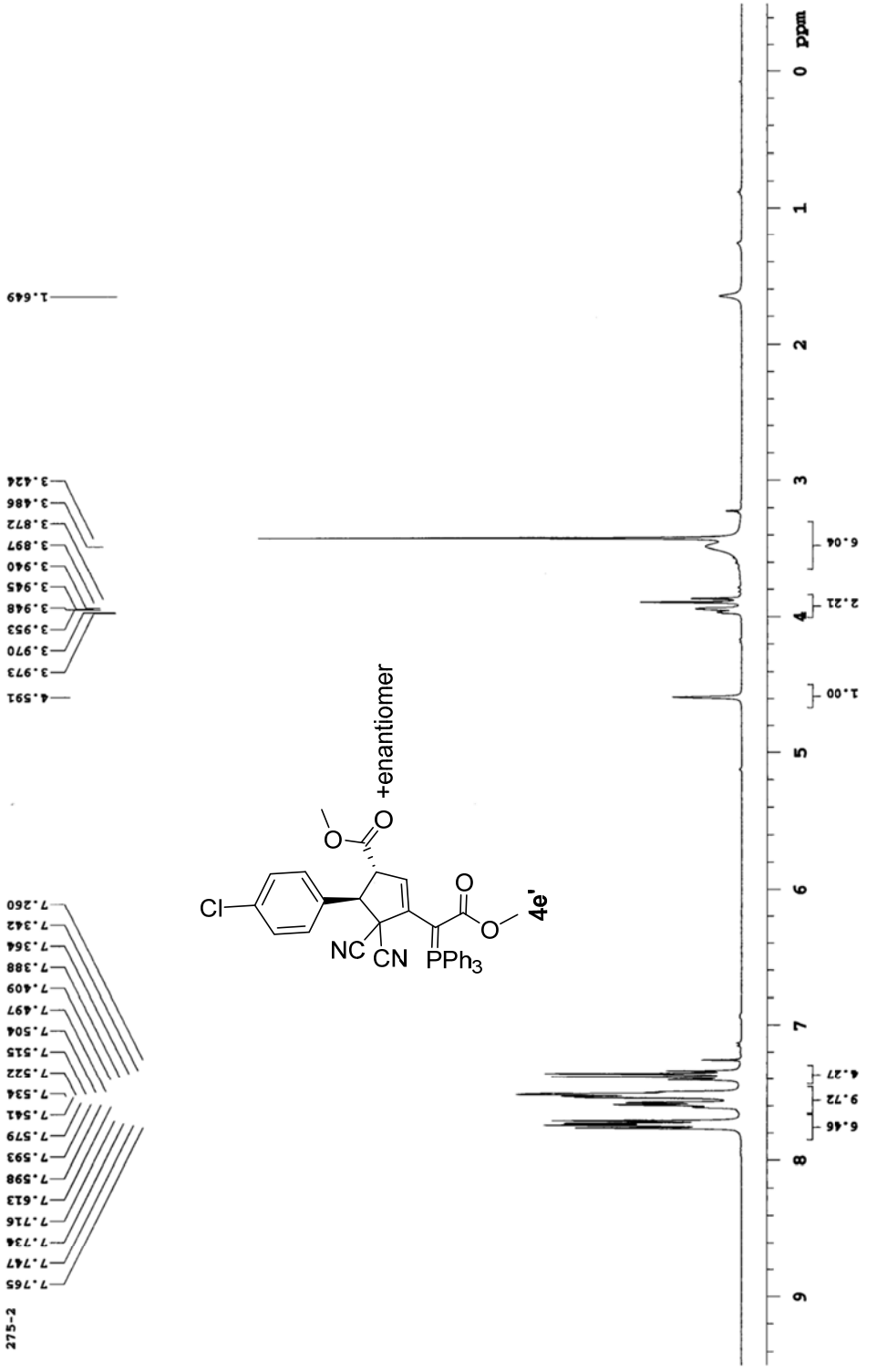

Fig. S20. ^{13}C NMR spectrum of compound **4e'** (100 MHz, $CDCl_3$)

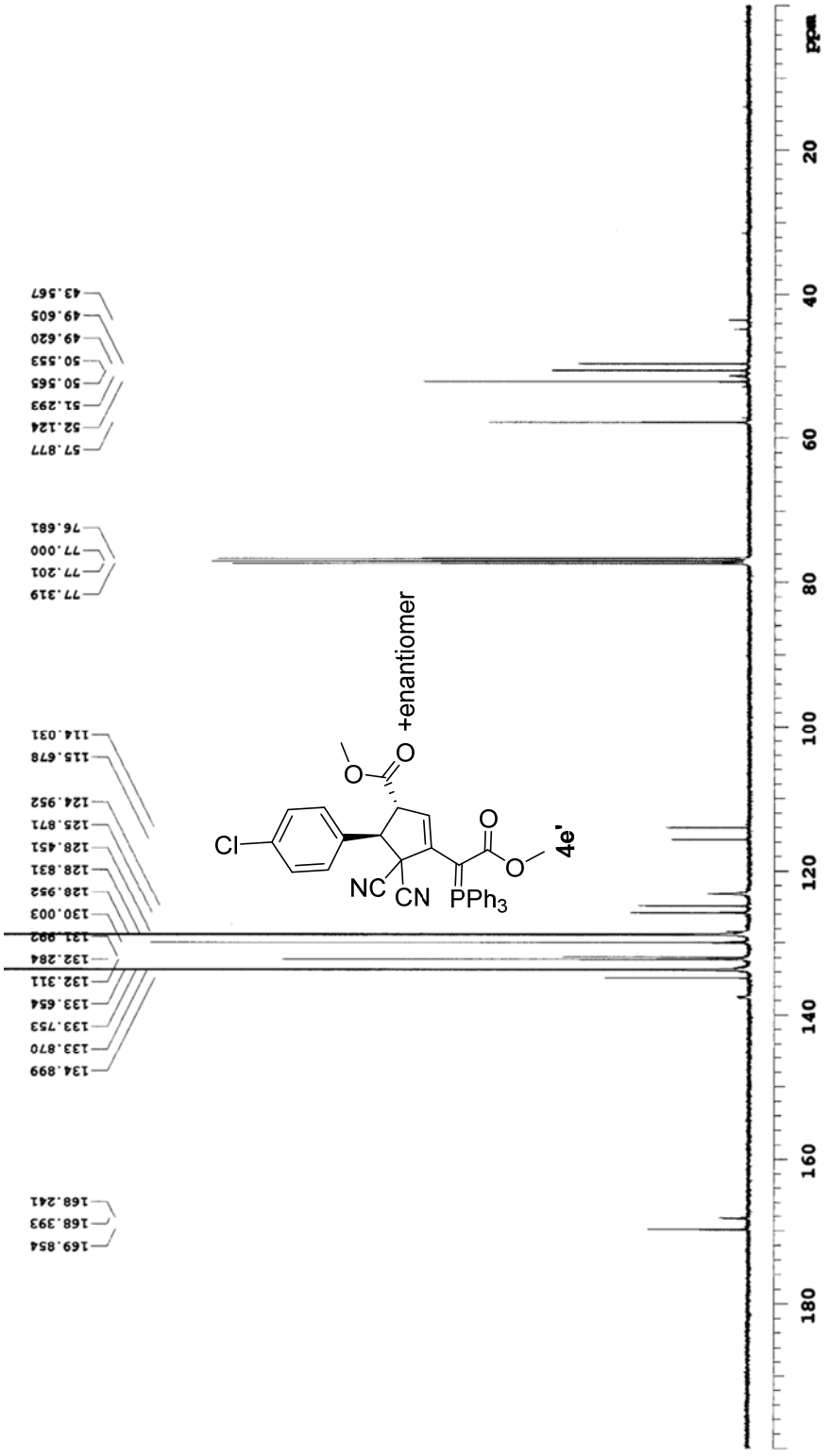

Fig. S21. ^{1}H NMR spectrum of compound **4f** (400 MHz, $CDCl_3$)

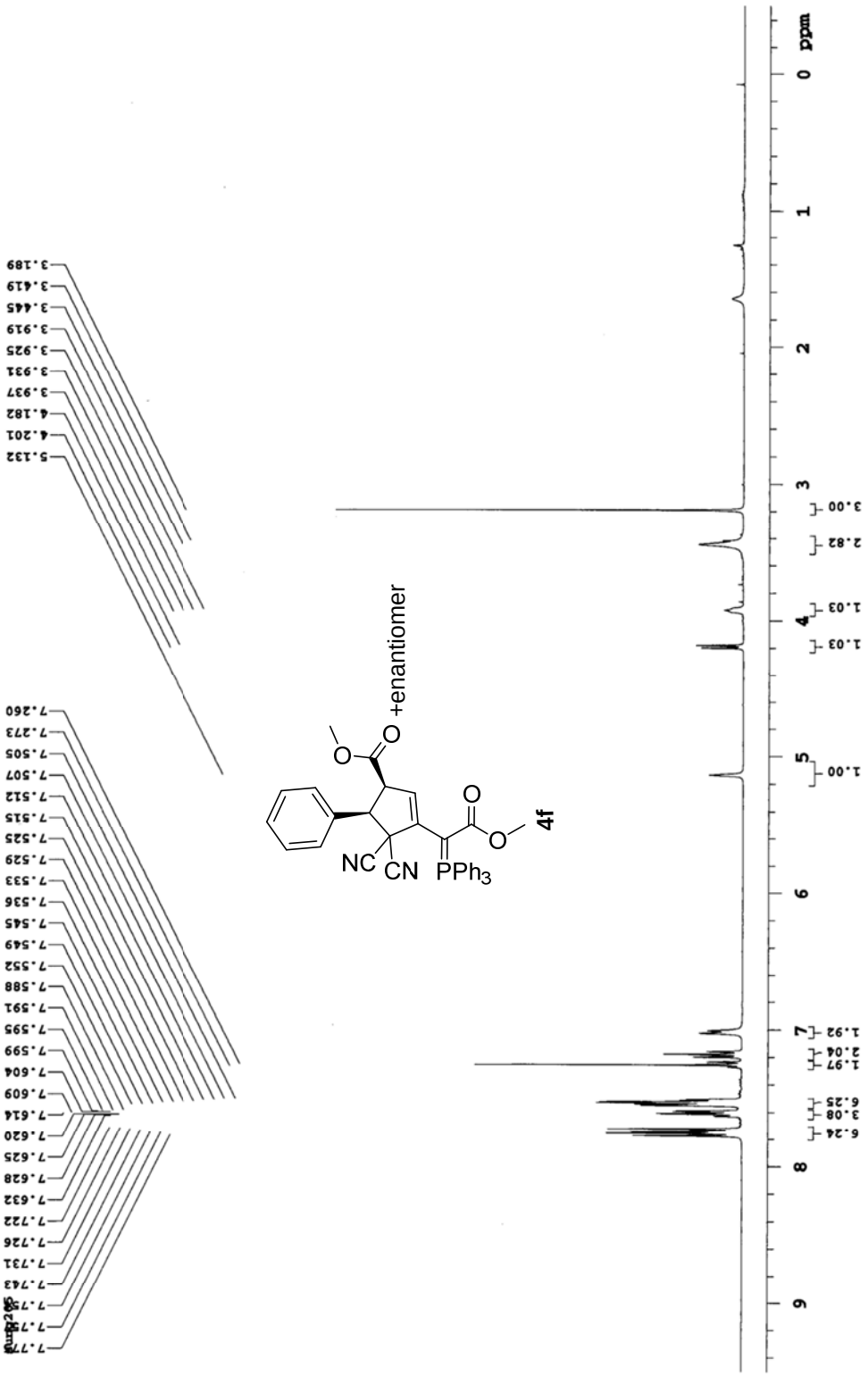

Fig. S22. ^{13}C NMR spectrum of compound **4f** (100 MHz, $CDCl_3$)

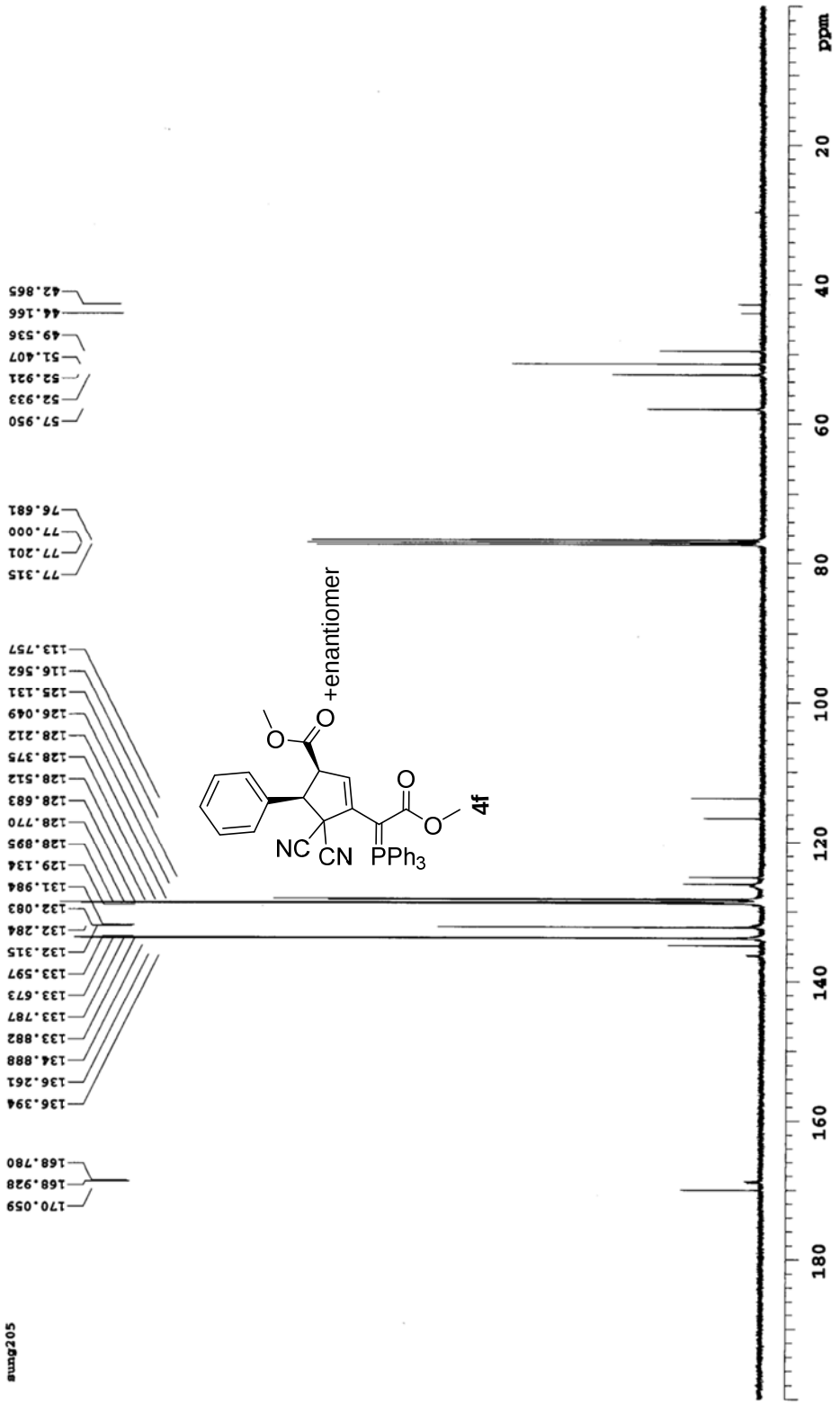

Fig. S23. ^{1}H NMR spectrum of compound **4f′** (300 MHz, $CDCl_3$)

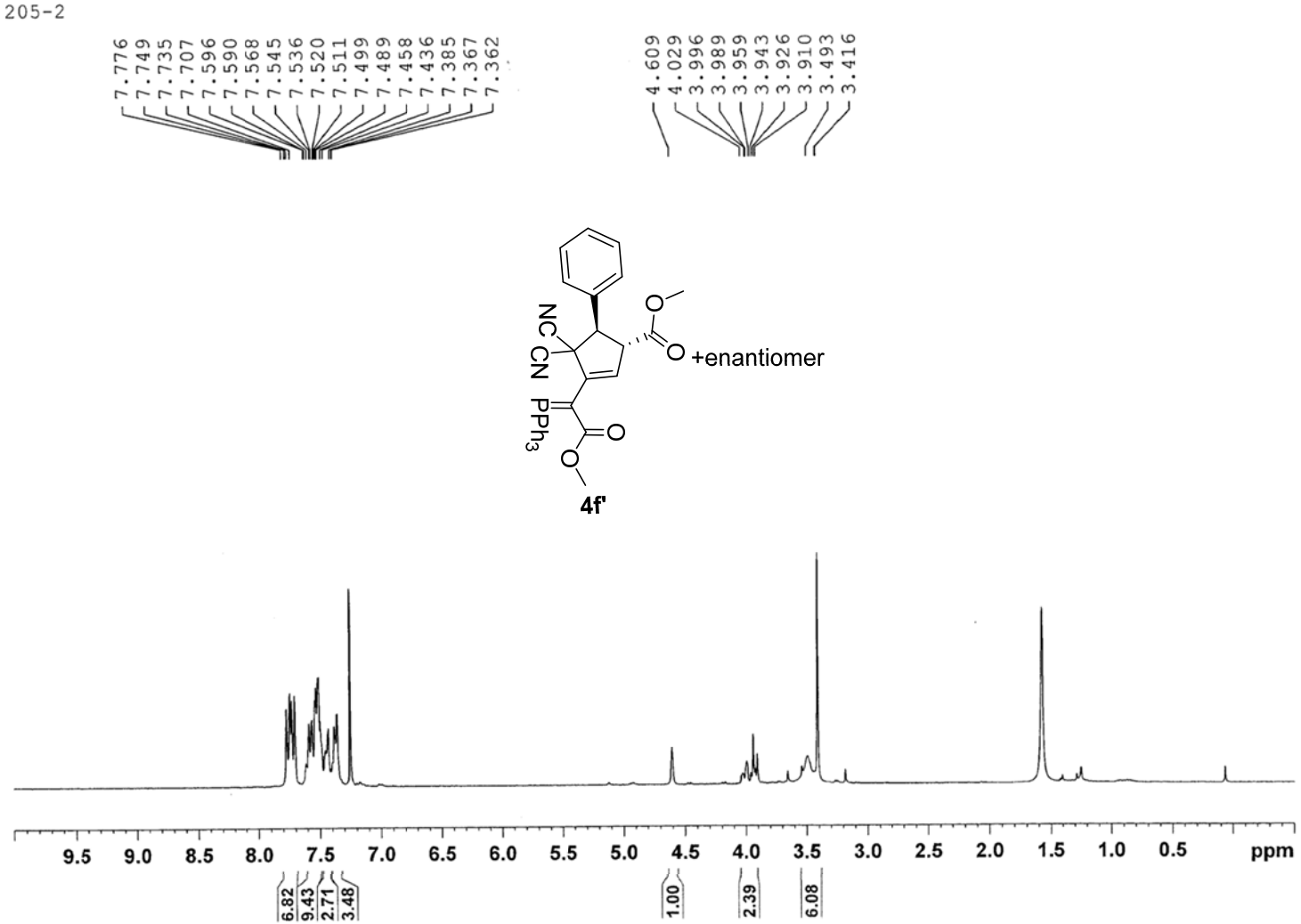

Fig. S24. ^{13}C NMR spectrum of compound **4f′** (175.9 MHz, $CDCl_3$)

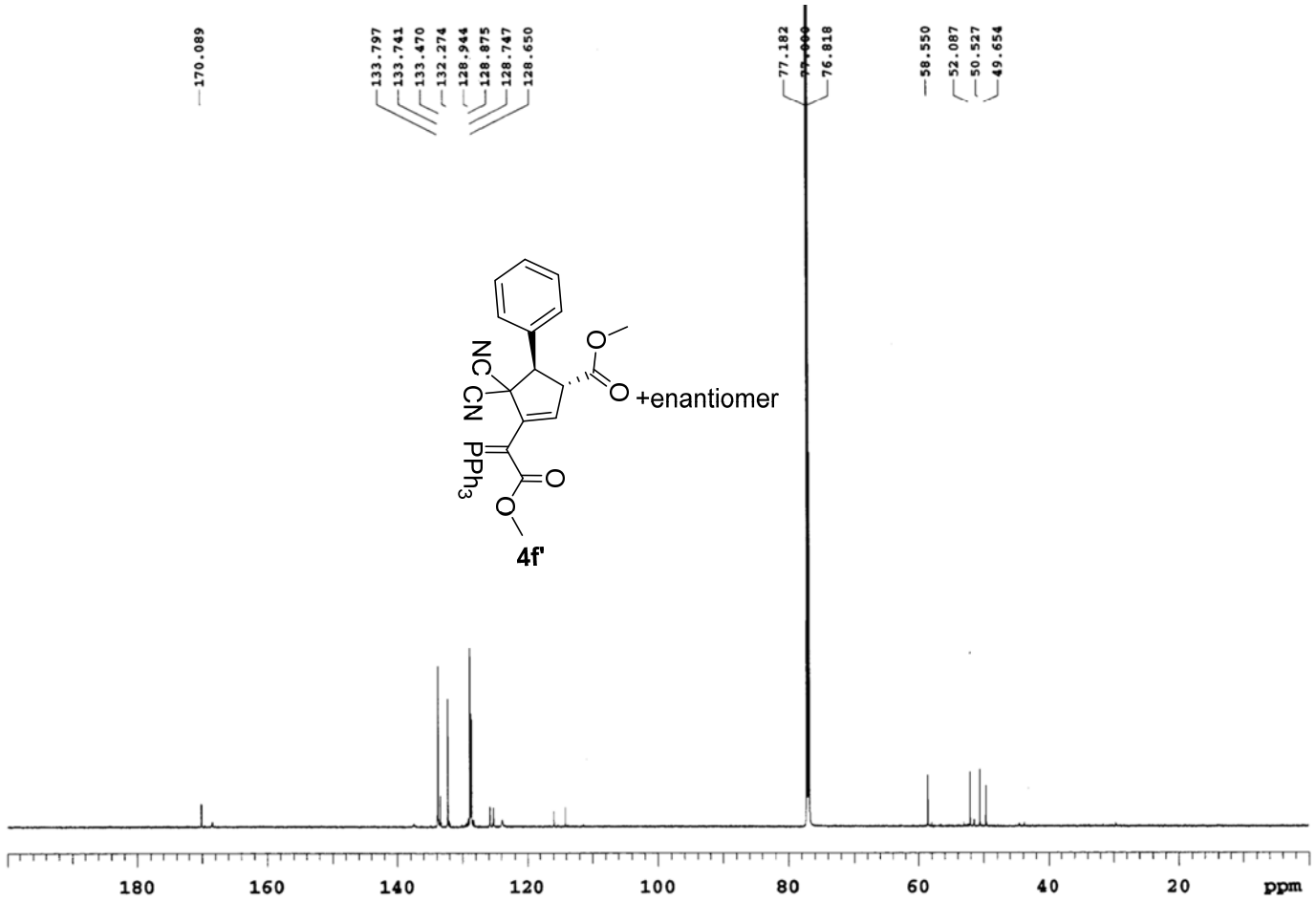

Fig. S25. ^{1}H NMR spectrum of compound **4g** (300 MHz, $CDCl_3$)

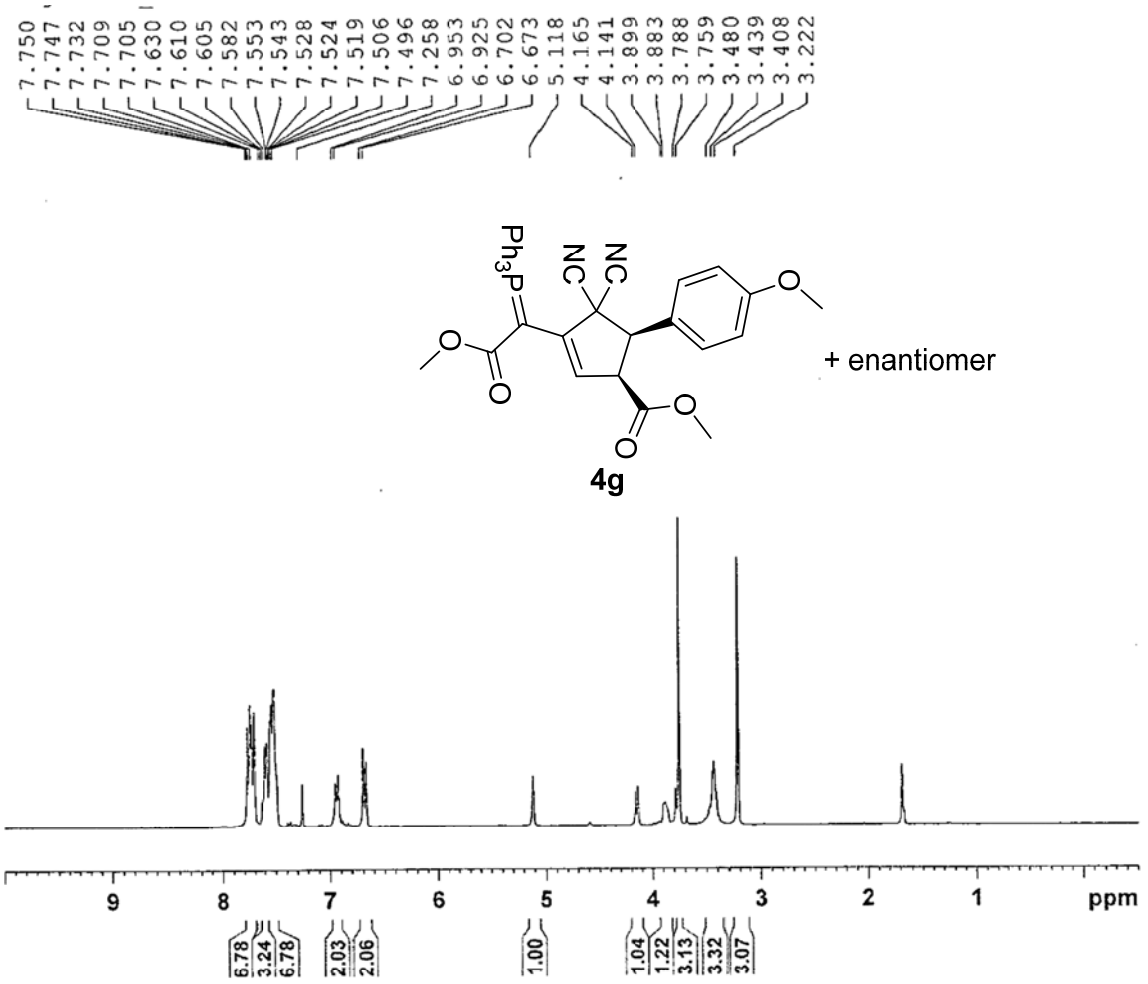


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Fig. S26. ^{13}C NMR spectrum of compound **4g** (100 MHz, $CDCl_3$)

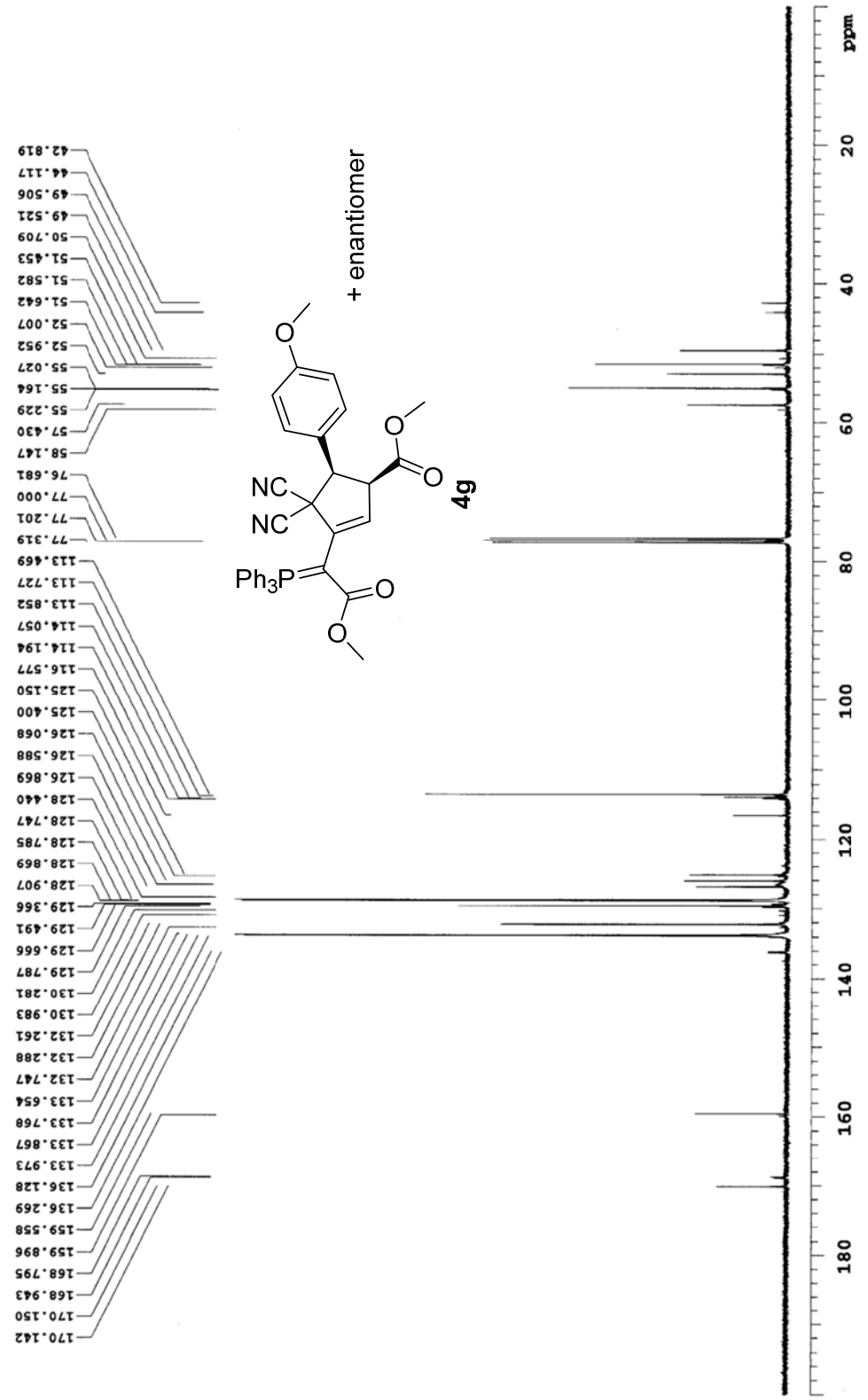


Fig. S27. ^{1}H NMR spectrum of compound **4g''** (300 MHz, $CDCl_3$)

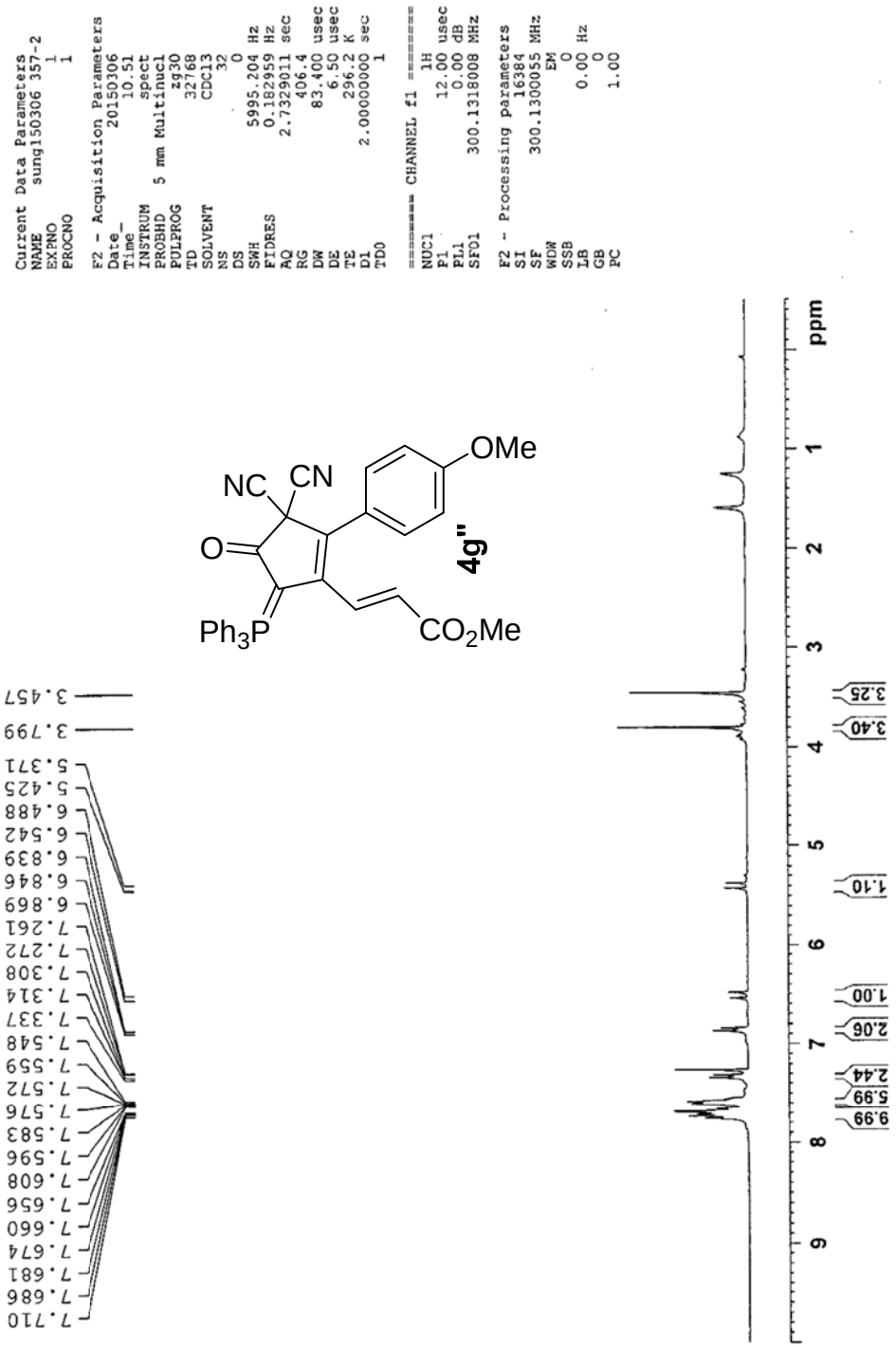


Fig. S28. ^{13}C NMR spectrum of compound **4g''** (100 MHz, $CDCl_3$)

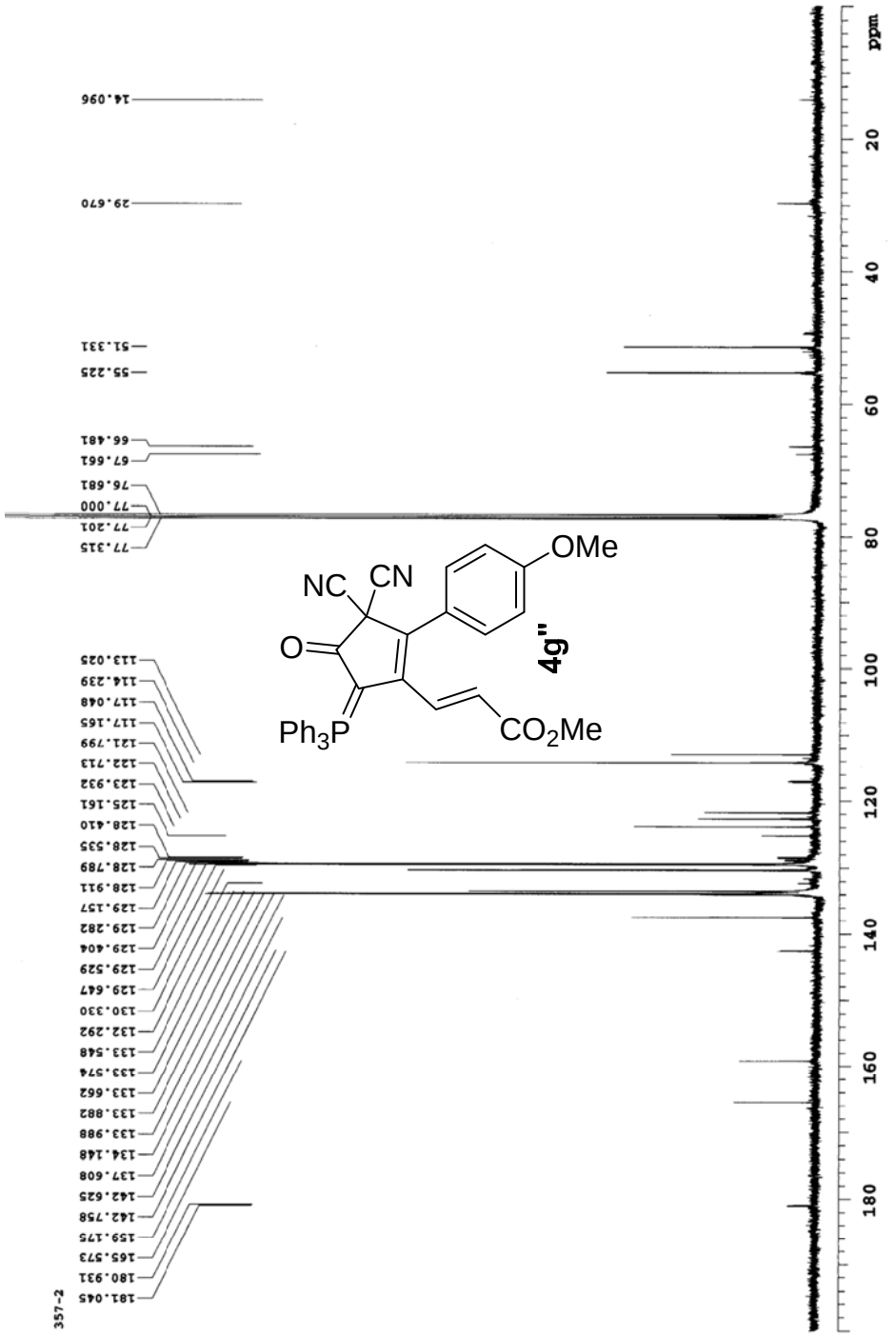
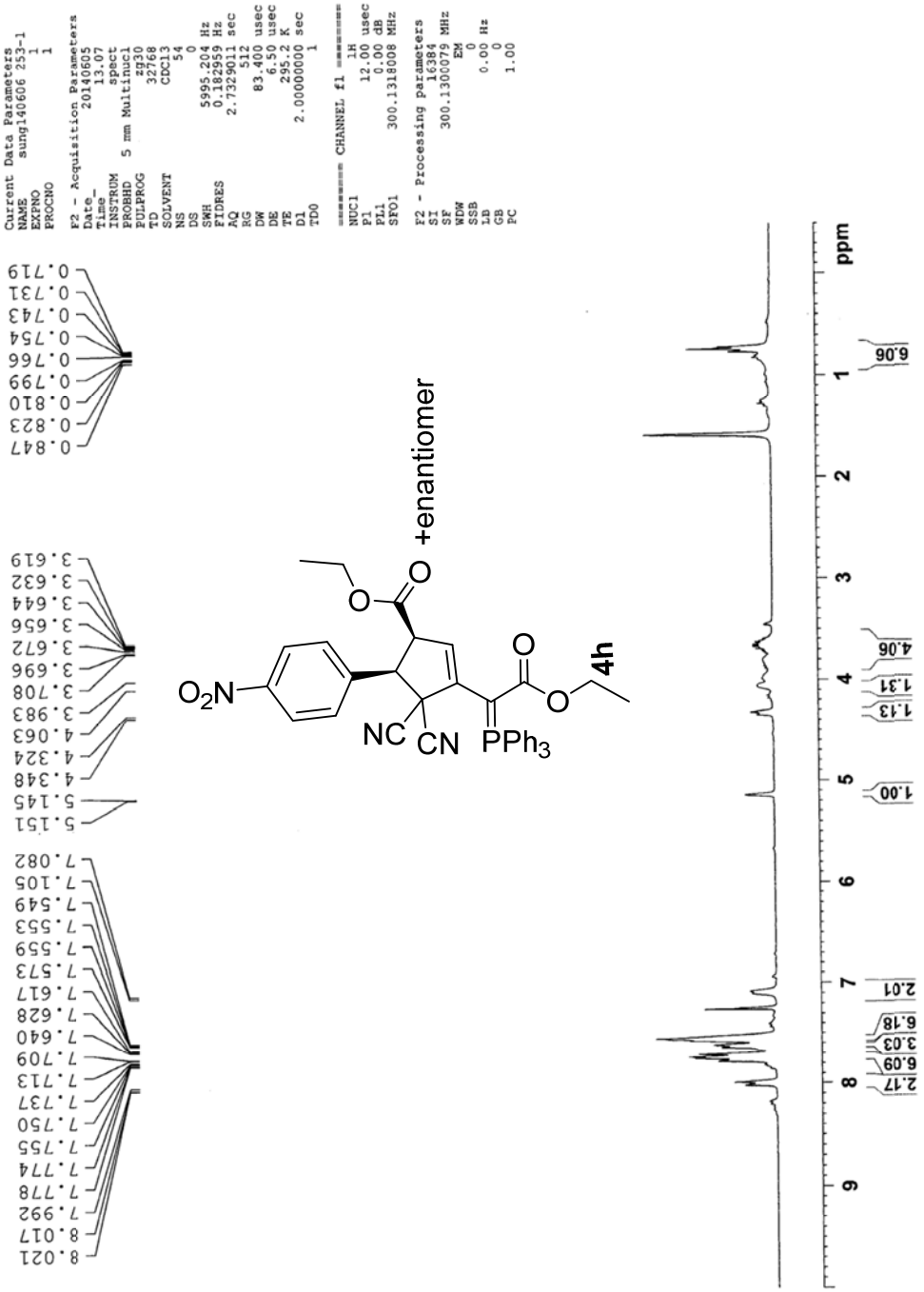


Fig. S29. ^{1}H NMR spectrum of compound **4h** (300 MHz, $CDCl_3$)



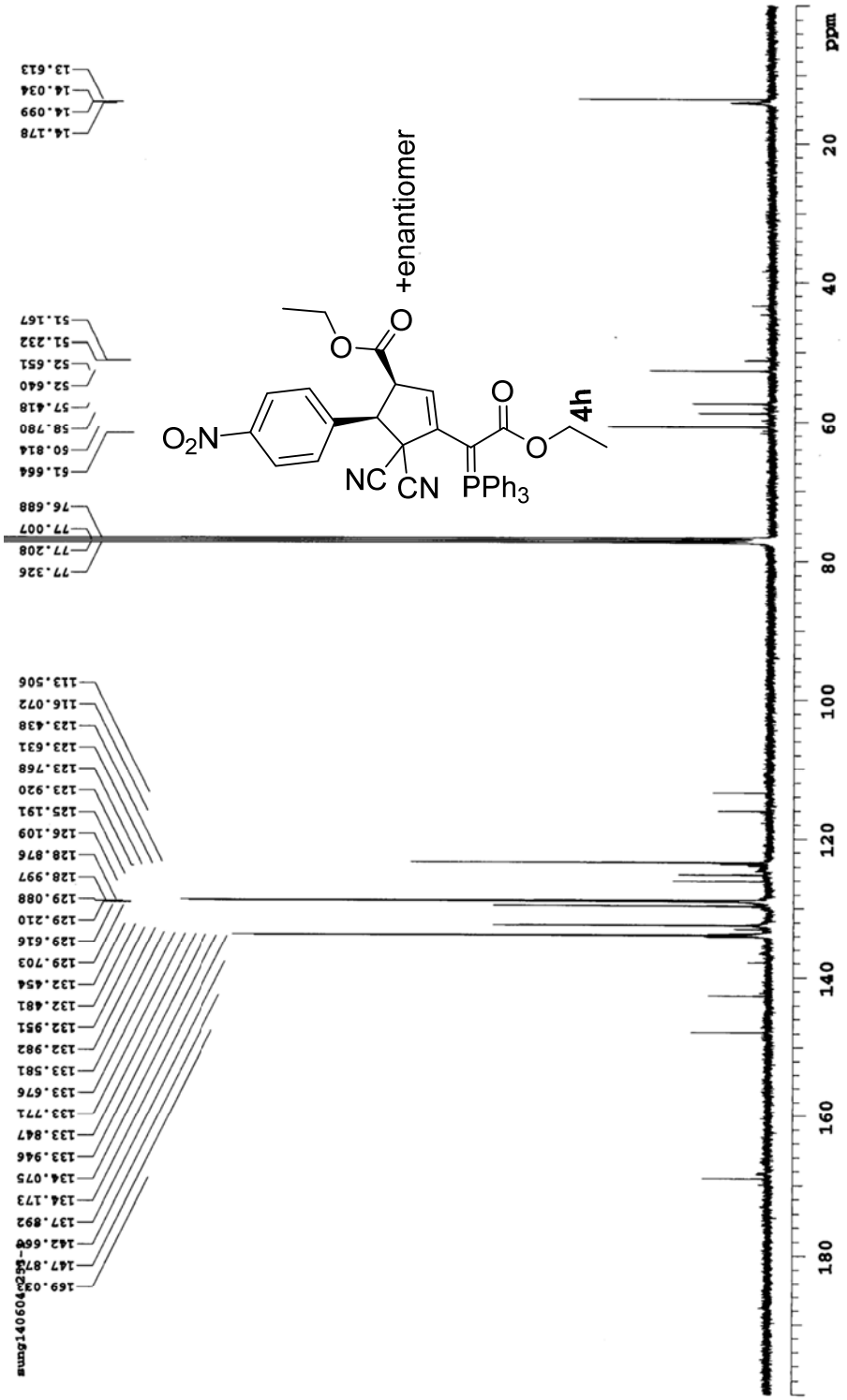


Fig. S30. ^{13}C NMR spectrum of compound **4h** (100 MHz, $CDCl_3$)

Fig. S31. ^{1}H NMR spectrum of compound **4h′** (300 MHz, $CDCl_3$)

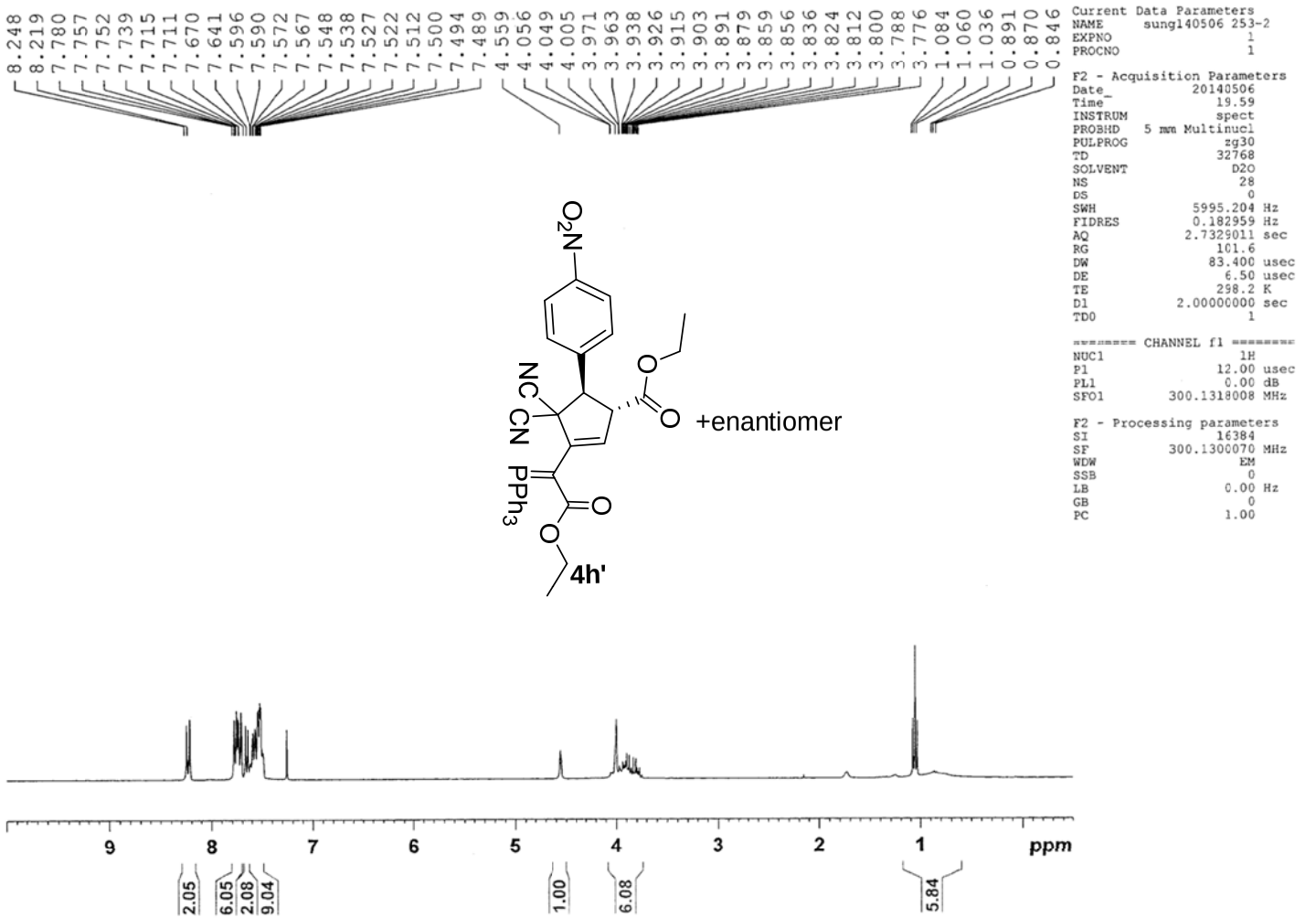


Fig. S32. ^{13}C NMR spectrum of compound **4h'** (100 MHz, $CDCl_3$)

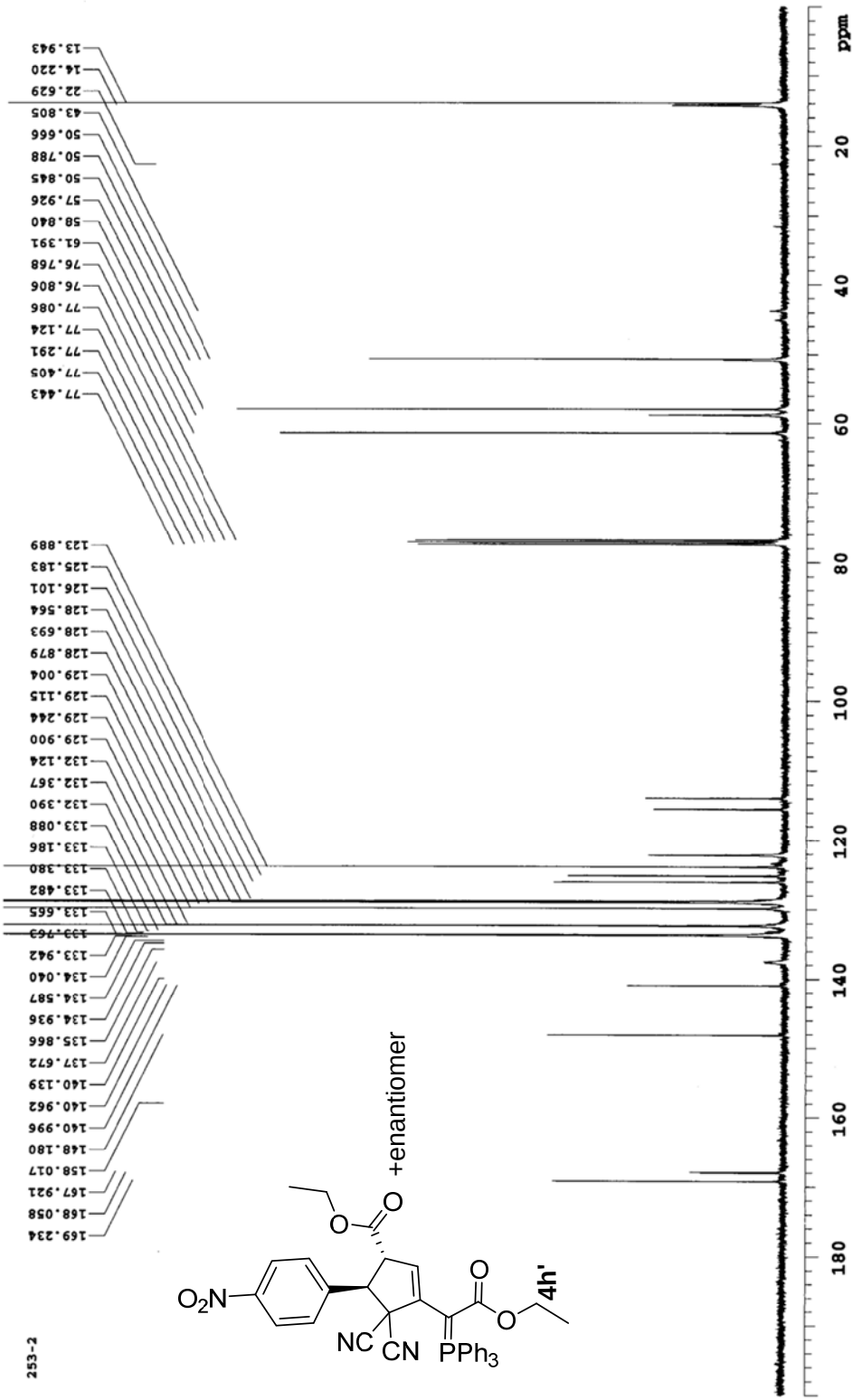


Fig. S33. ^{1}H NMR spectrum of compound **4i** and **4i'** (300 MHz, $CDCl_3$)

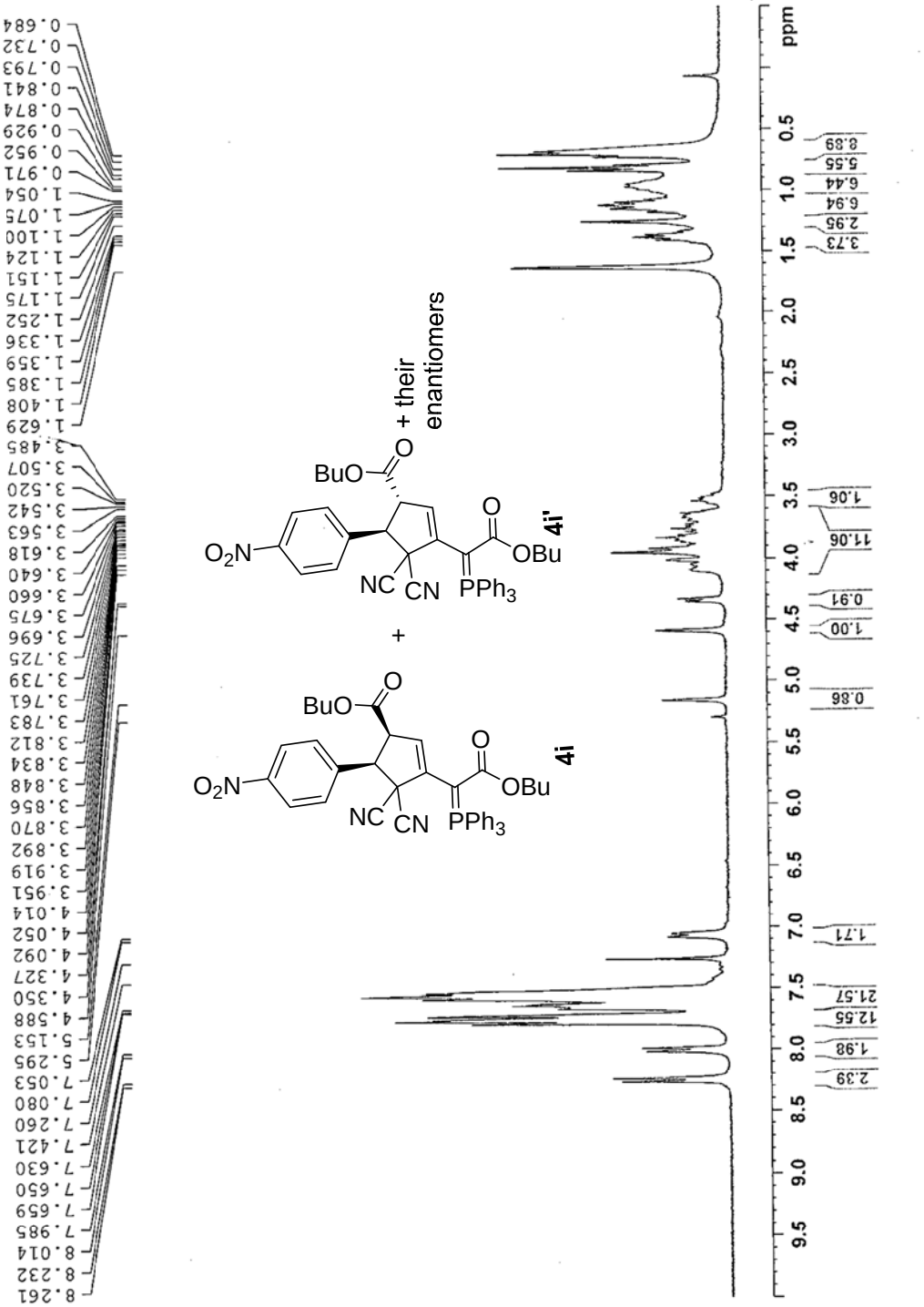


Fig. S34. ^{13}C NMR spectrum of compound **4i** and **4i'** (100 MHz, $CDCl_3$)

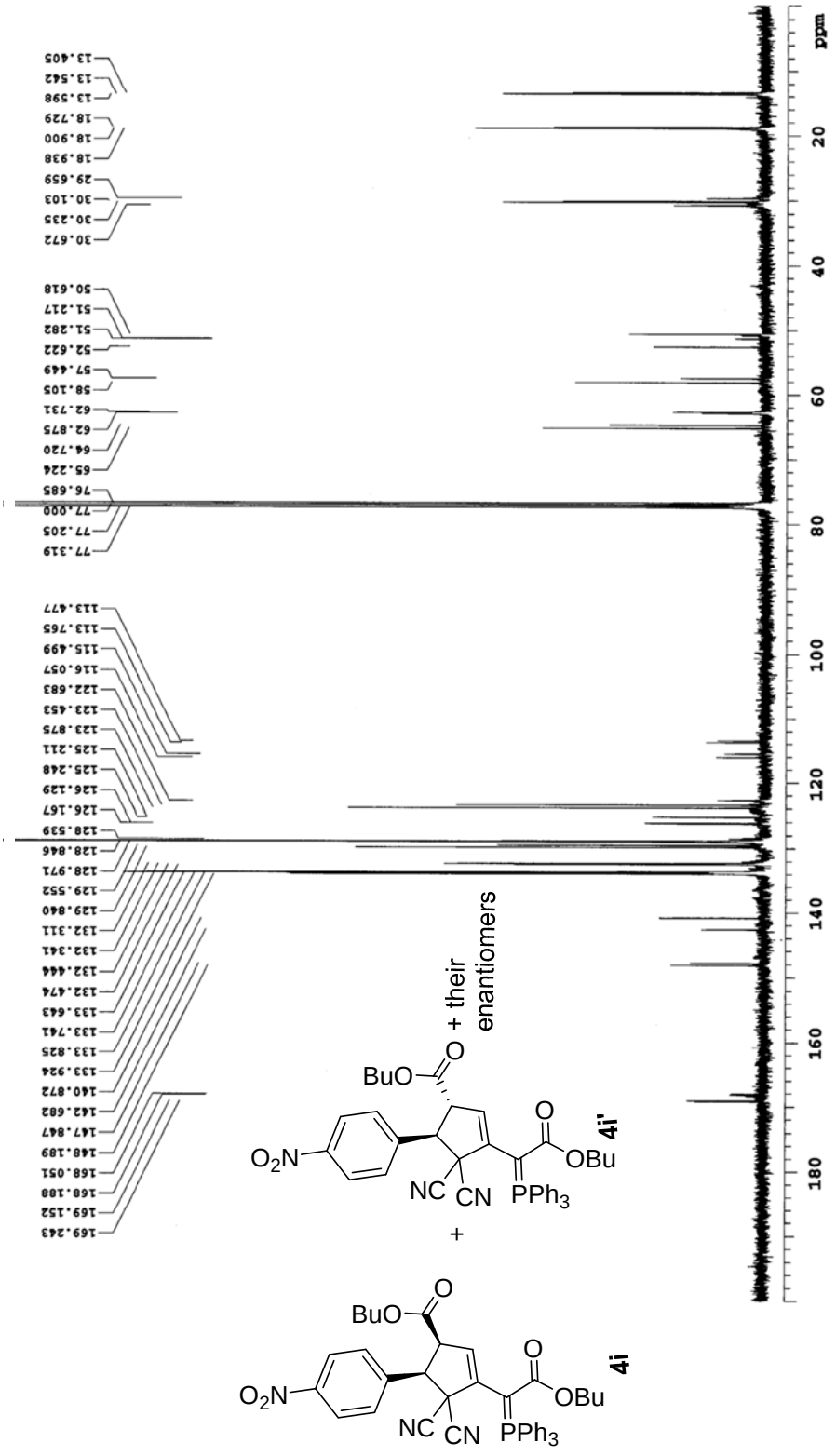
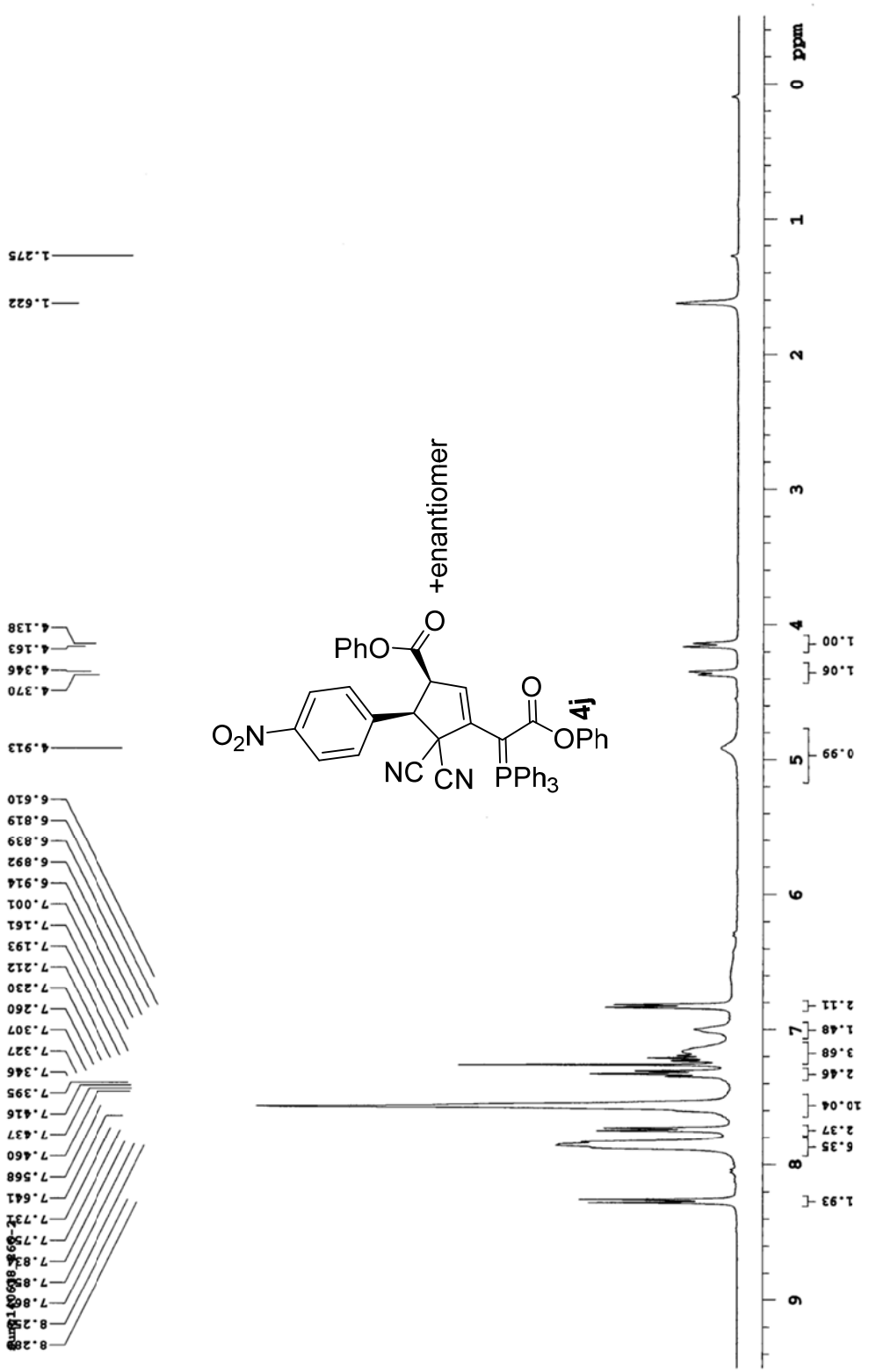


Fig. S35. ^{1}H NMR spectrum of compound **4j** (400 MHz, $CDCl_3$)



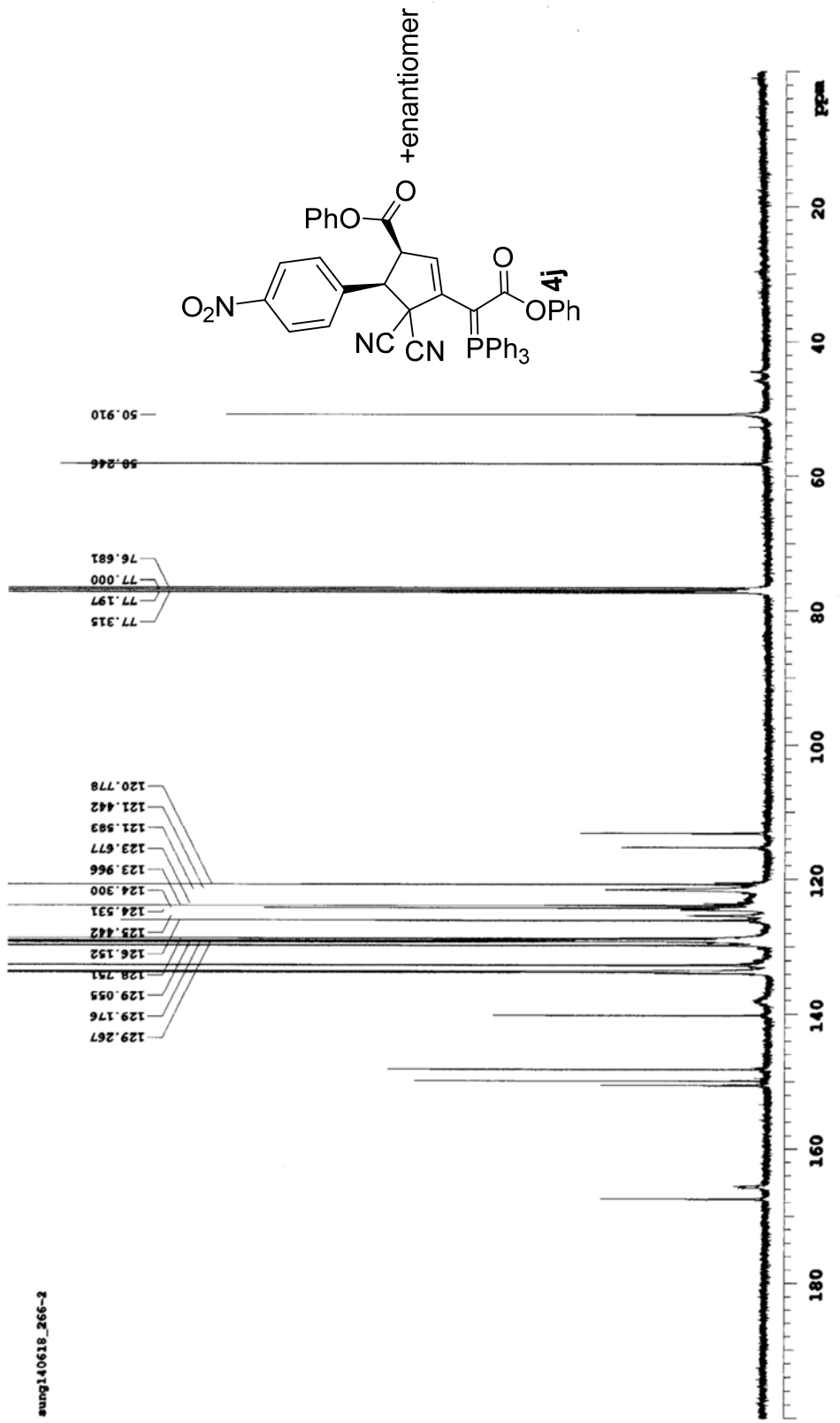


Fig. S36. ^{13}C NMR spectrum of compound **4j** (100 MHz, $CDCl_3$)

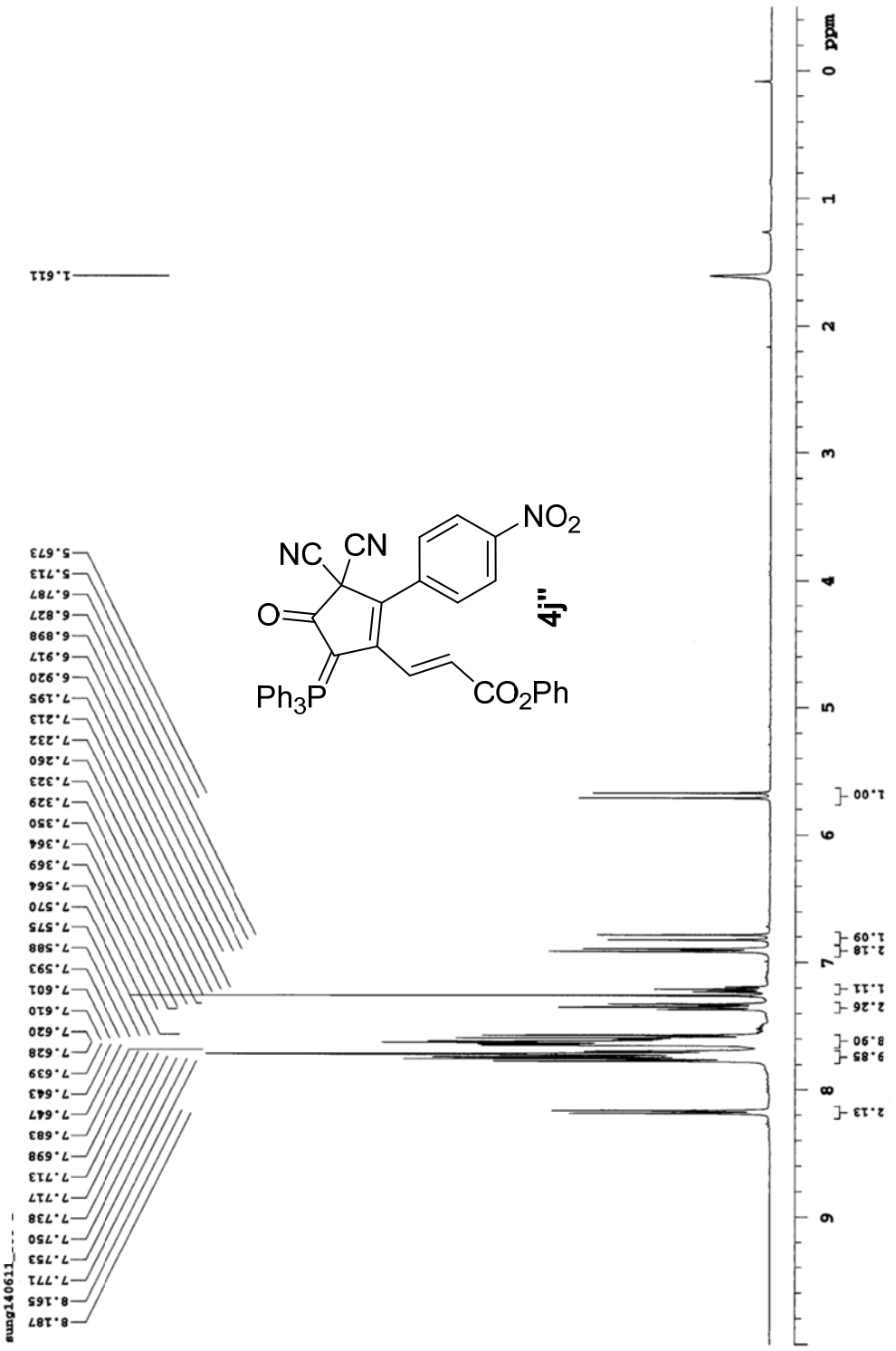


Fig. S37. ^{1}H NMR spectrum of compound **4j''** (400 MHz, $CDCl_3$)

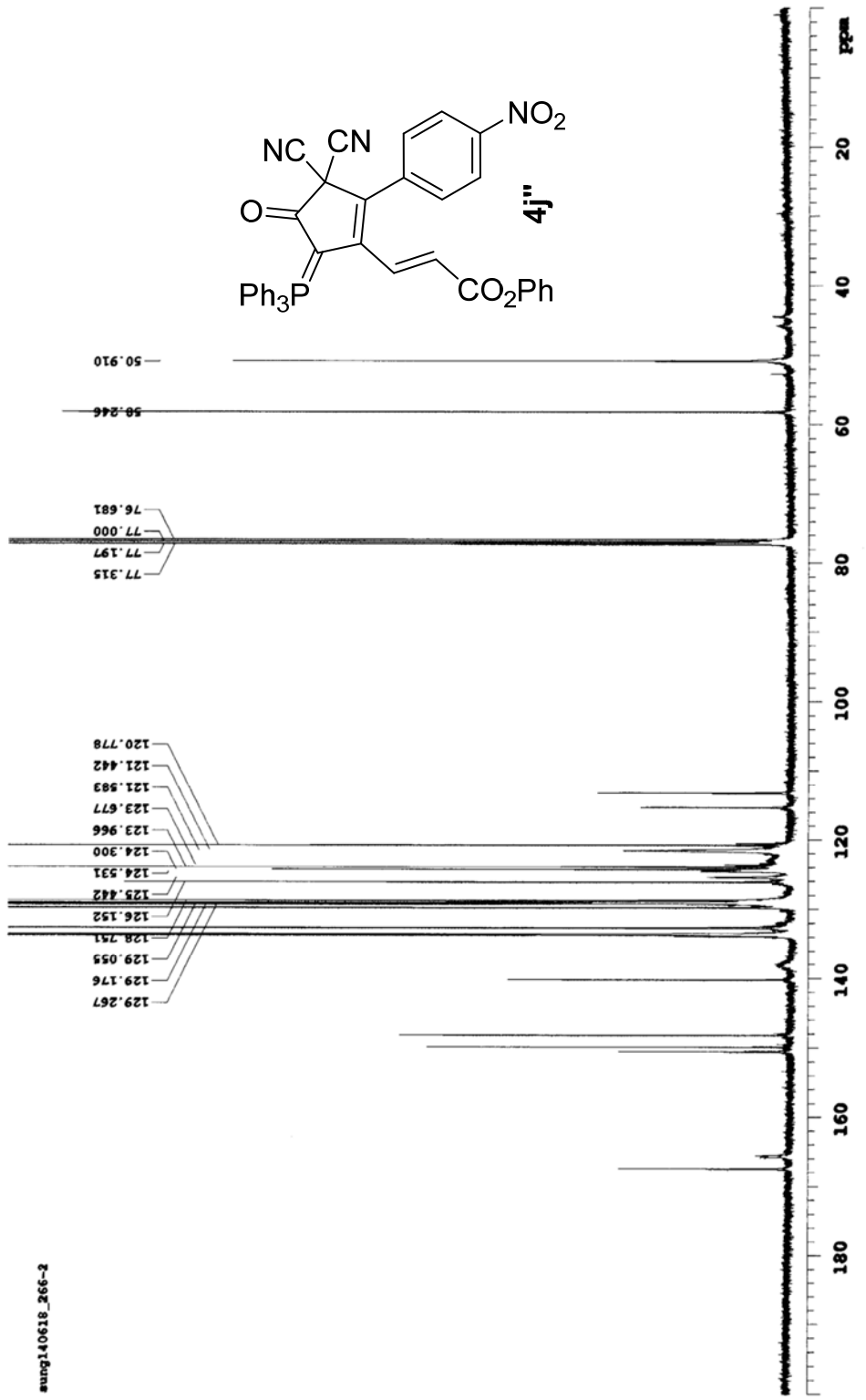


Fig. S38. ^{13}C NMR spectrum of compound **4j''** (100 MHz, $CDCl_3$)

Fig. S39. ^{1}H NMR spectrum of compound **4k** and **4k′** (300 MHz, $CDCl_3$)

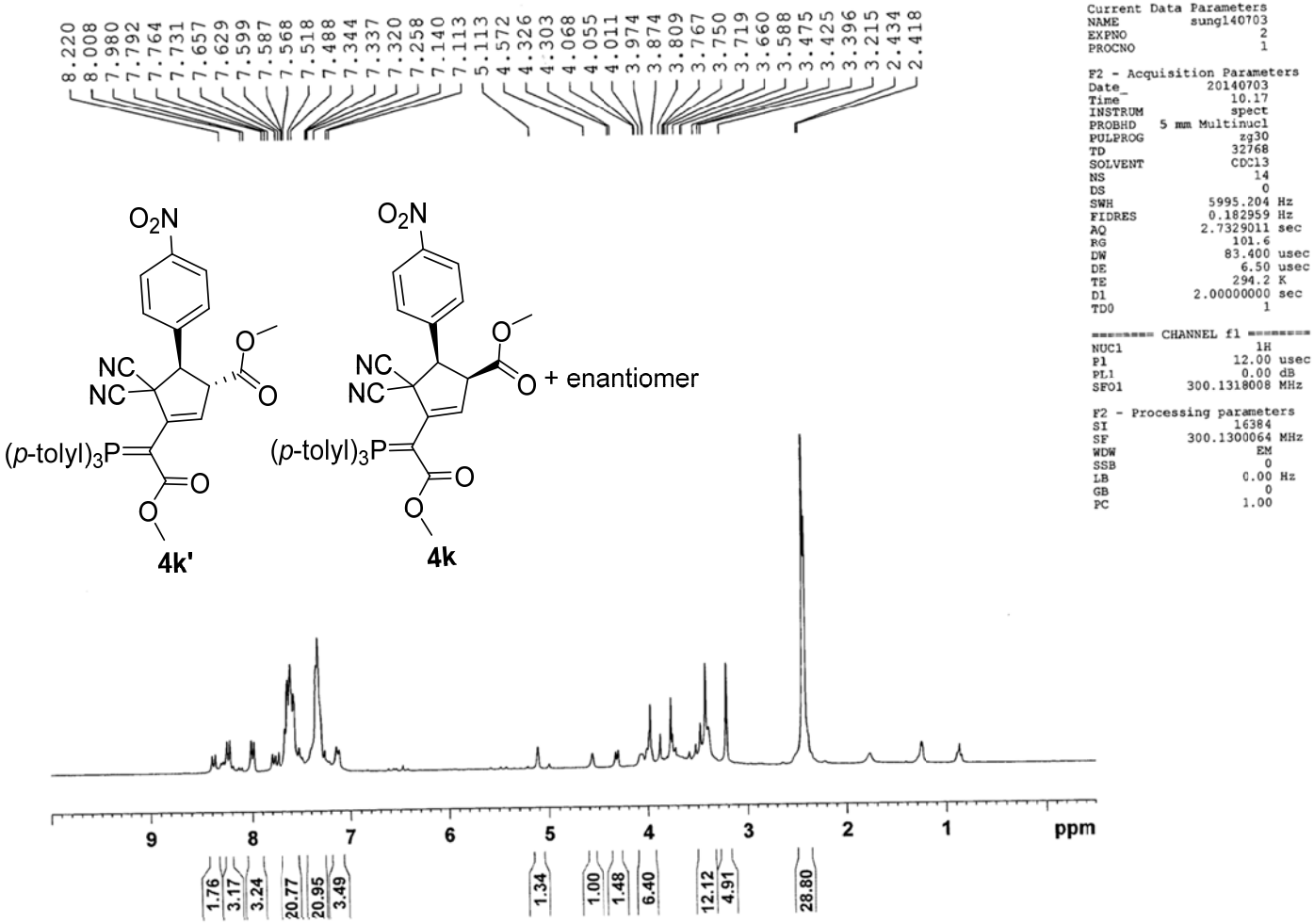


Fig. S40. ^{1}H NMR spectrum of compound **4k'** (300 MHz, $CDCl_3$)

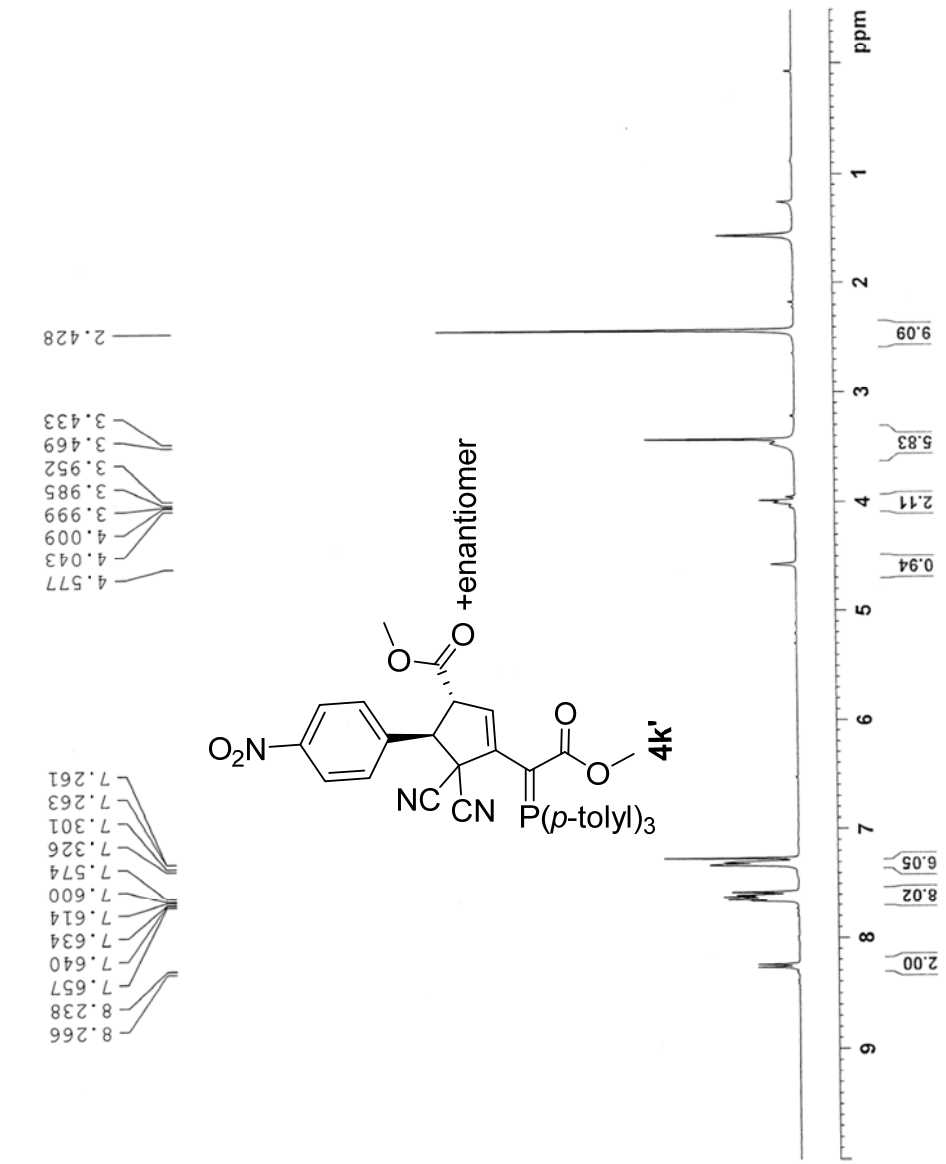


Fig. S41. ^{13}C NMR spectrum of compound **4k'** (100 MHz, $CDCl_3$)

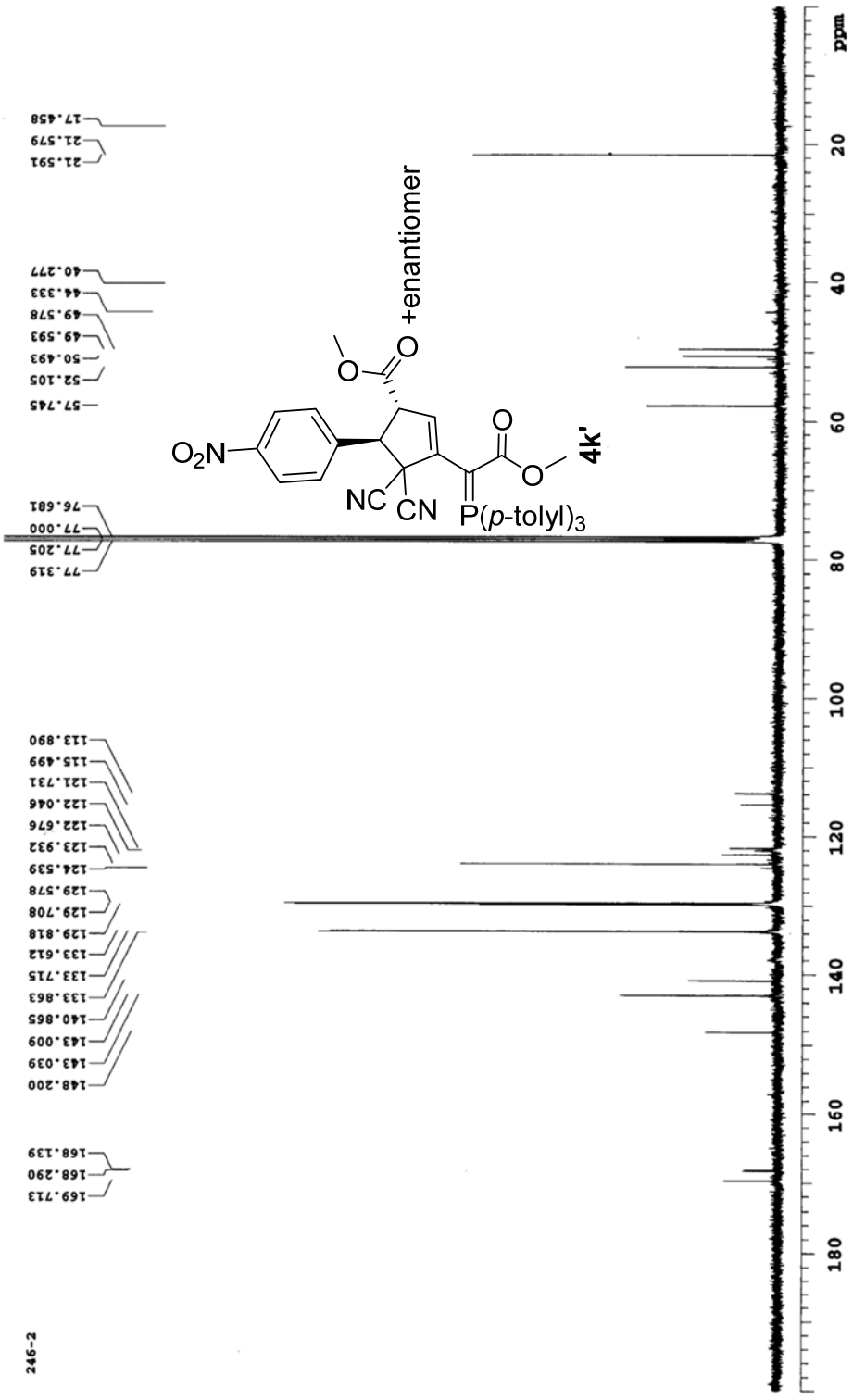


Fig. S42. ^{1}H NMR spectrum of compound **4l** (300 MHz, $CDCl_3$)

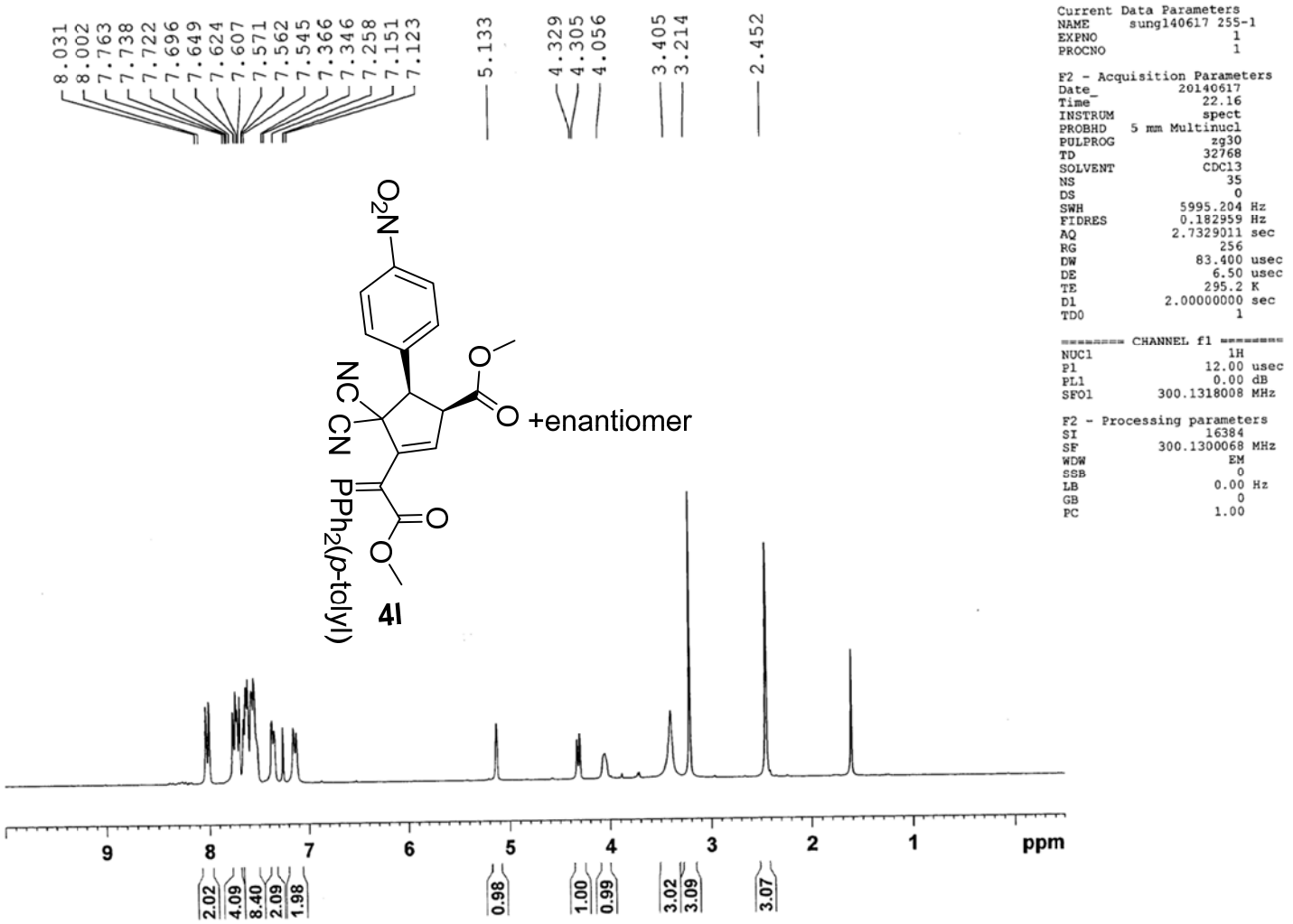



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Fig. S43. ^{13}C NMR spectrum of compound **4l** (100 MHz, $CDCl_3$)

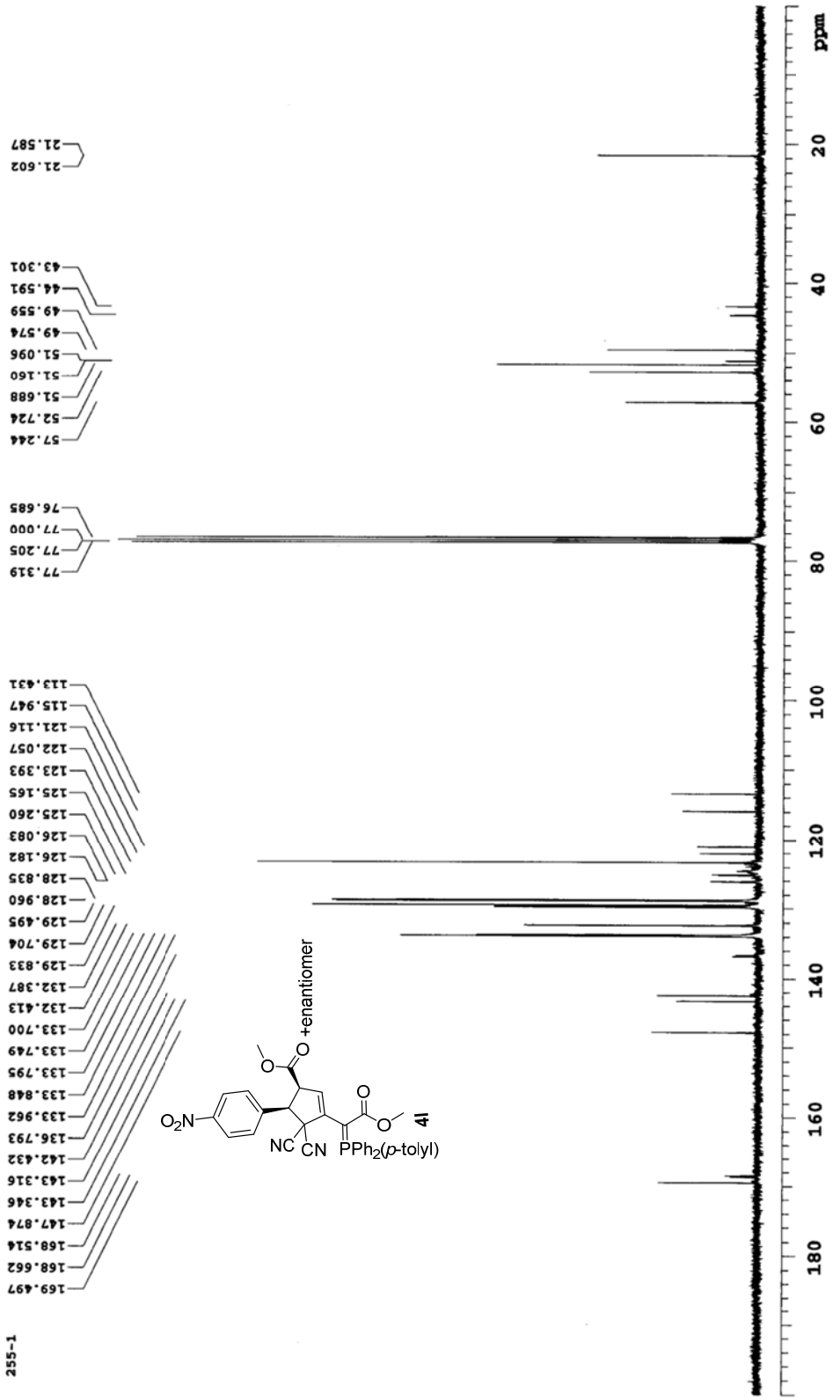


Fig. S44. ^{1}H NMR spectrum of compound **4l'** (300 MHz, $CDCl_3$)

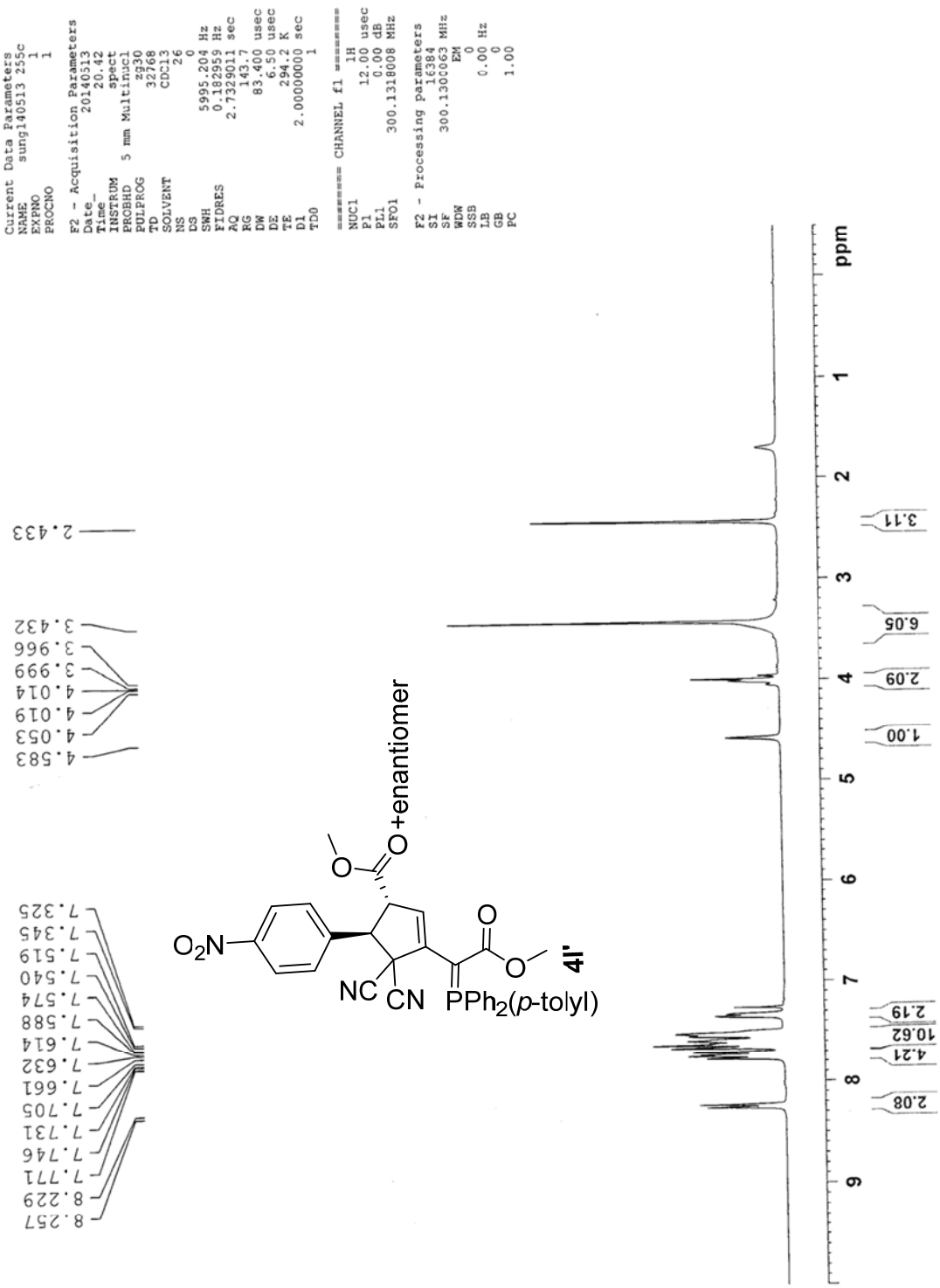


Fig. S45. ^{13}C NMR spectrum of compound **4l'** (100 MHz, $CDCl_3$)

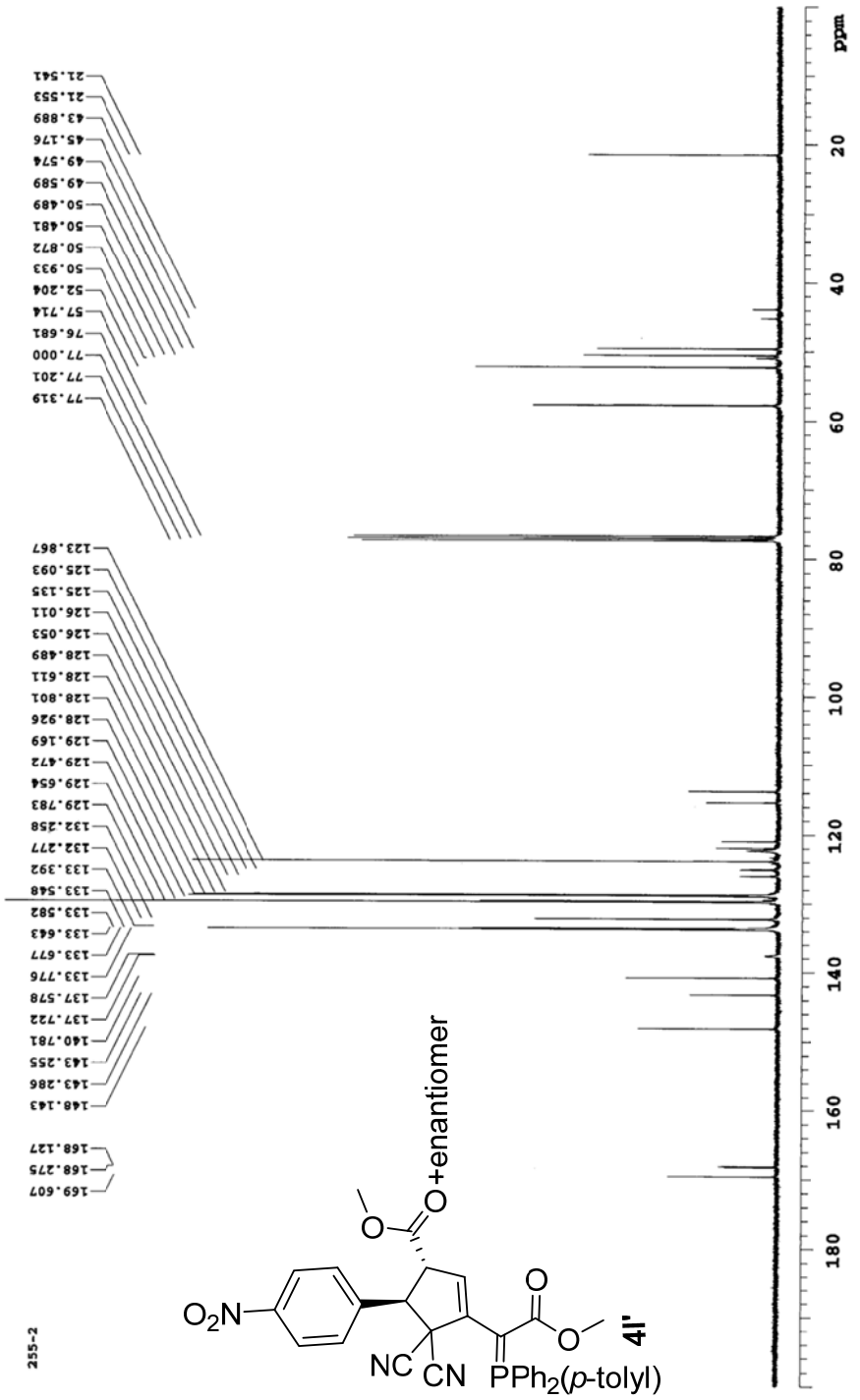


Fig. S46. ^{1}H NMR spectrum of compound **4m** (300 MHz, $CDCl_3$)

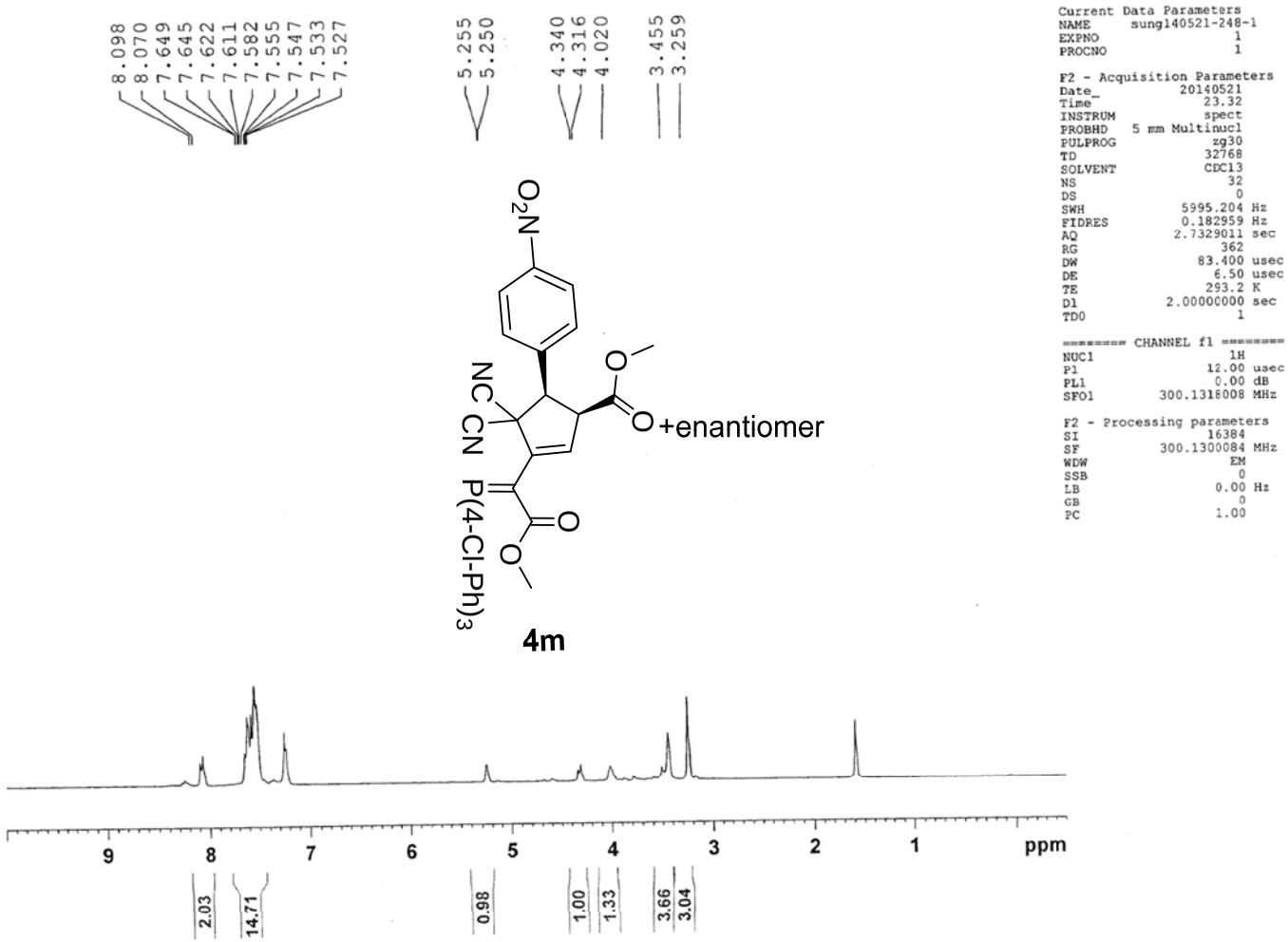


Fig. S47. ^{13}C NMR spectrum of compound **4m** (100 MHz, $CDCl_3$)

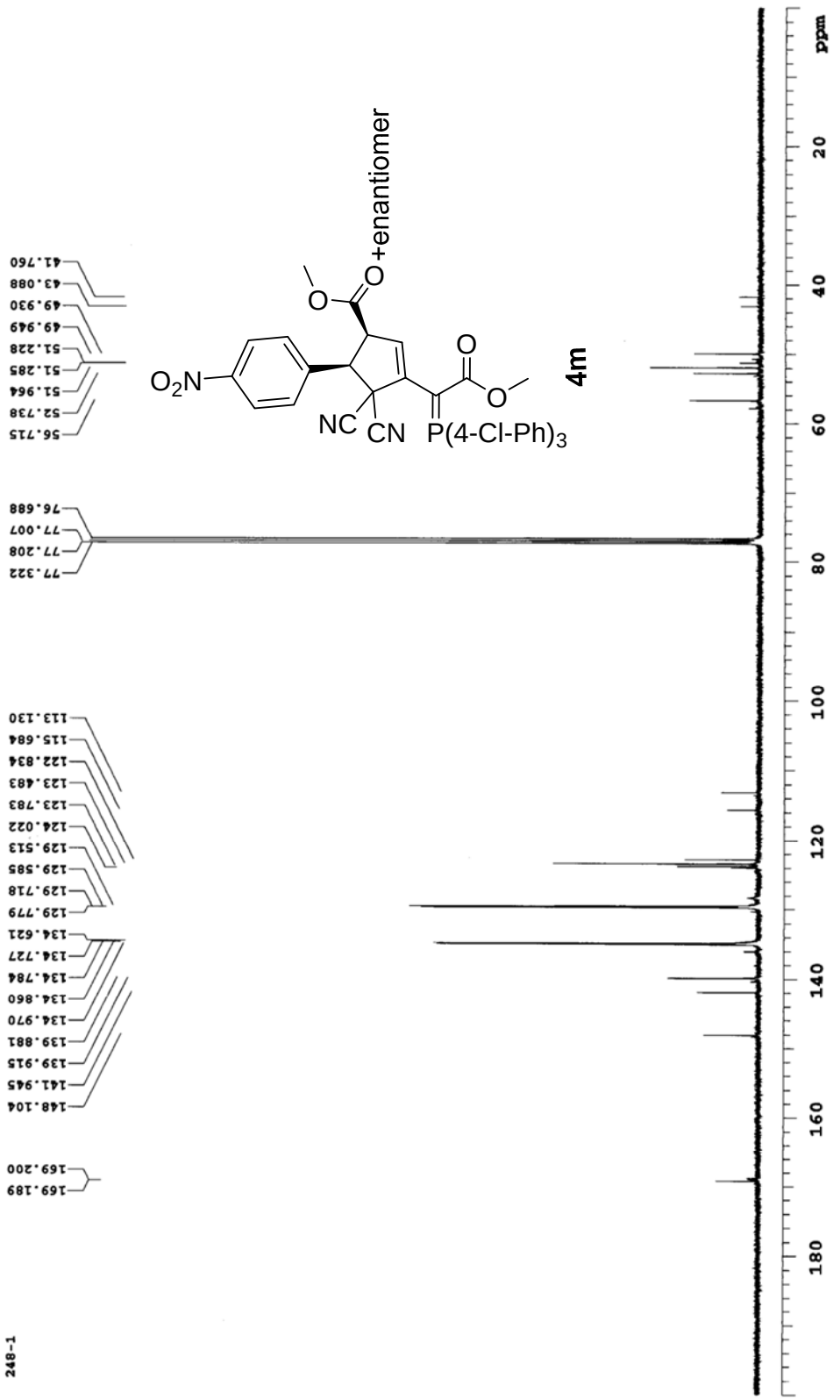
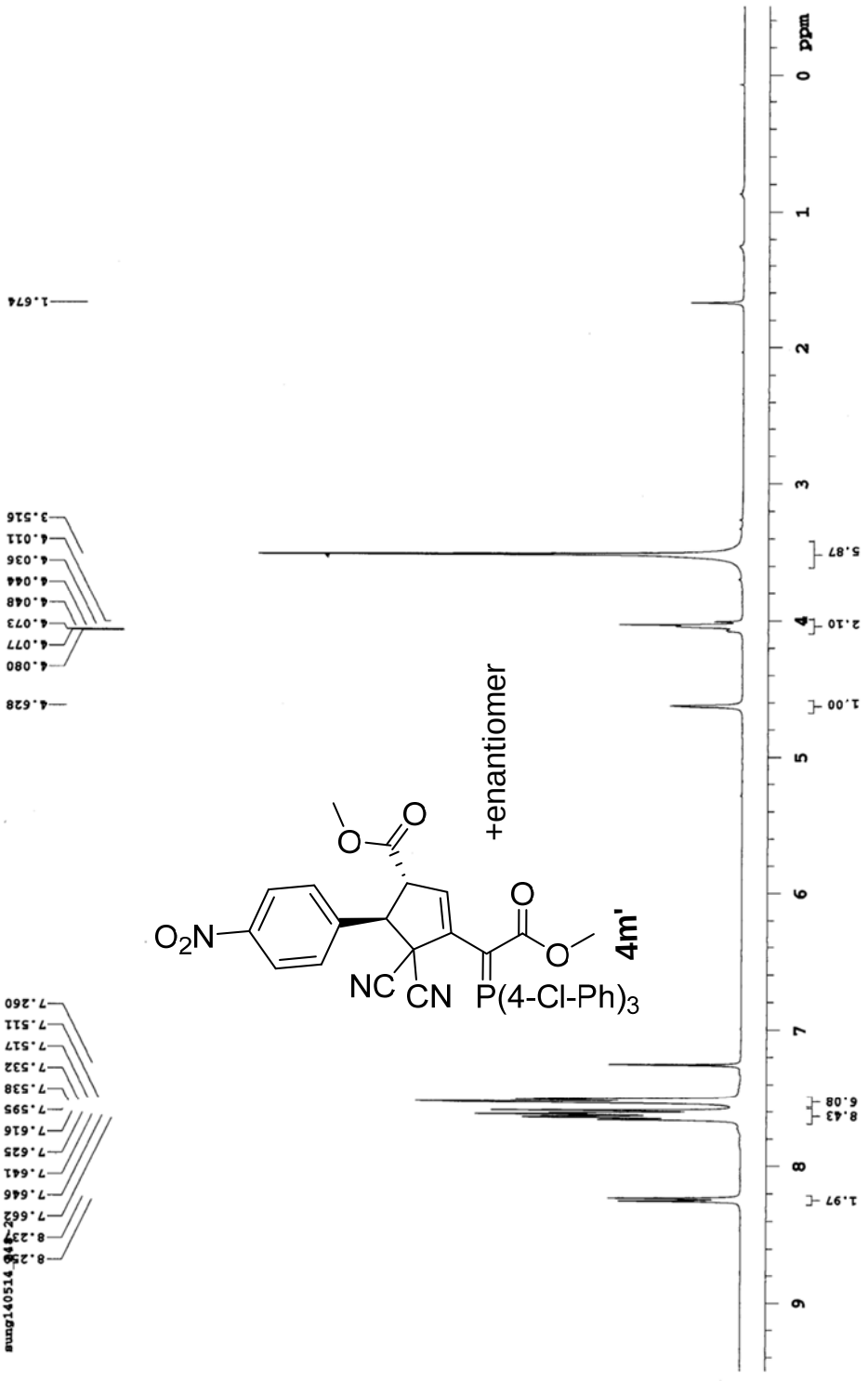


Fig. S48. ^{1}H NMR spectrum of compound **4m'** (400 MHz, $CDCl_3$)



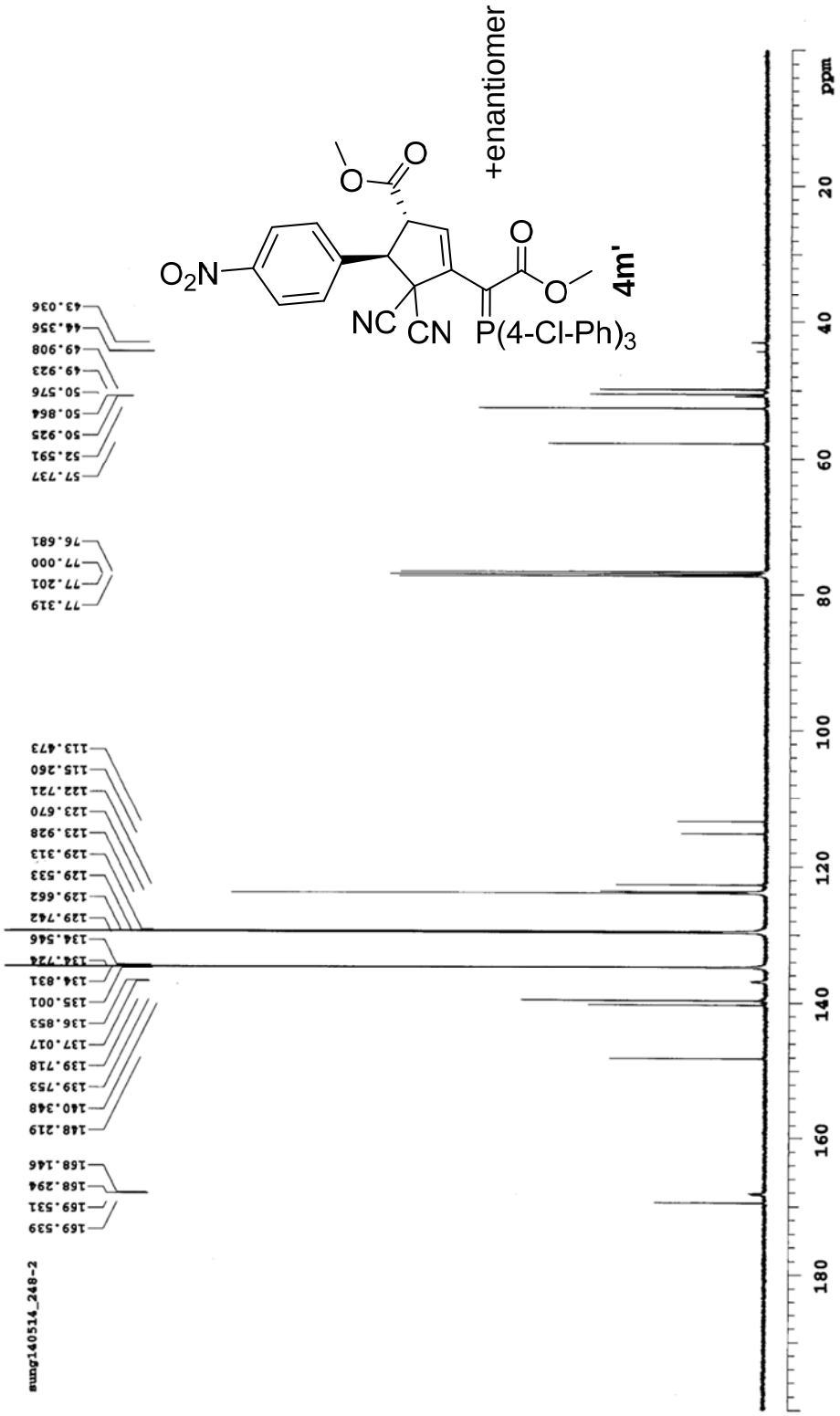
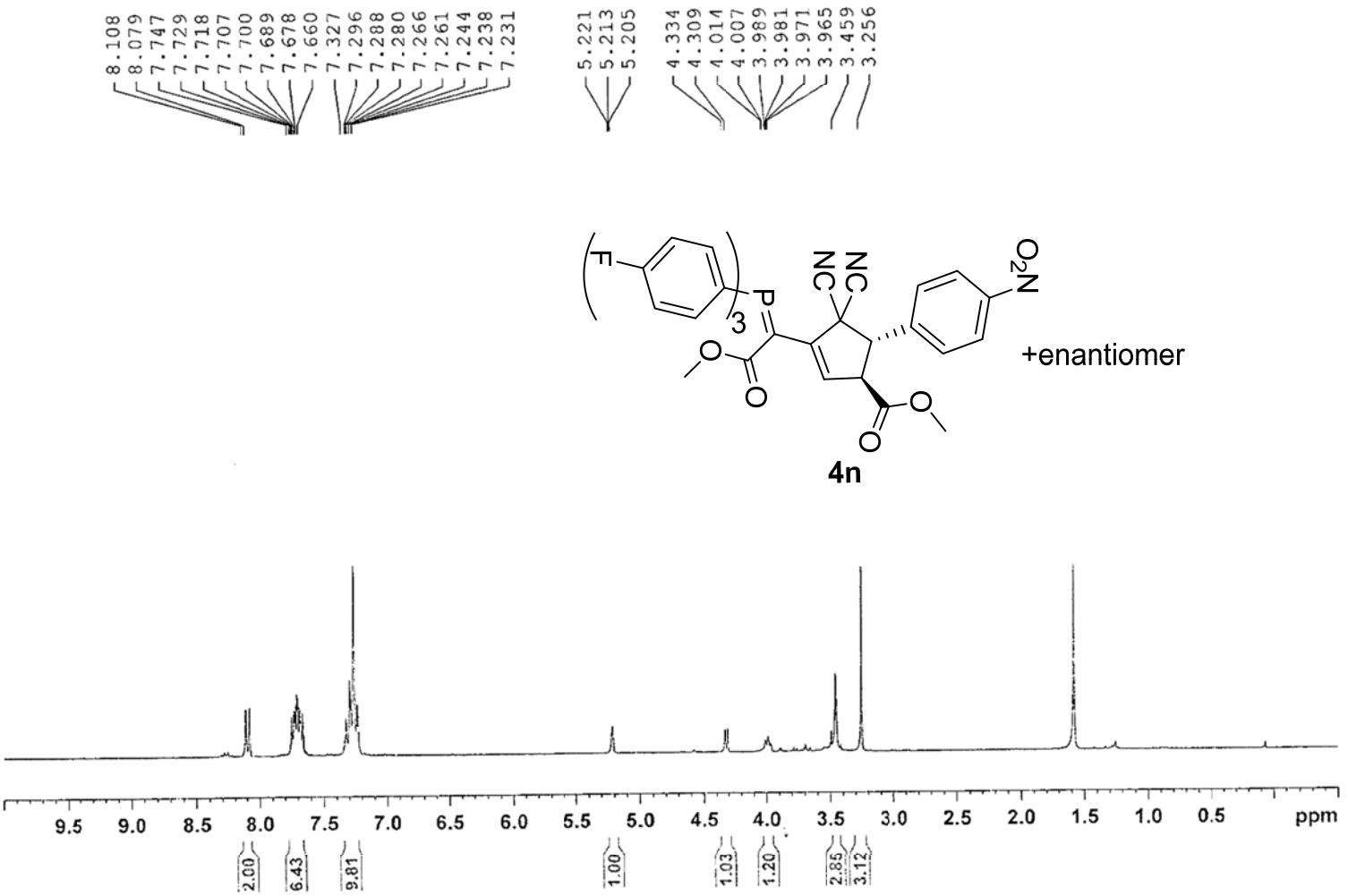


Fig. S49. ^{13}C NMR spectrum of compound **4m'** (100 MHz, $CDCl_3$)

Fig. S50. ^{1}H NMR spectrum of compound **4n** (300 MHz, $CDCl_3$)



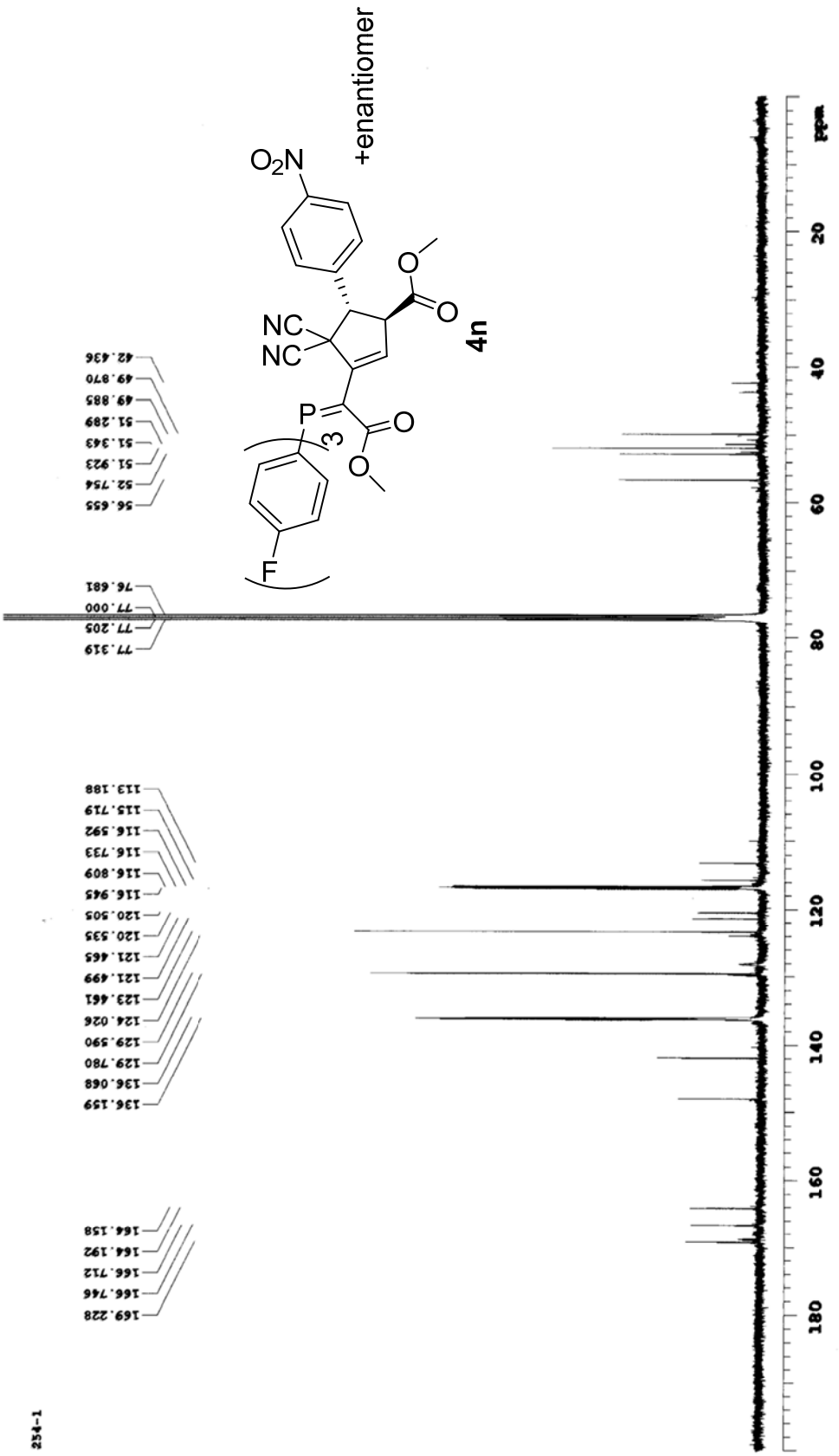


Fig. S51. ^{13}C NMR spectrum of compound **4n** (100 MHz, $CDCl_3$)

Fig. S52. ^{1}H NMR spectrum of compound **4n'** (400 MHz, $CDCl_3$)

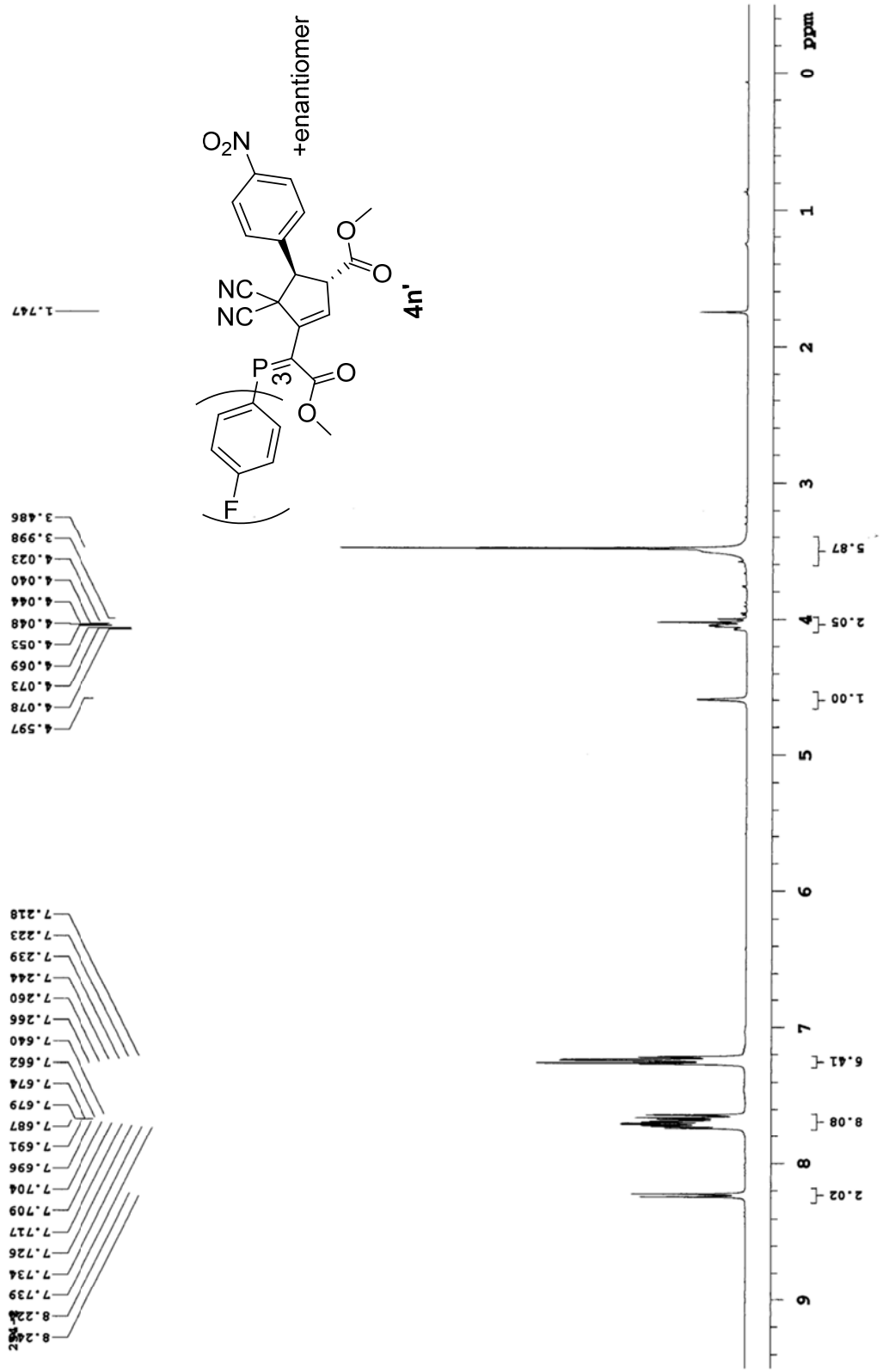


Fig. S53. ^{13}C NMR spectrum of compound **4n'** (100 MHz, $CDCl_3$)

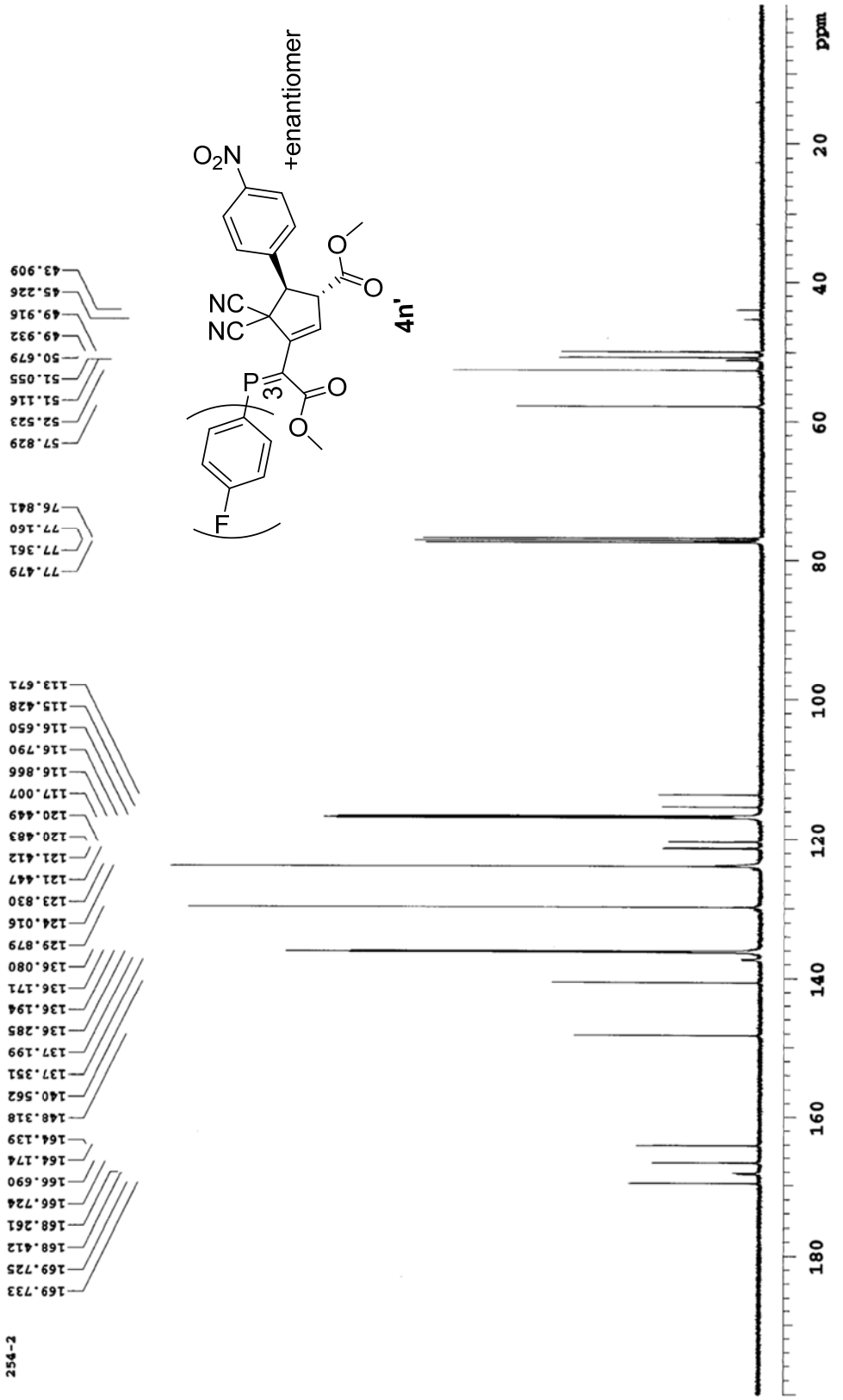


Fig. S54. ^{1}H NMR spectrum of compound **4o** (400 MHz, $CDCl_3$)

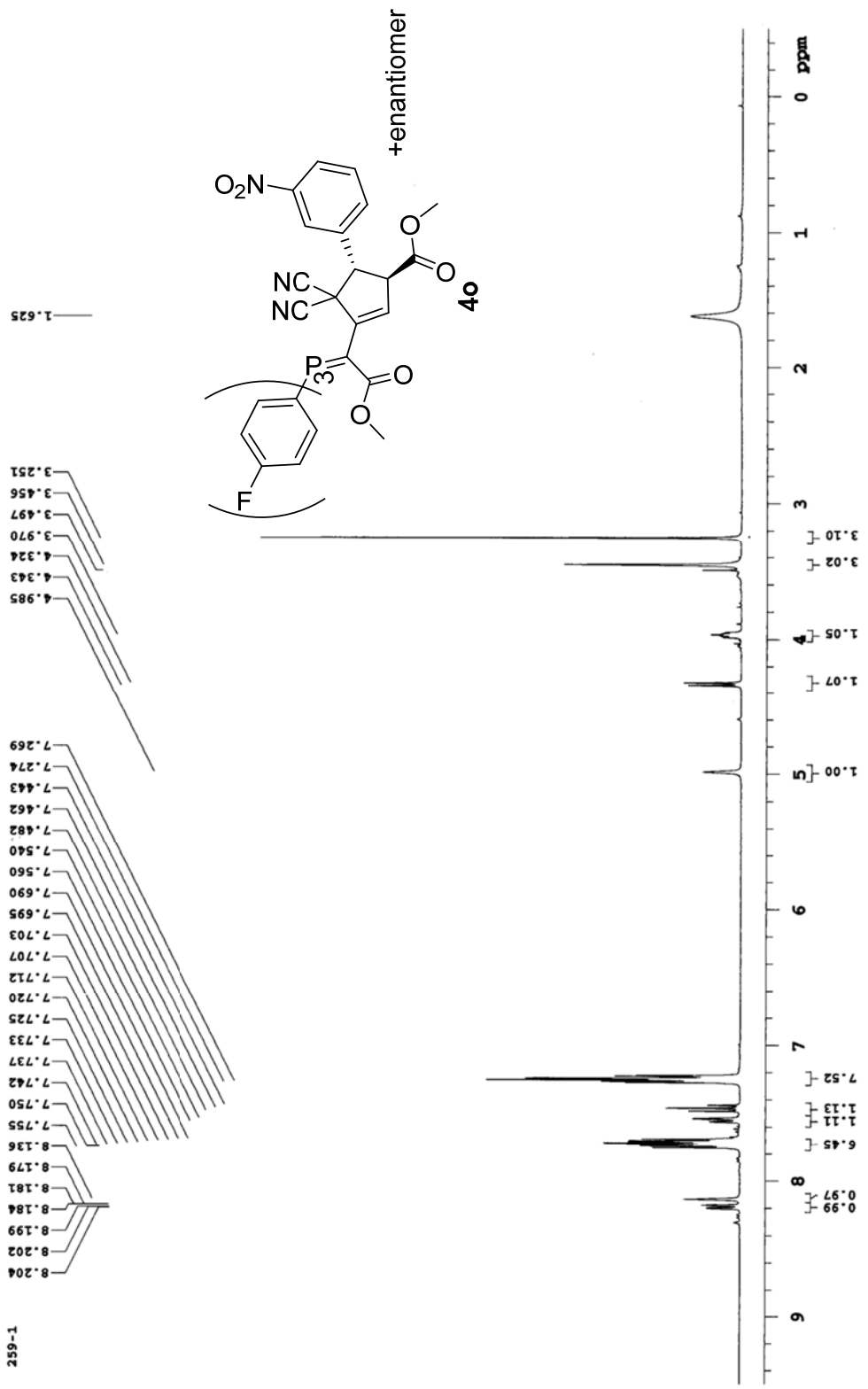


Fig. S55. ^{13}C NMR spectrum of compound **4o** (100 MHz, $CDCl_3$)

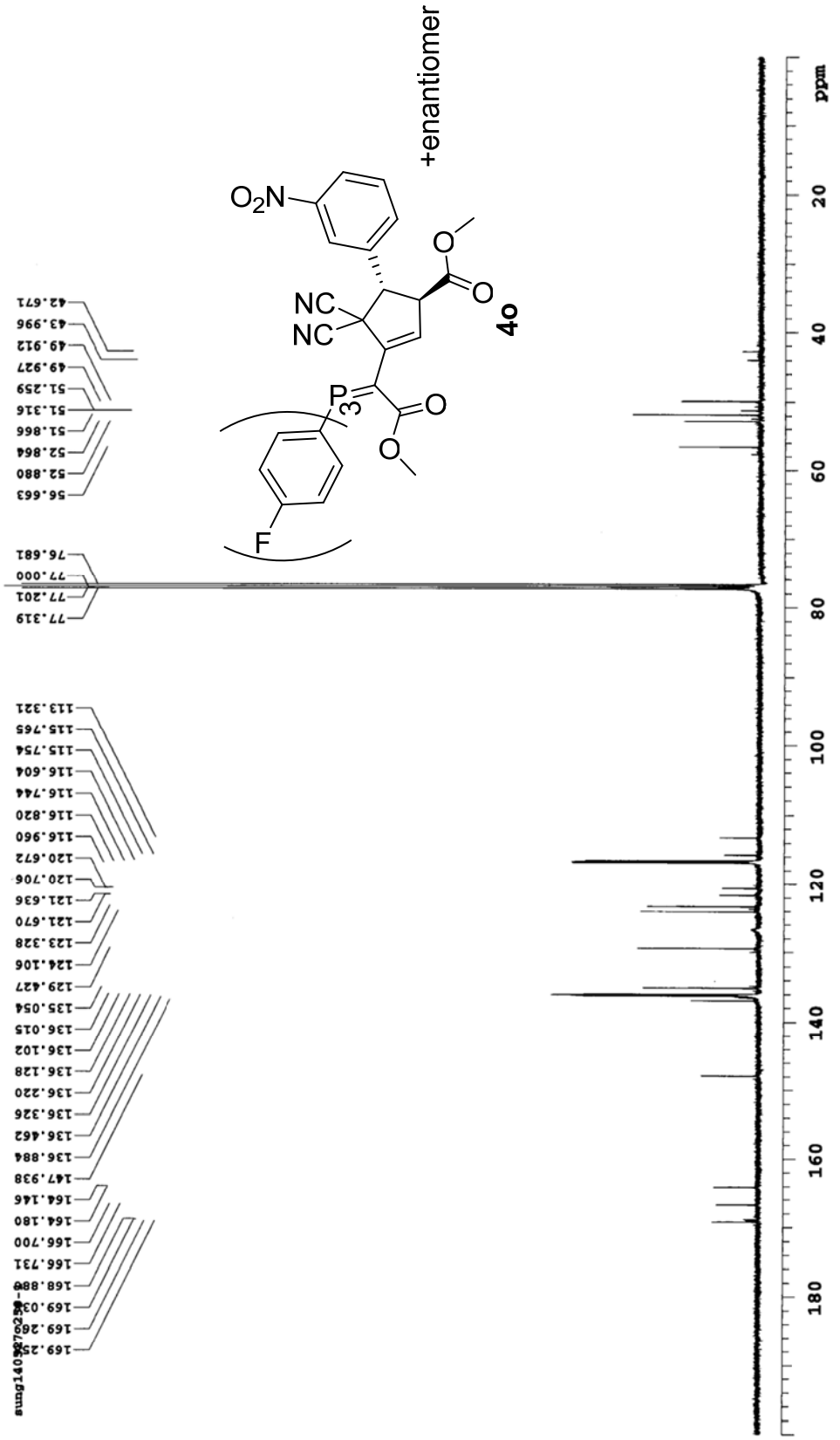
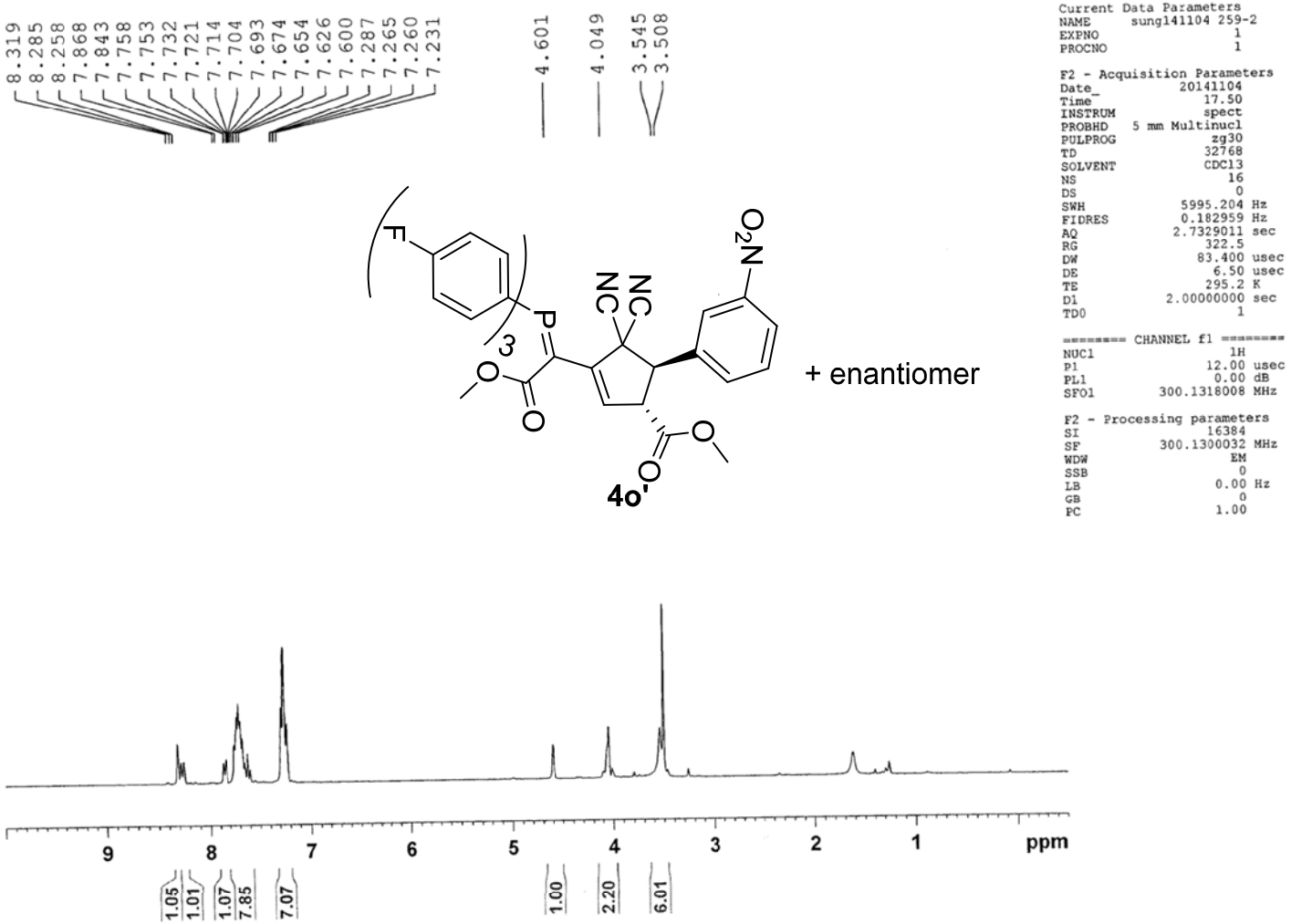


Fig. S56. ^{1}H NMR spectrum of compound **4o′** (300 MHz, $CDCl_3$)



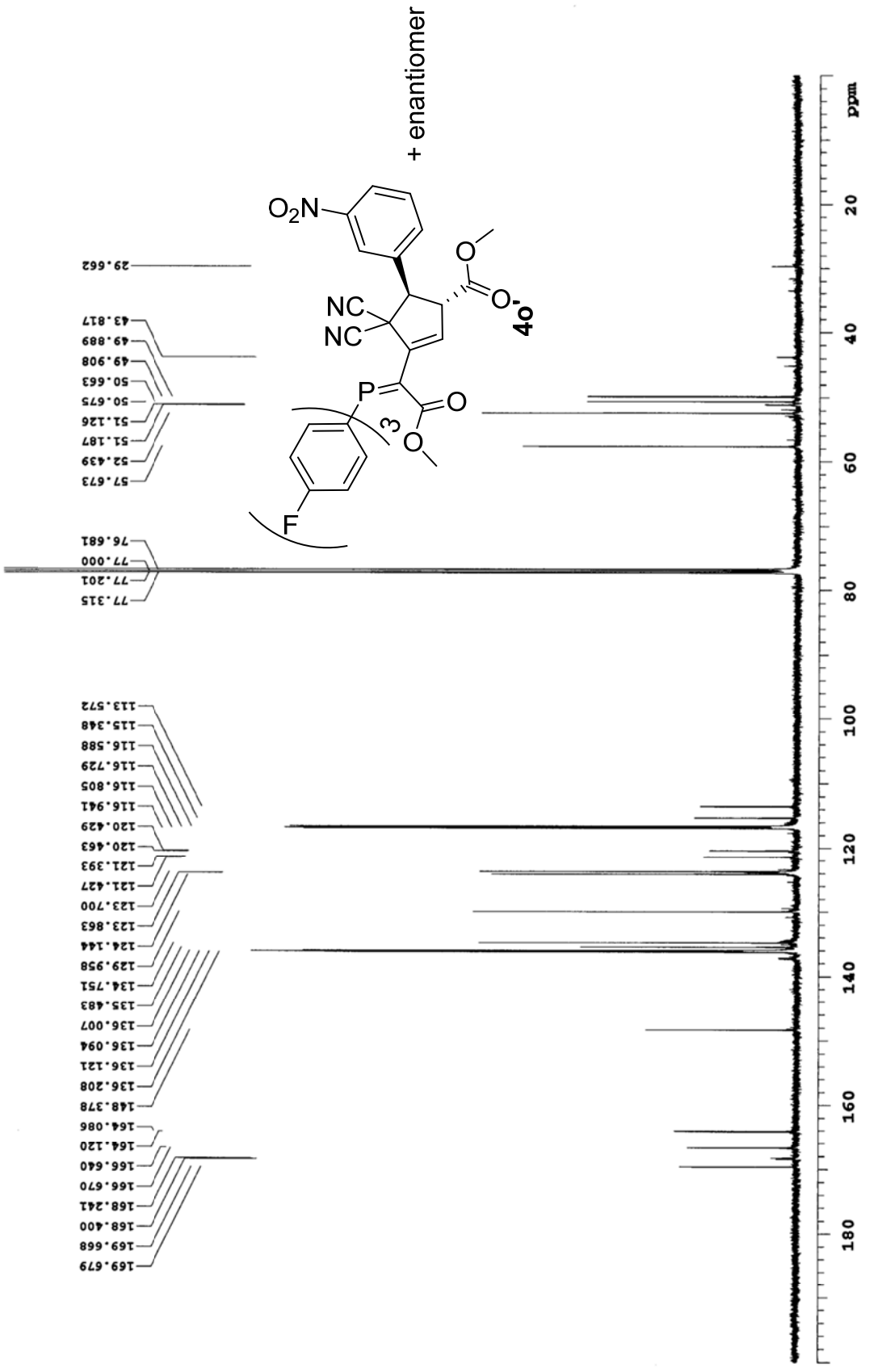
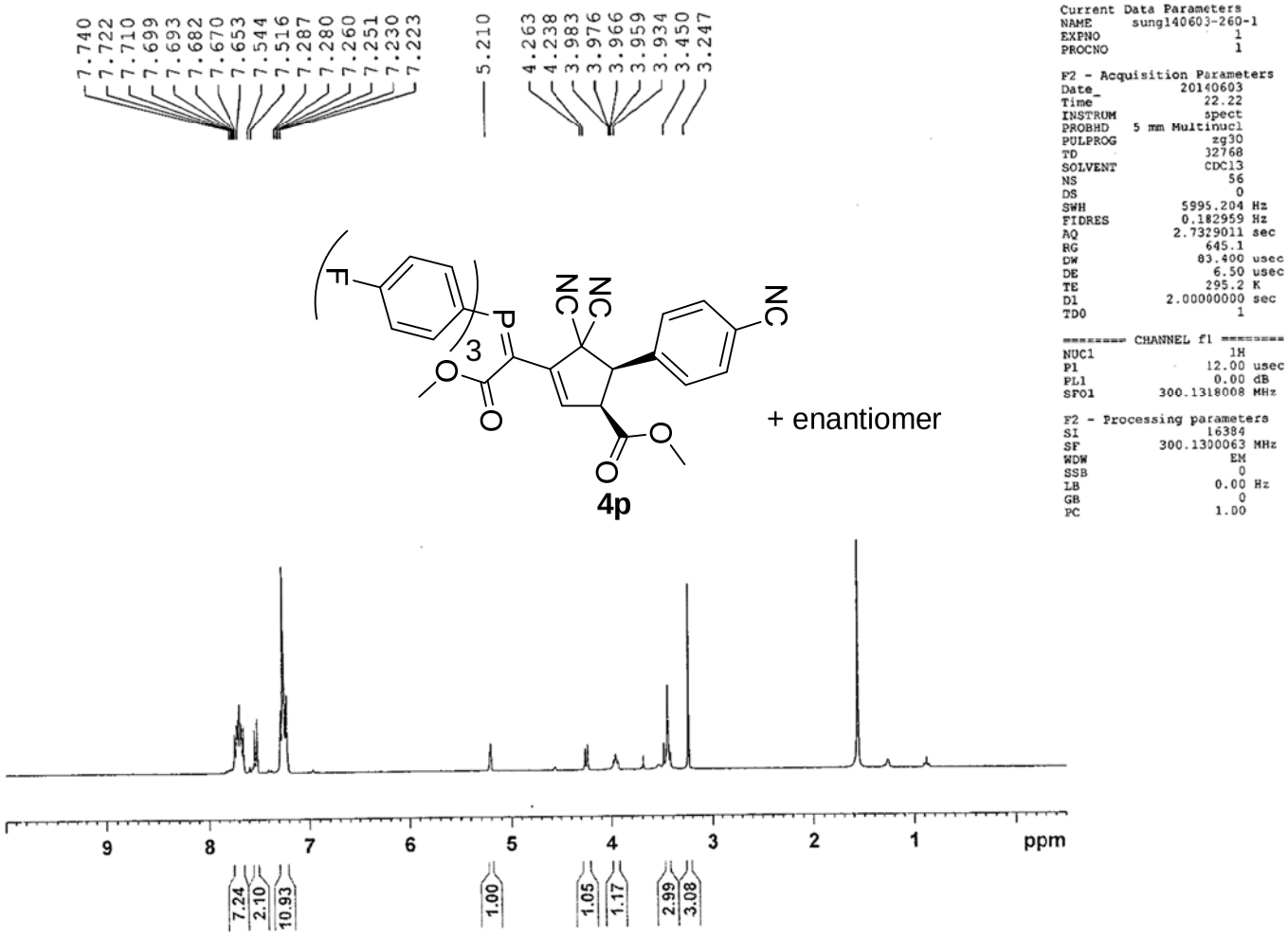


Fig. S57. ^{13}C NMR spectrum of compound **4o'** (100 MHz, $CDCl_3$)

Fig. S58. ^{1}H NMR spectrum of compound **4p** (300 MHz, $CDCl_3$)



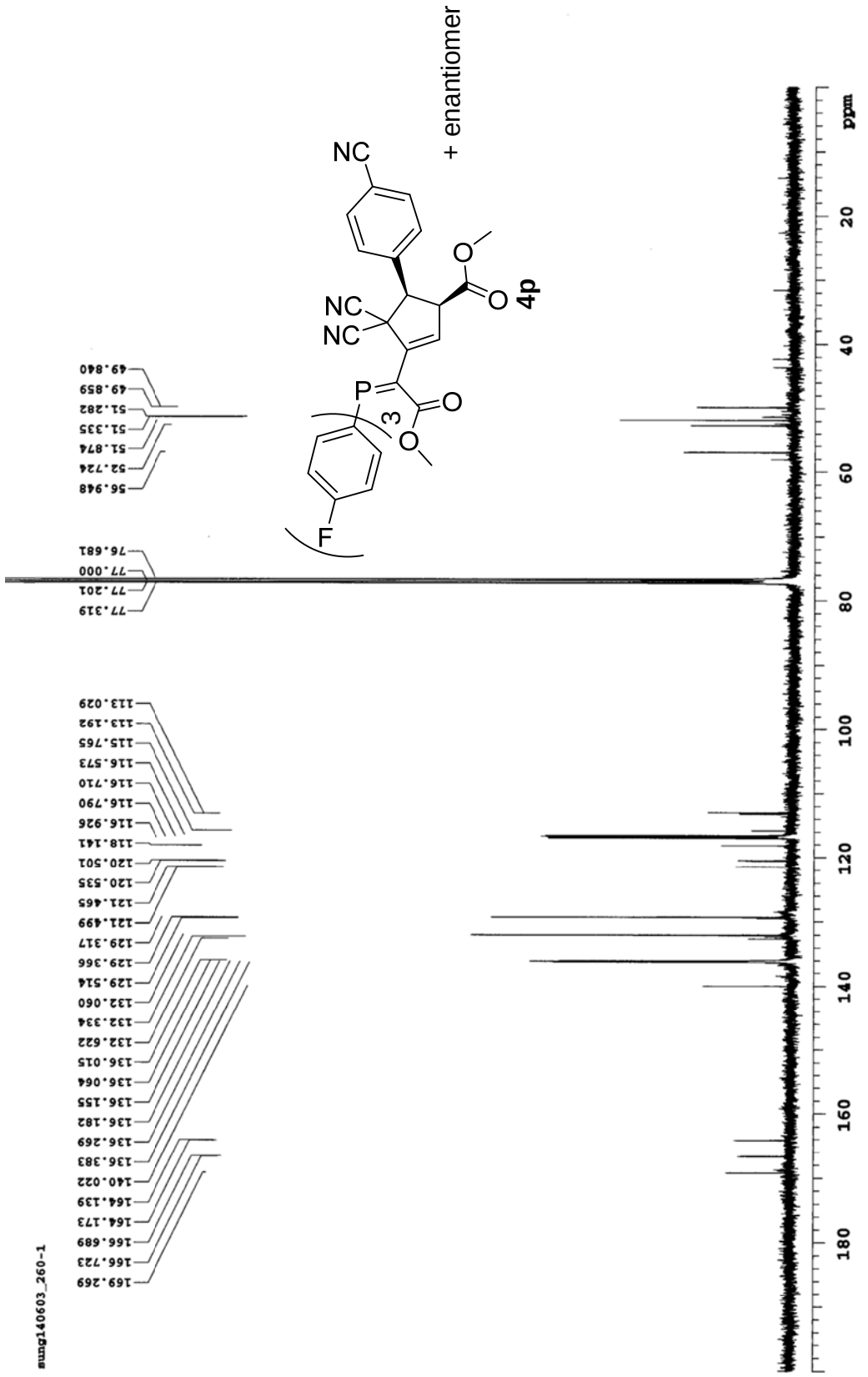
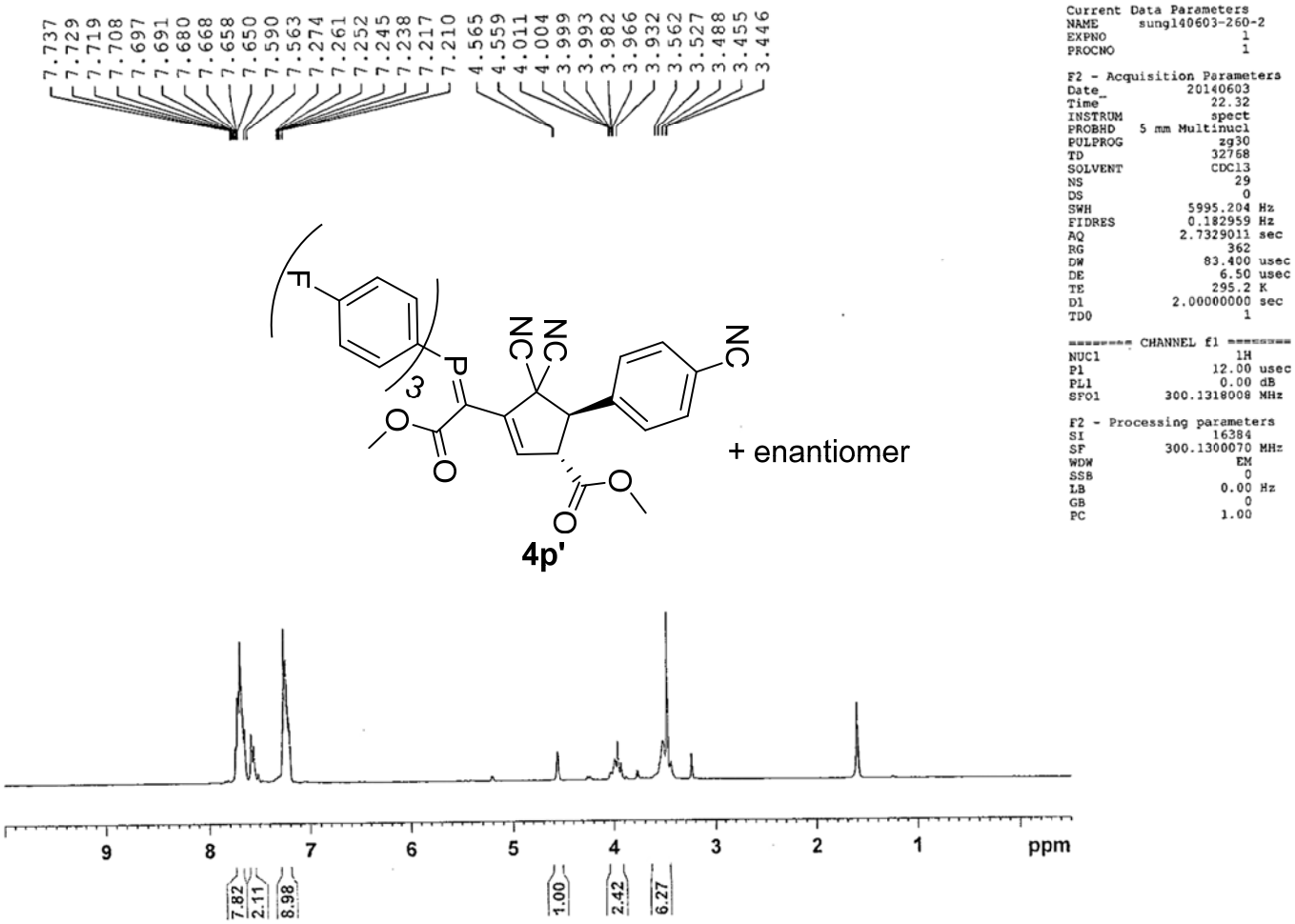


Fig. S59. ^{13}C NMR spectrum of compound **4p** (100 MHz, $CDCl_3$)

Fig. S60. ^{1}H NMR spectrum of compound **4p′** (300 MHz, $CDCl_3$)

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F2 - Processing parameters
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Fig. S61. ^{13}C NMR spectrum of compound **4p′** (100 MHz, $CDCl_3$)

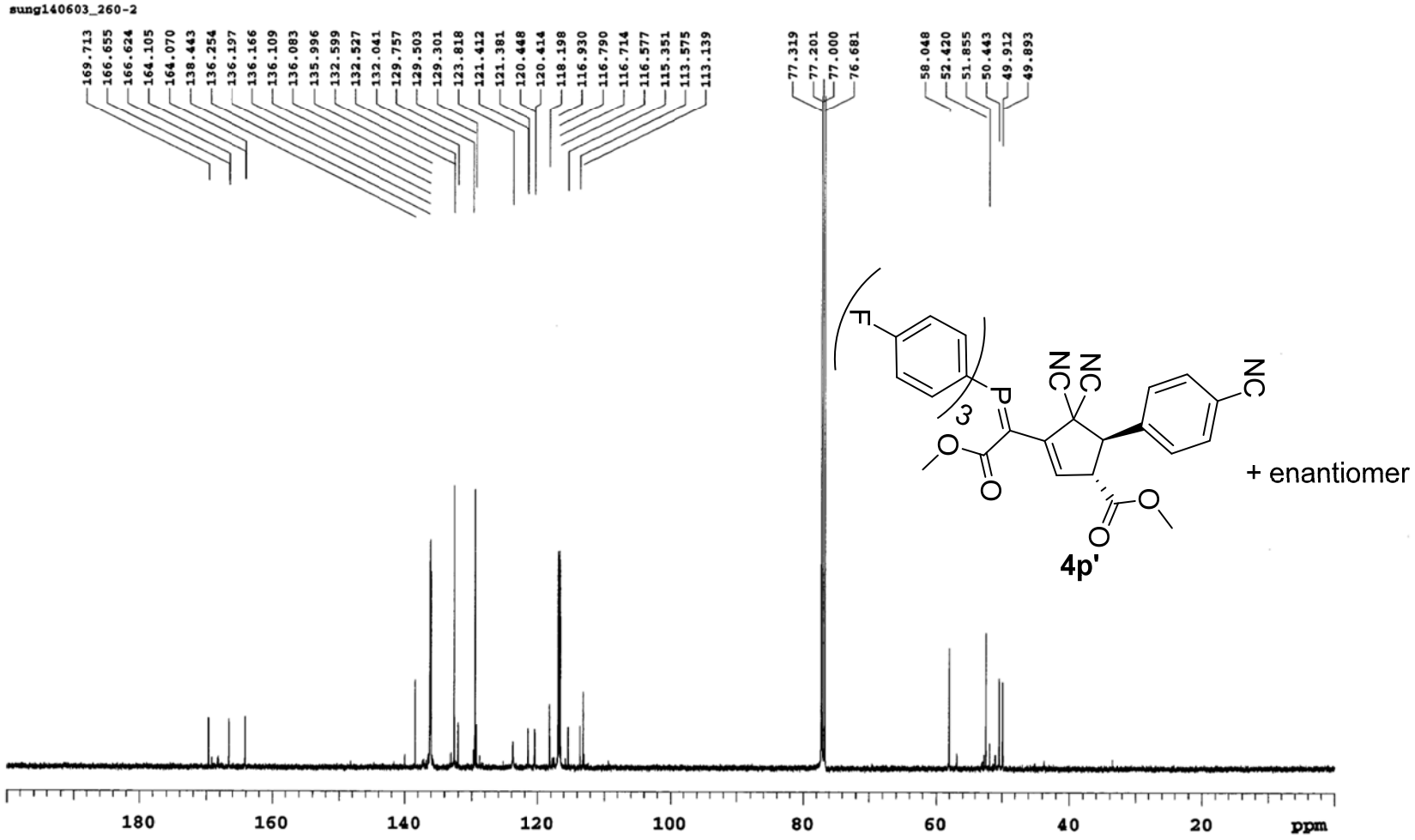
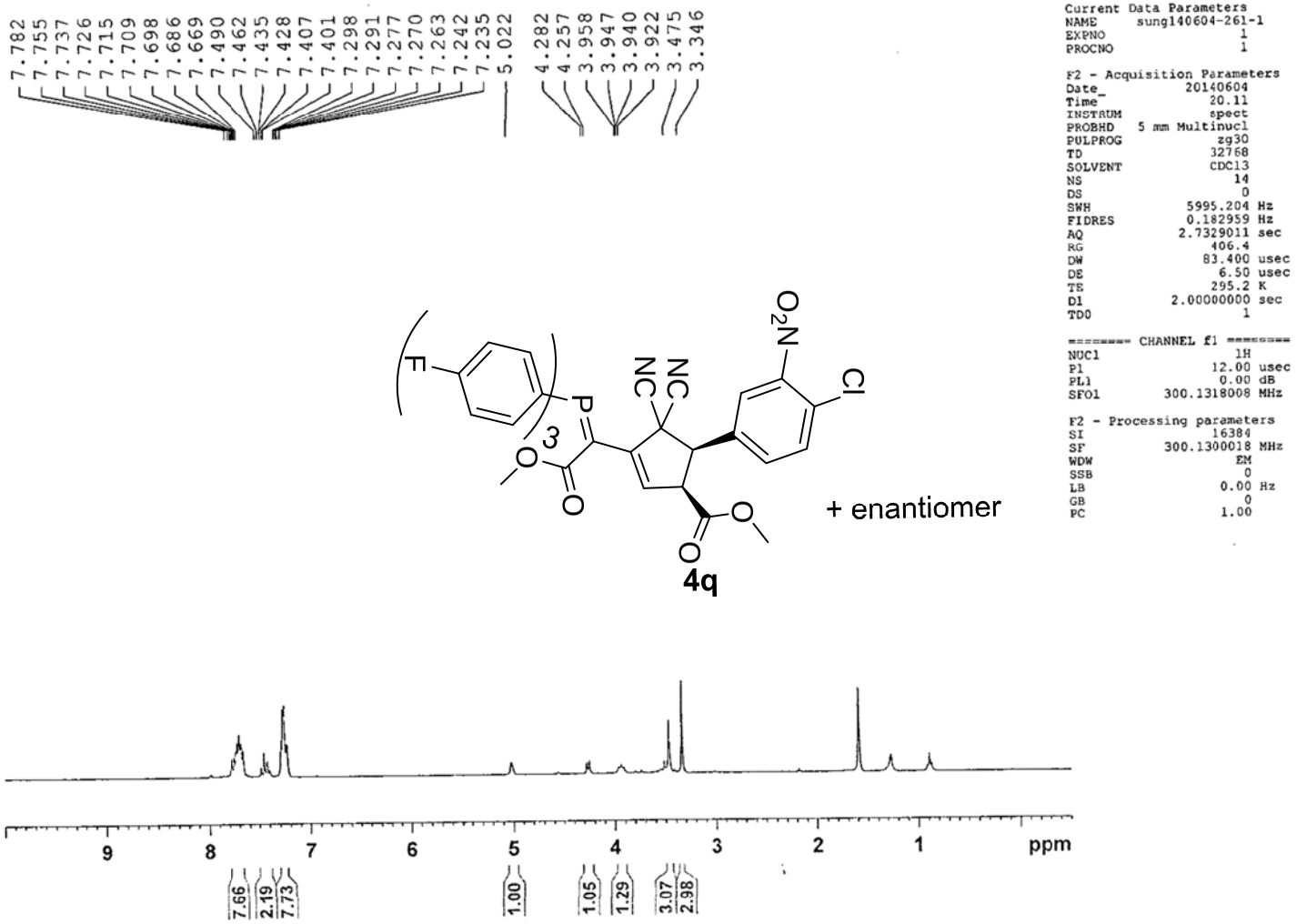


Fig. S62. ^{1}H NMR spectrum of compound **4q** (300 MHz, $CDCl_3$)



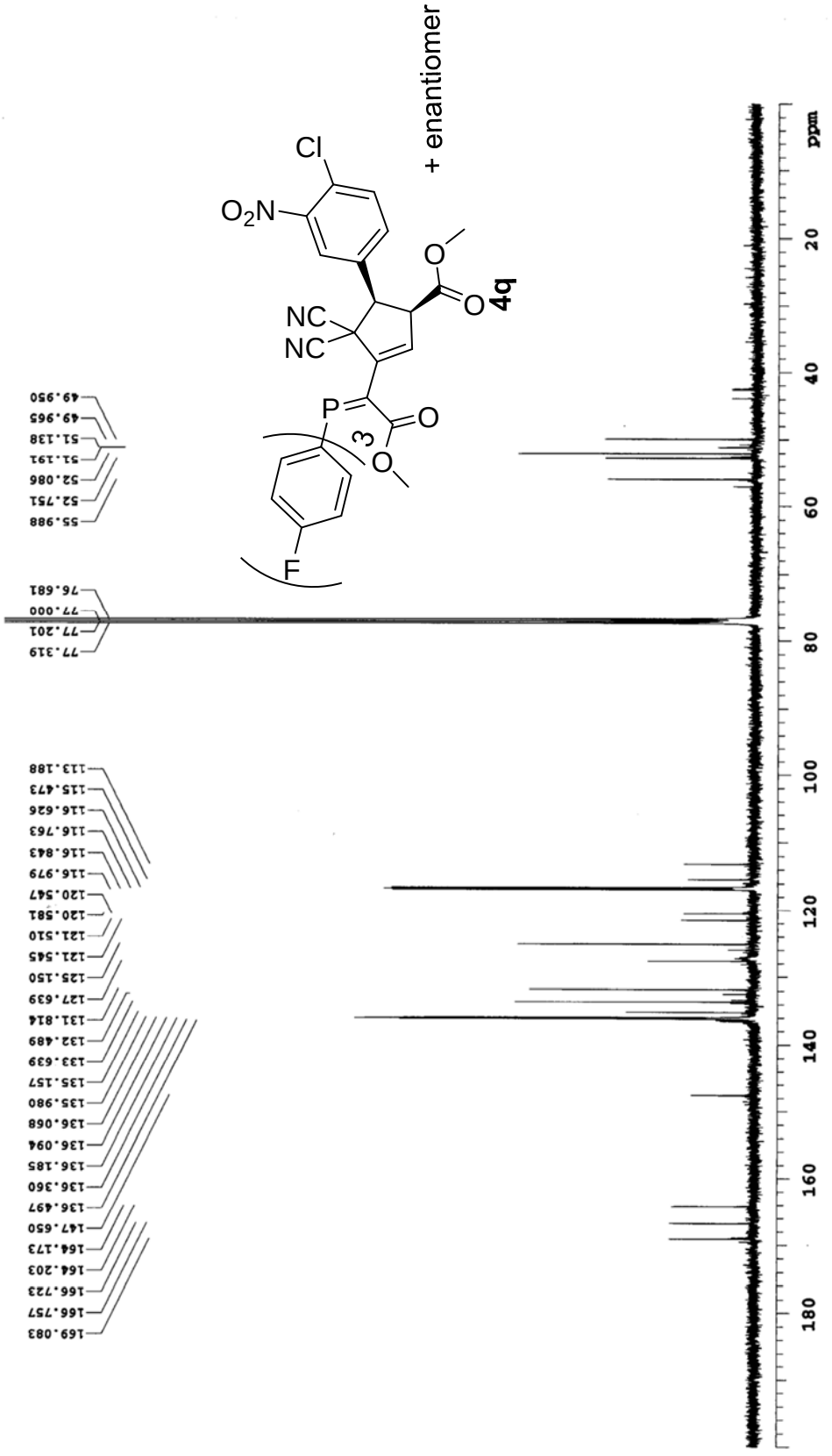


Fig. S63. ^{13}C NMR spectrum of compound **4q** (100 MHz, $CDCl_3$)

Fig. S64. ^{1}H NMR spectrum of compound **4q′** (300 MHz, $CDCl_3$)

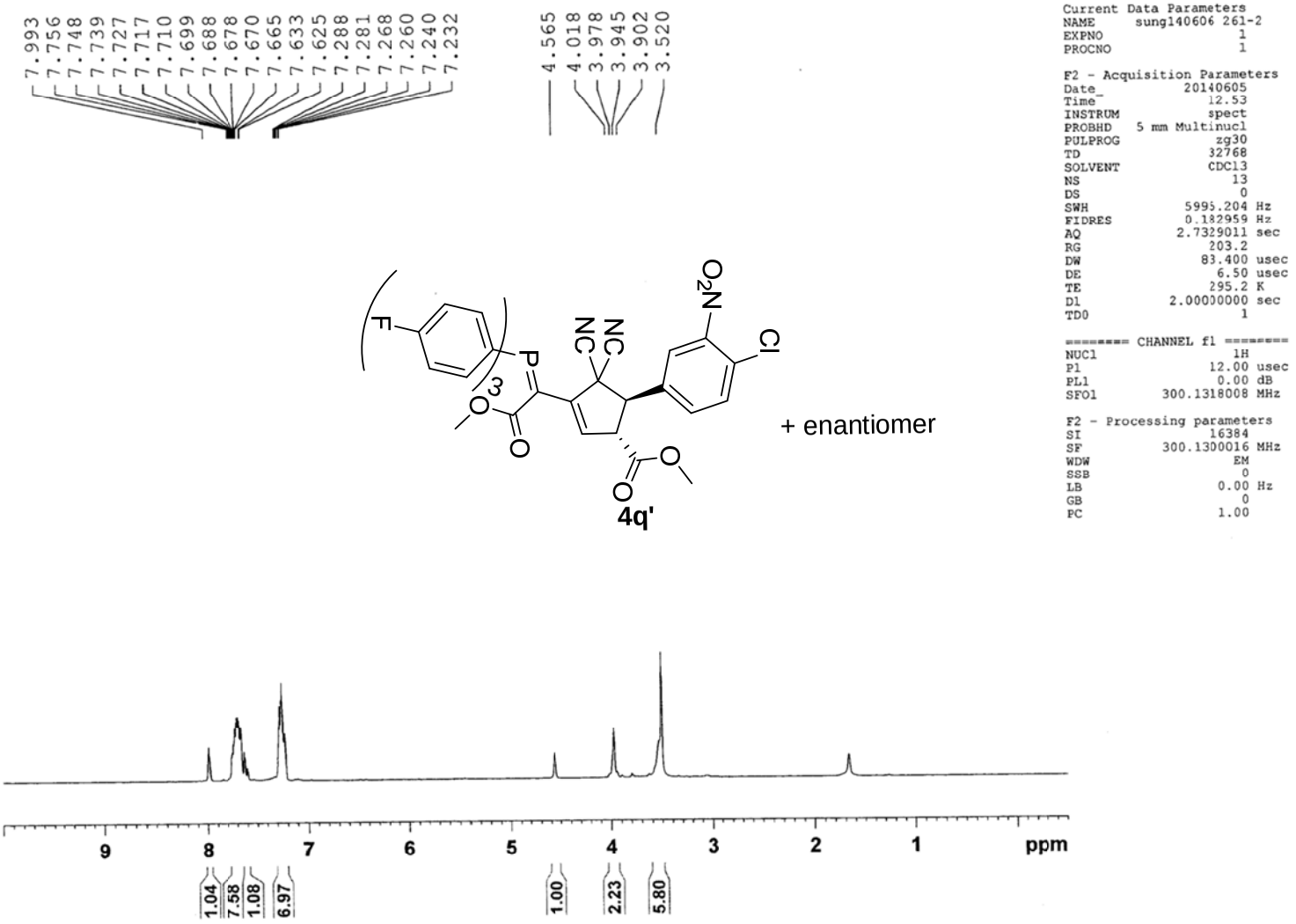


Fig. S65. ^{13}C NMR spectrum of compound **4q′** (100 MHz, $CDCl_3$)

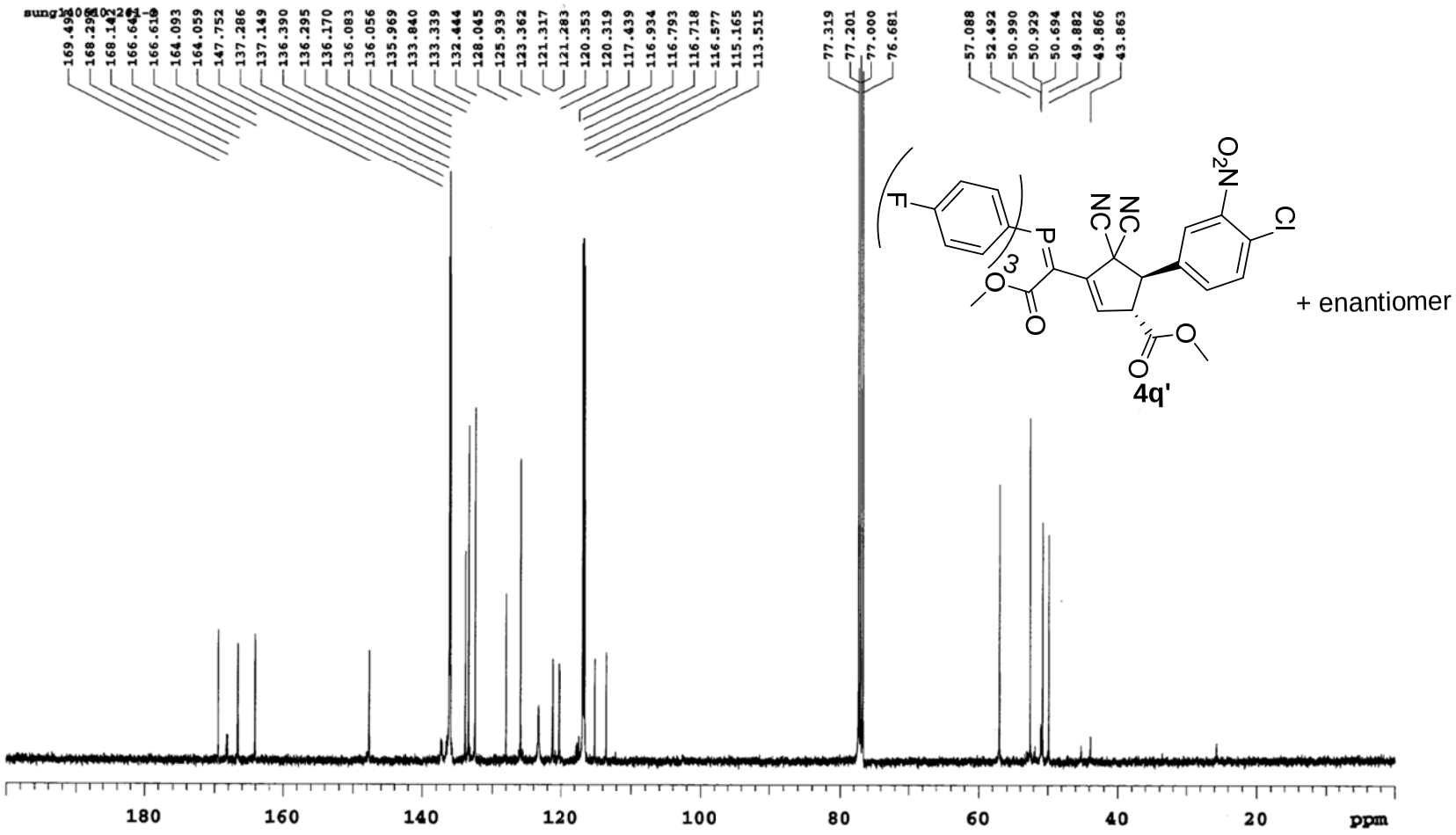


Fig. S66. ^{1}H NMR spectrum of compound **4r** (300 MHz, $CDCl_3$)

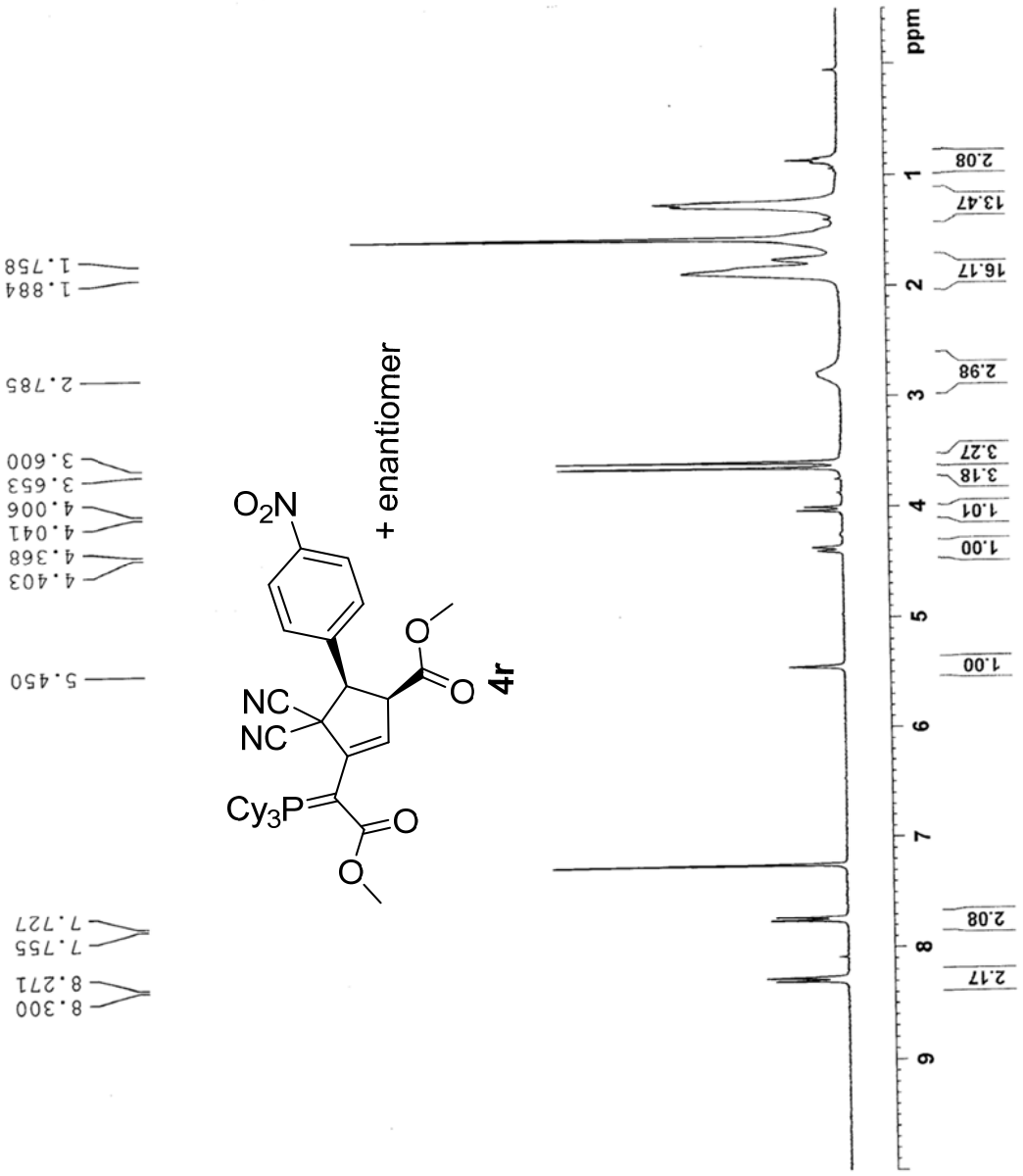


Fig. S67. ^{13}C NMR spectrum of compound **4r** (100 MHz, $CDCl_3$)

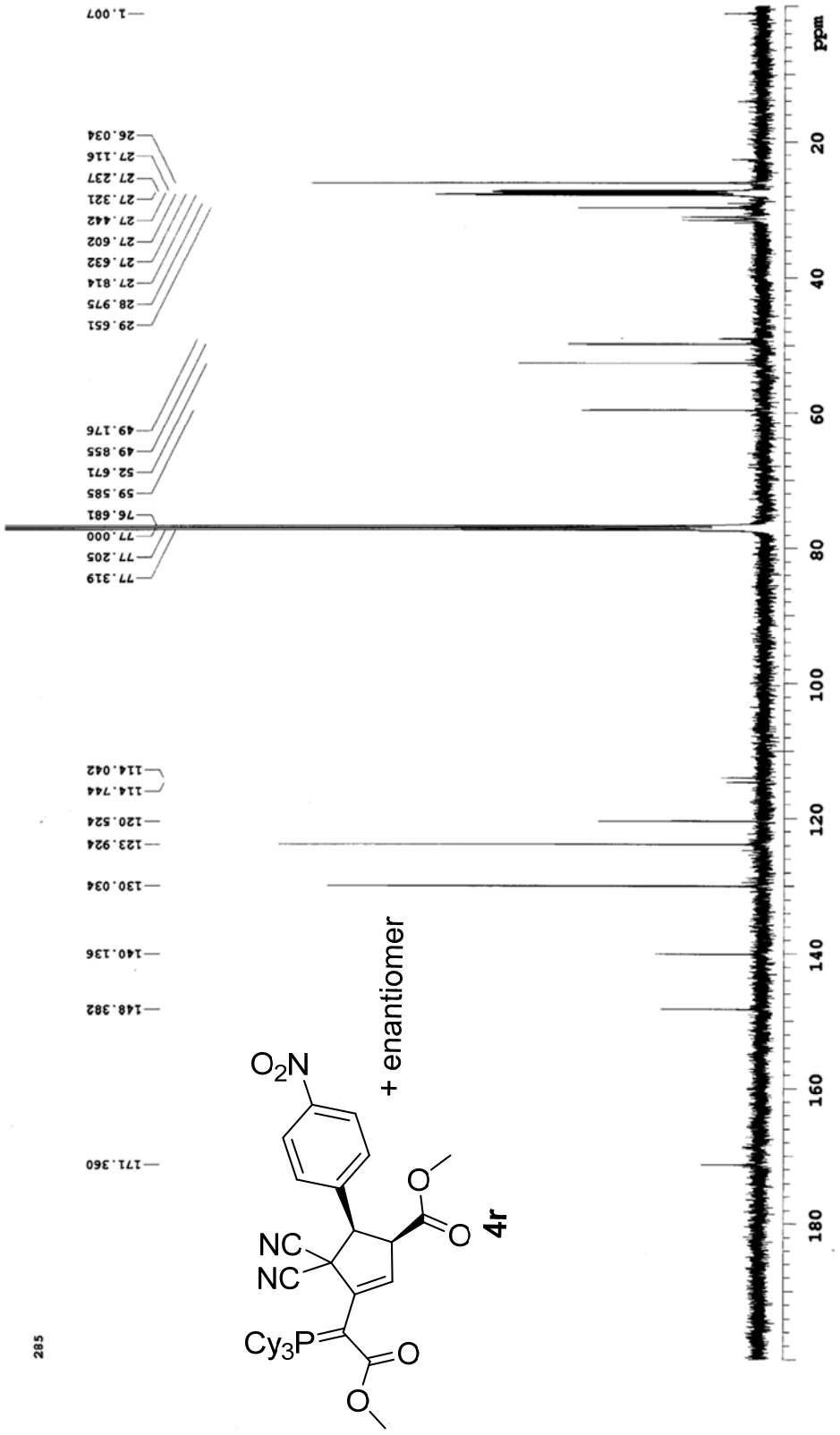


Fig. S68. ^{1}H NMR spectrum of compound **4s** (400 MHz, $CDCl_3$)

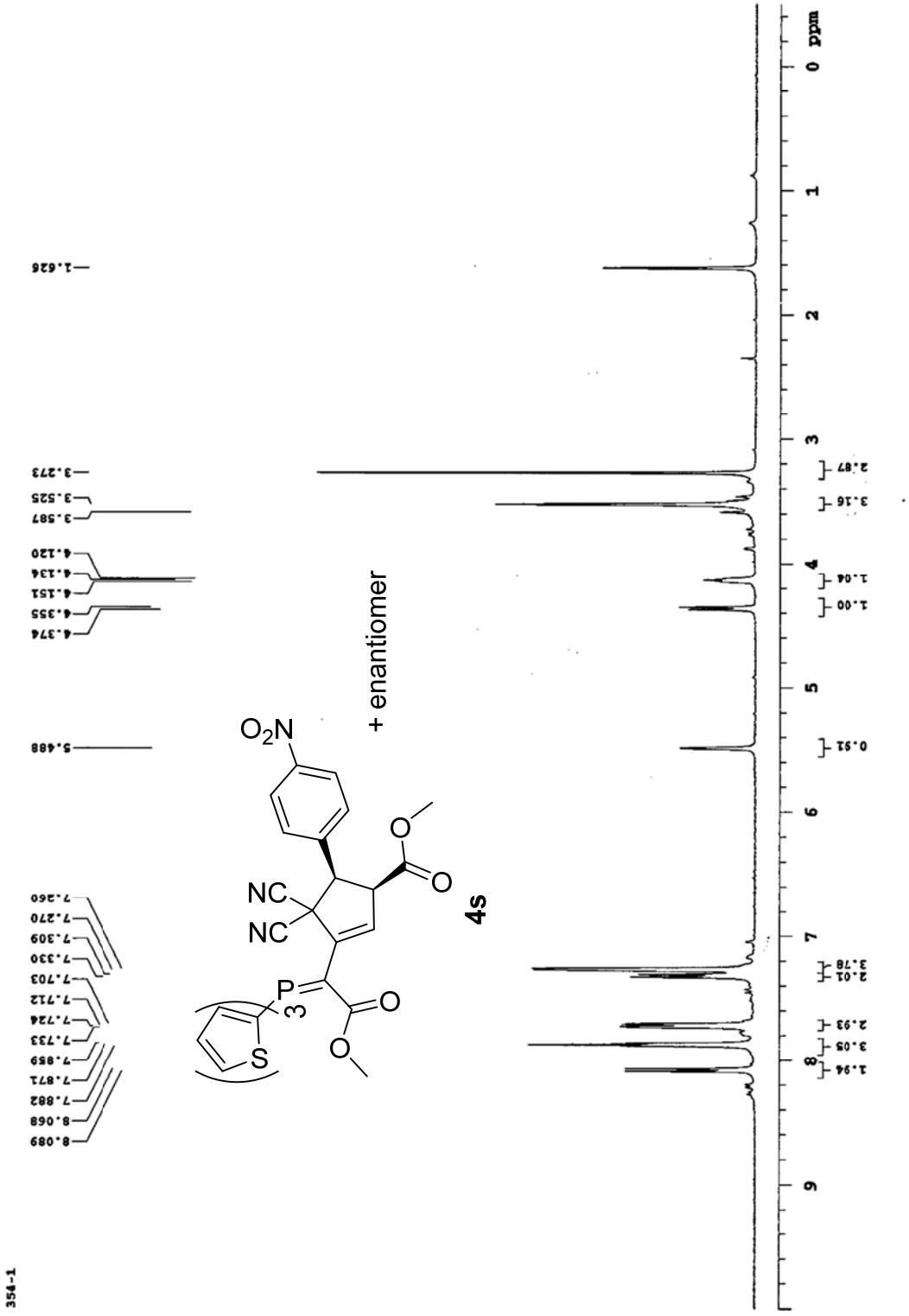


Fig. S69. ^{13}C NMR spectrum of compound **4s** (100 MHz, $CDCl_3$)

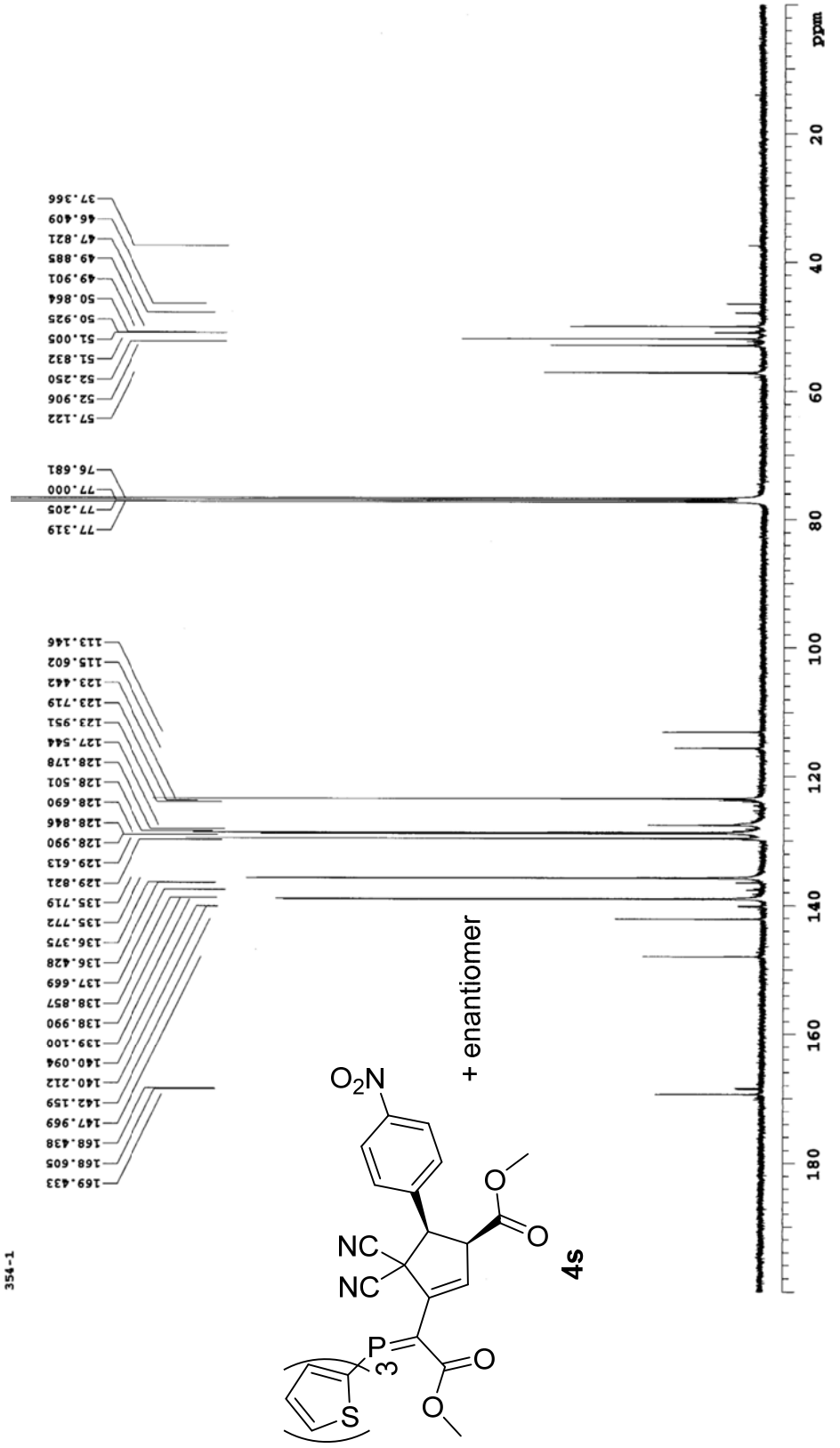


Fig. S70. ^{1}H NMR spectrum of compound **4s'** (400 MHz, $CDCl_3$)

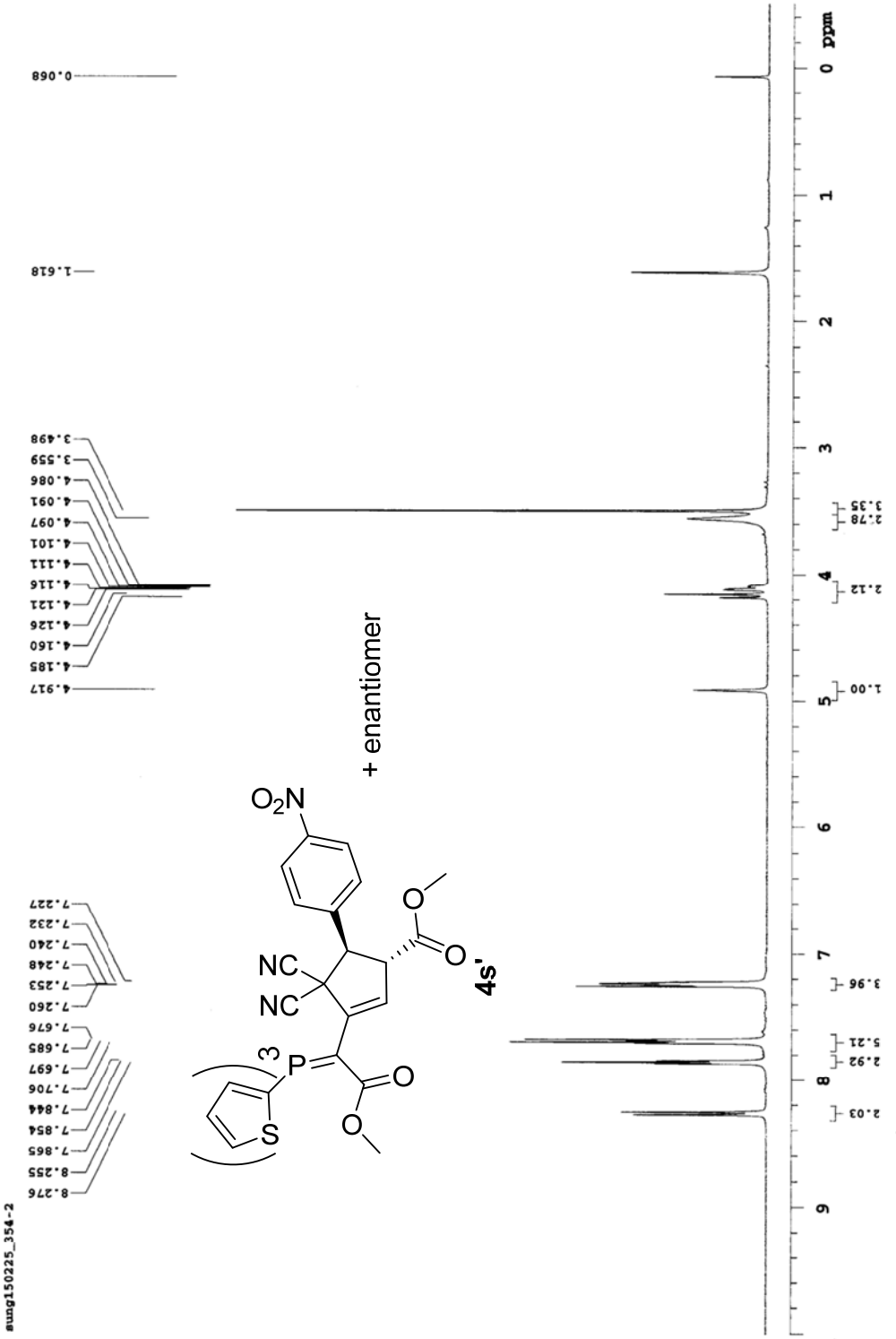


Fig. S71. ^{13}C NMR spectrum of compound **4s'** (100 MHz, $CDCl_3$)

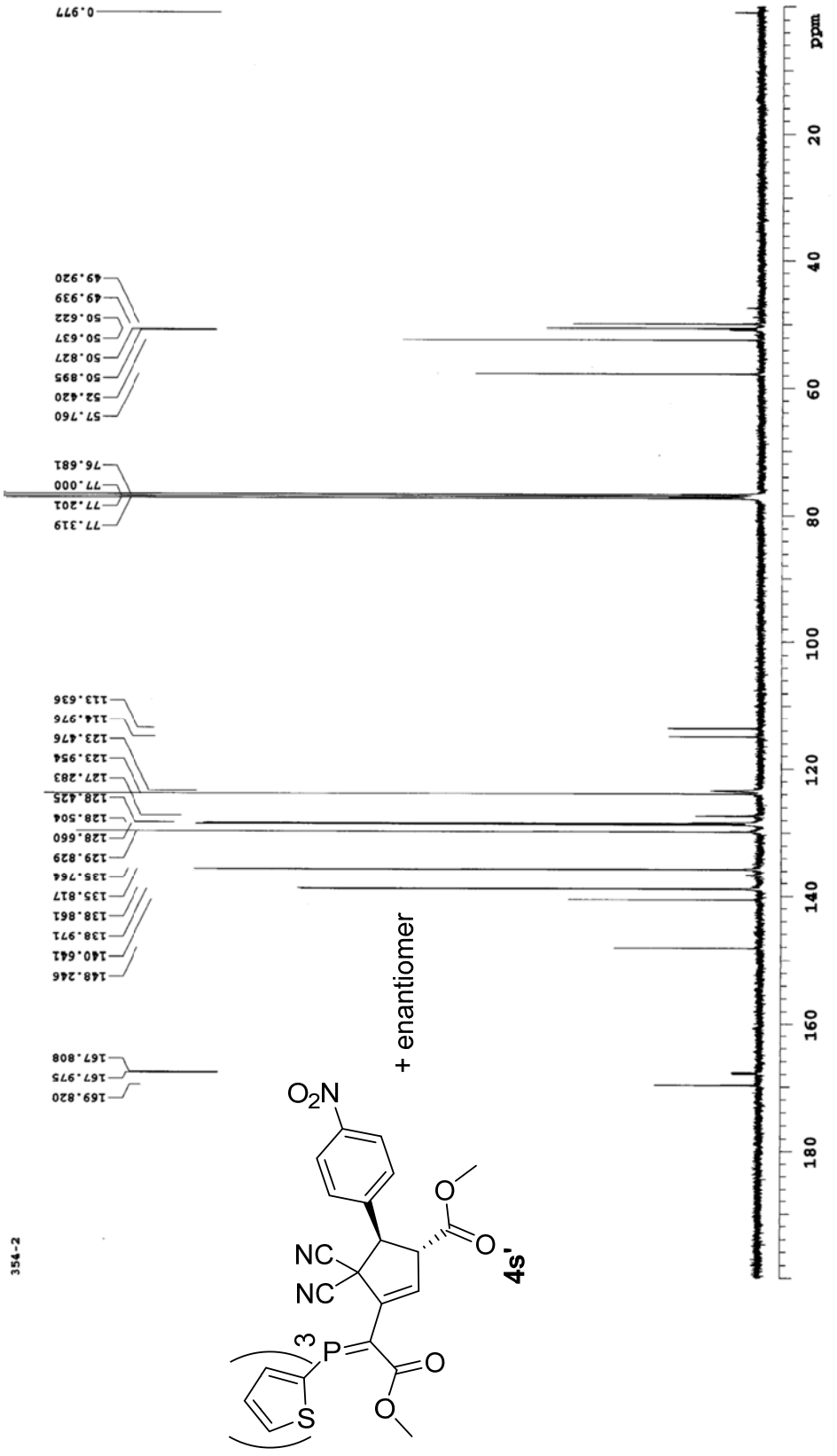
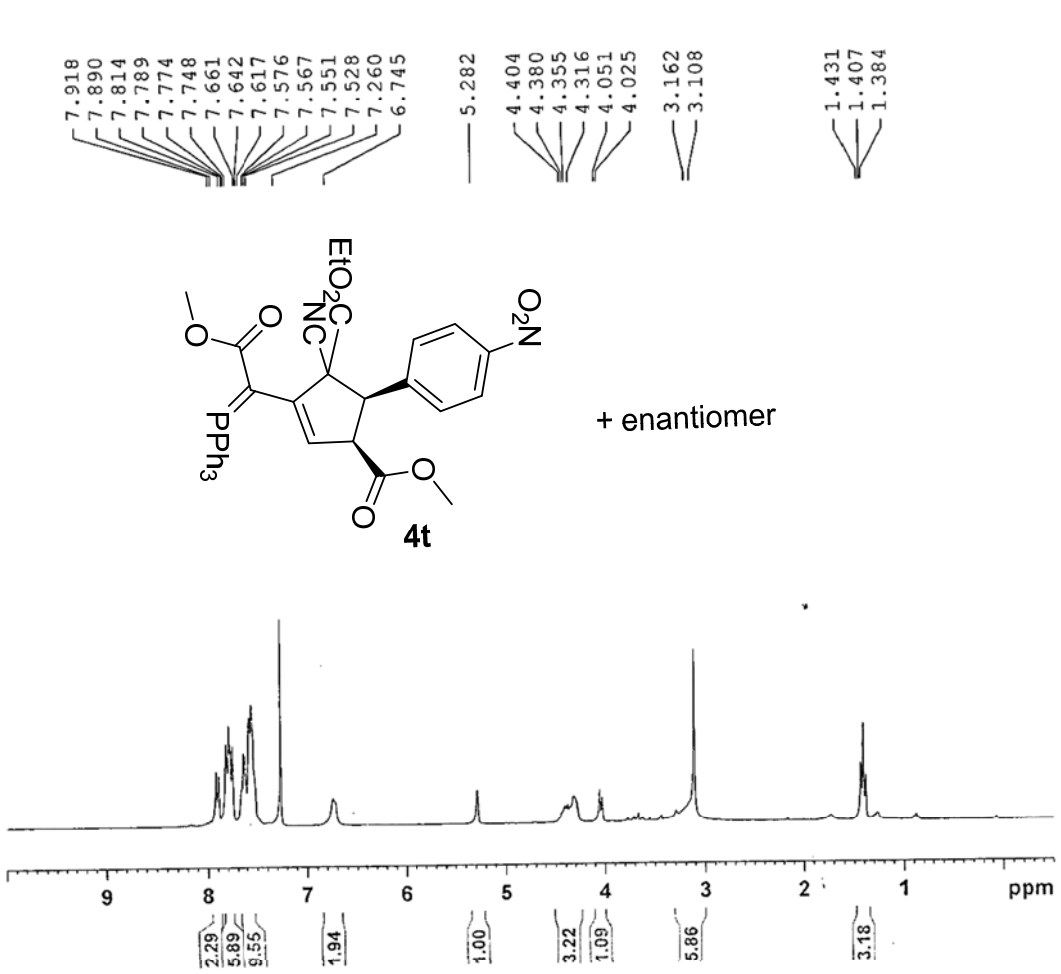


Fig. S72. ^{1}H NMR spectrum of compound **4t** (300 MHz, $CDCl_3$)

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RG                   143.7
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DE                    6.50 usec
TE                   297.2 K
D1             2.00000000 sec
TD0                      1

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SFO1          300.1318008 MHz

F2 - Processing parameters
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WDW                     EM
SSB                      0
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GB                       0
PC                    1.00
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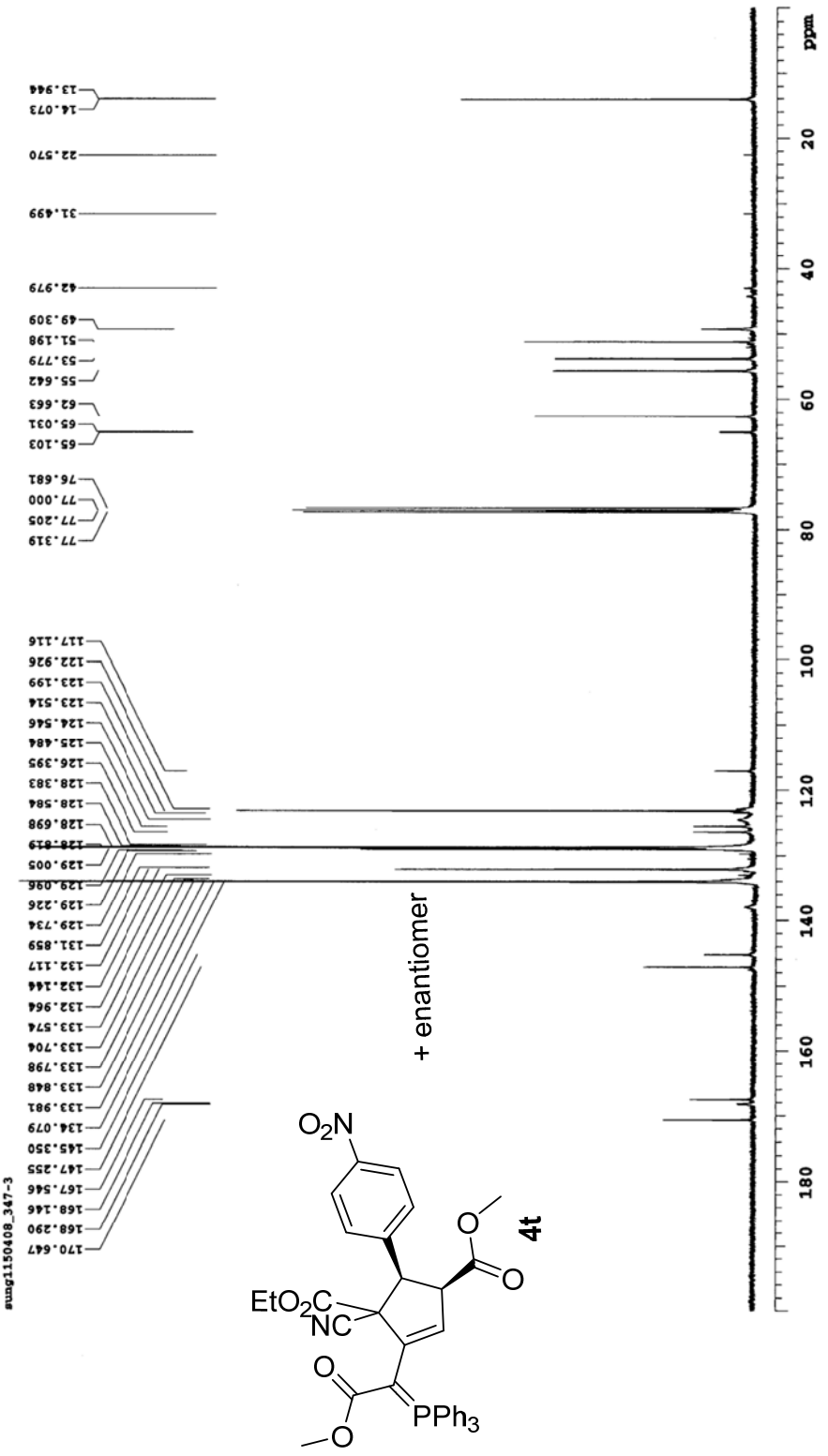
Fig. S73. ^{13}C NMR spectrum of compound **4t** (100 MHz, $CDCl_3$)



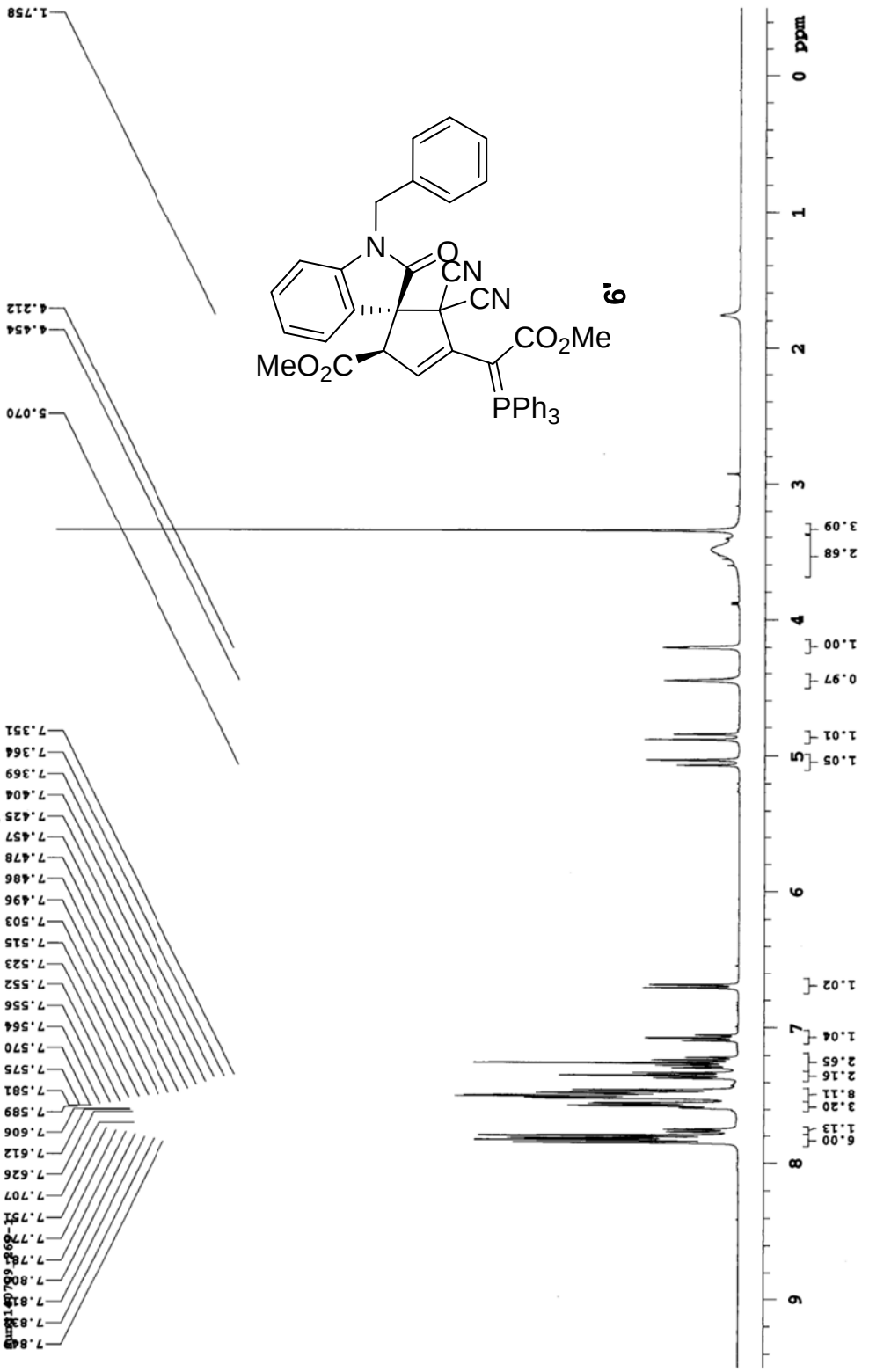


Fig. S74. ^{1}H NMR spectrum of compound **6'** (400 MHz, $CDCl_3$)

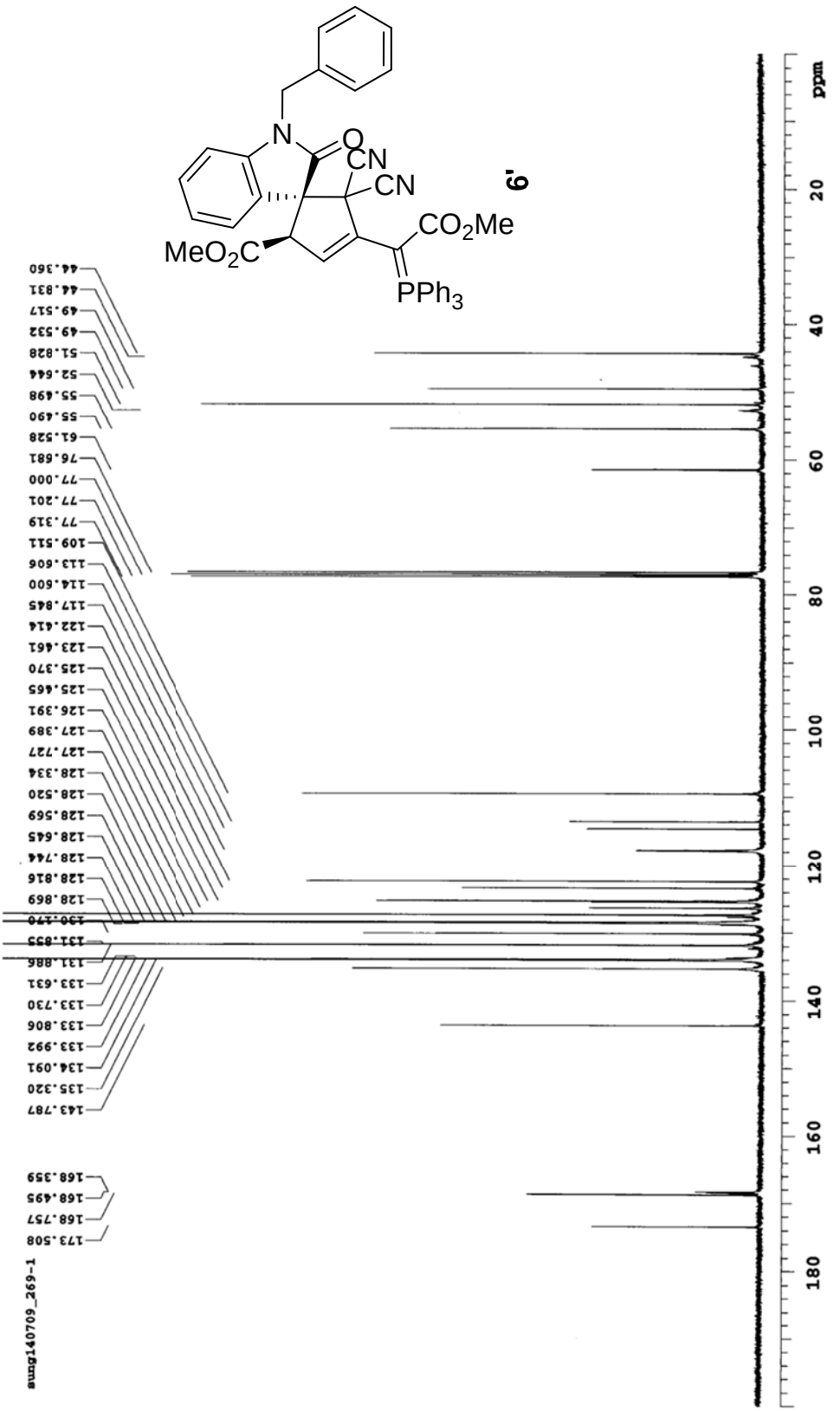


Fig. S75. ^{13}C NMR spectrum of compound **6'** (100 MHz, $CDCl_3$)

Fig. S76. Variable temperature ^{1}H NMR spectra of **4a** (600 MHz, $CDCl_3$)

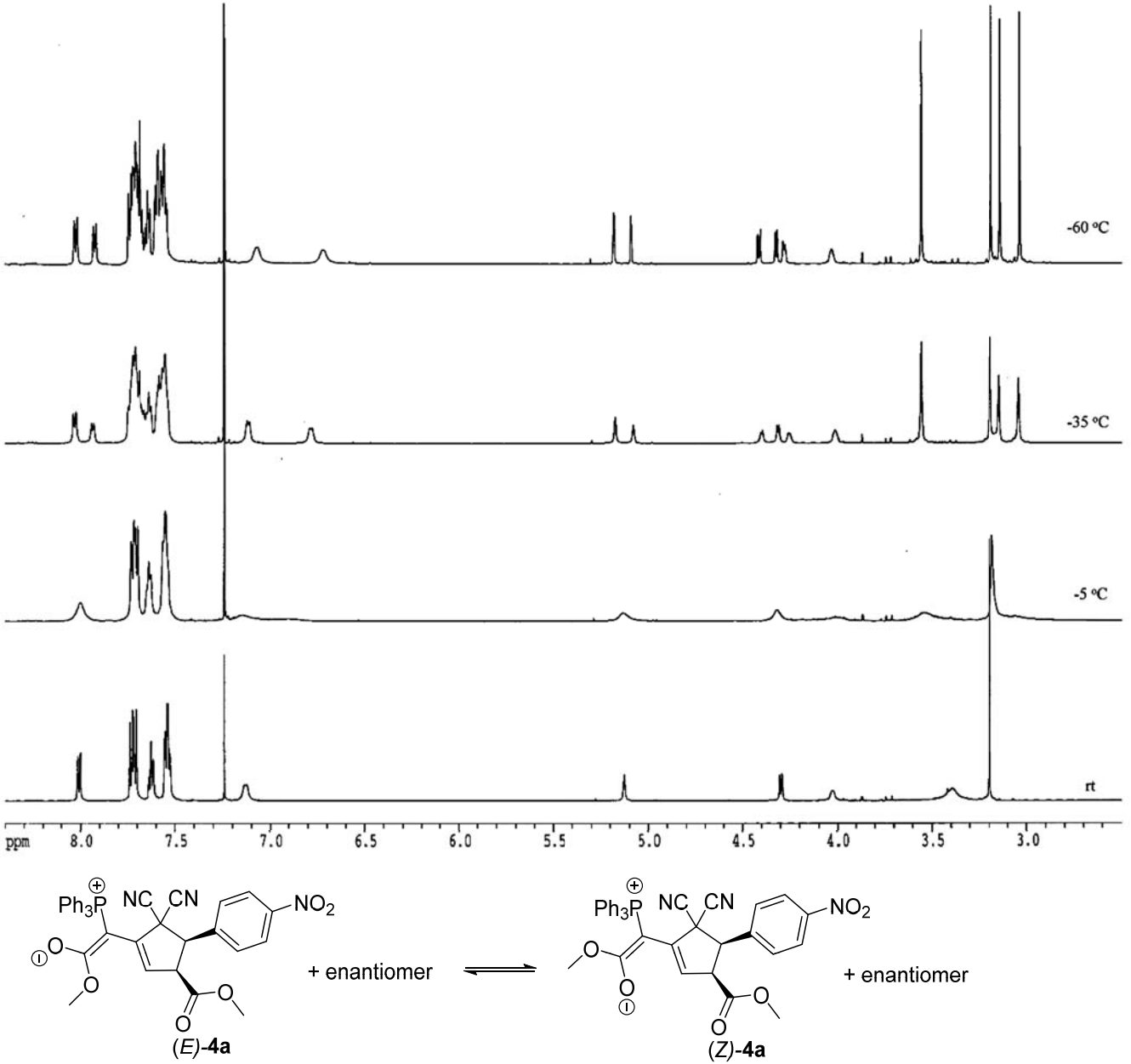


Fig. S77. Variable temperature ^{31}P NMR spectra of **4a** (242.5 MHz, $CDCl_3$)

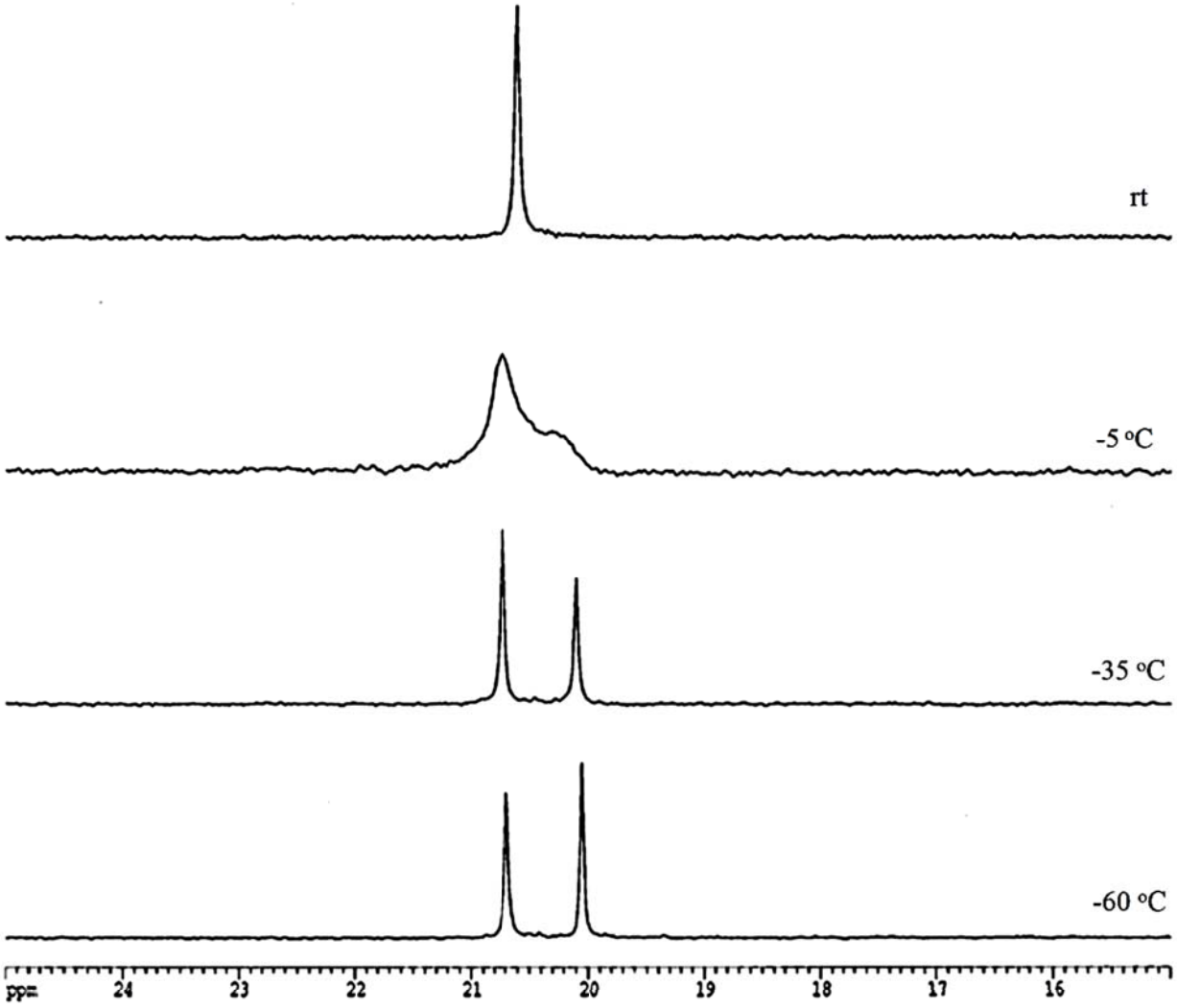


Fig. S78. Variable temperature ^{1}H NMR spectra of **4a′** (600 MHz, $CDCl_3$)

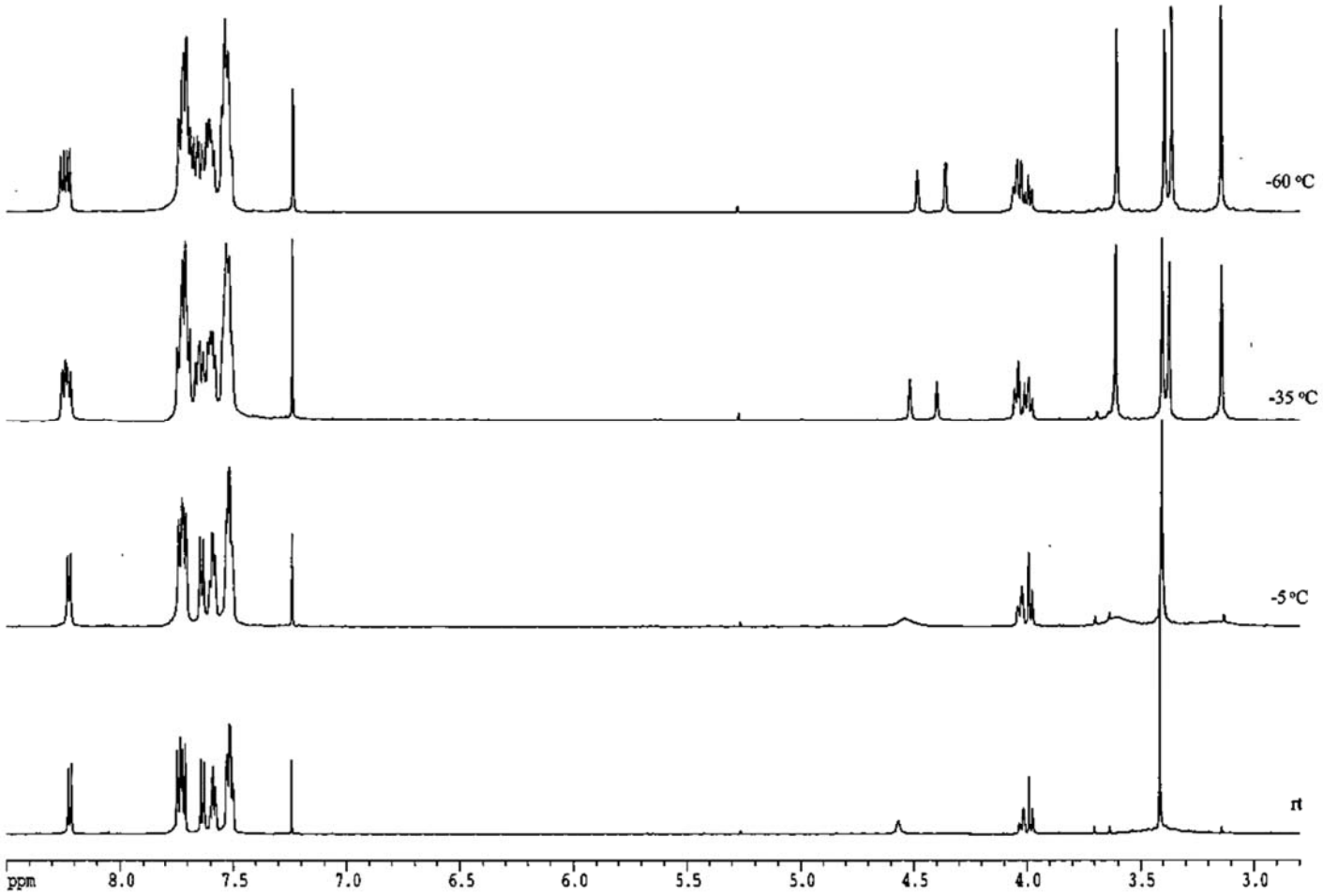


Fig. S79. Variable temperature ^{31}P NMR spectra of **4a′** (242.5 MHz, $CDCl_3$)

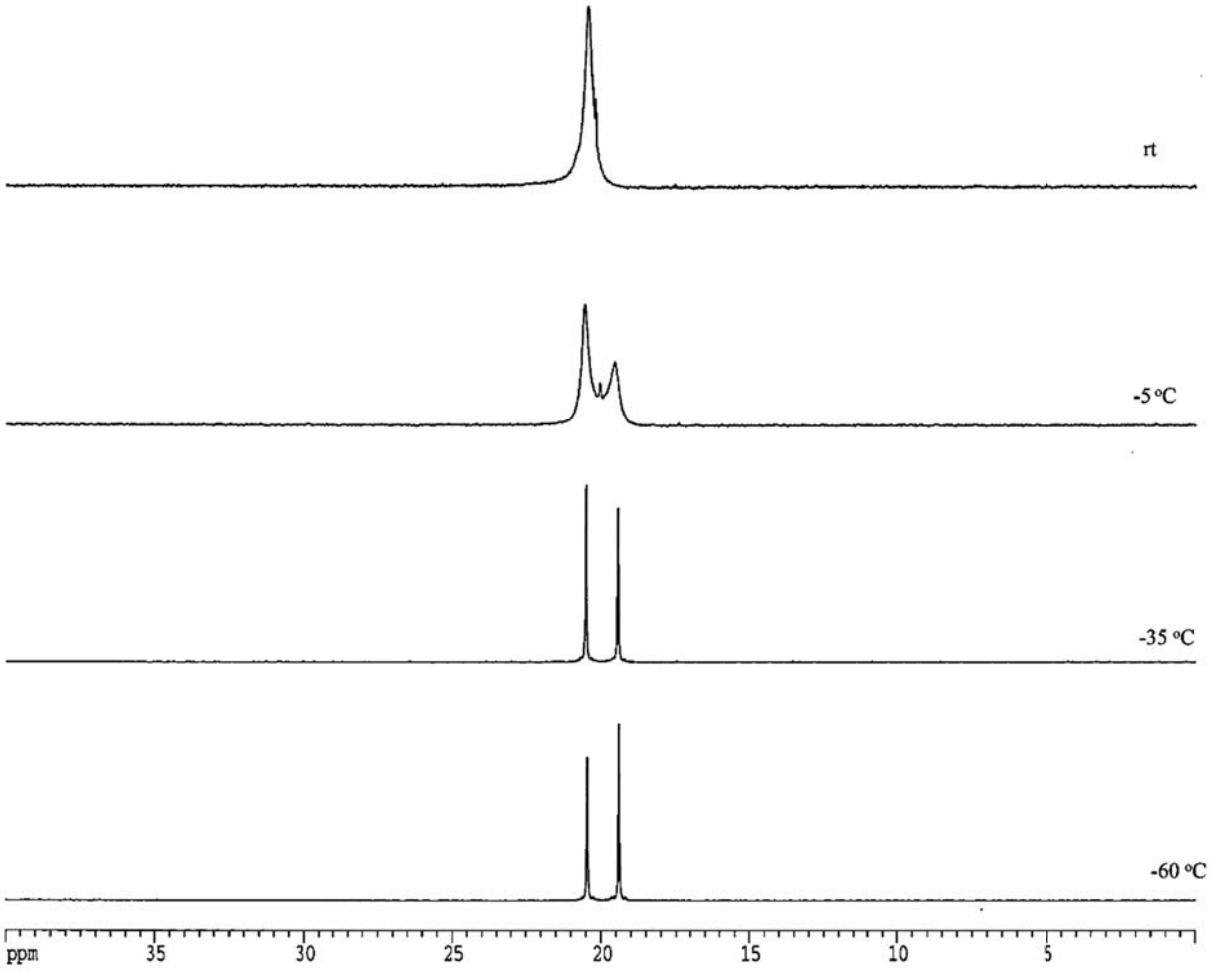


Fig. S80. nuclear Overhauser enhancement (NOE) spectra of **4a** (500 MHz, $CDCl_3$)

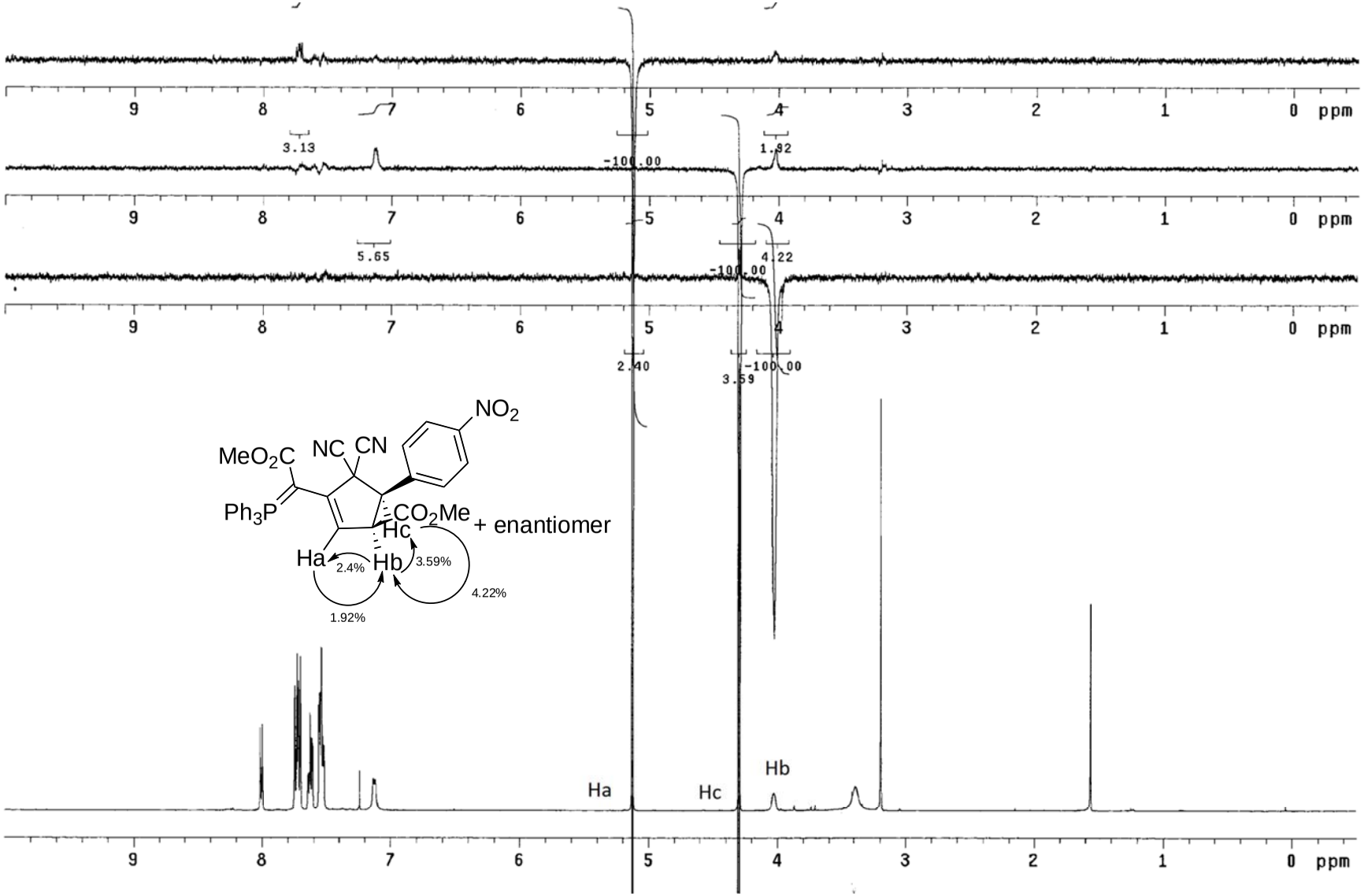


Fig. S81. nuclear Overhauser enhancement (NOE) spectra of **4a′** (500 MHz, $CDCl_3$)

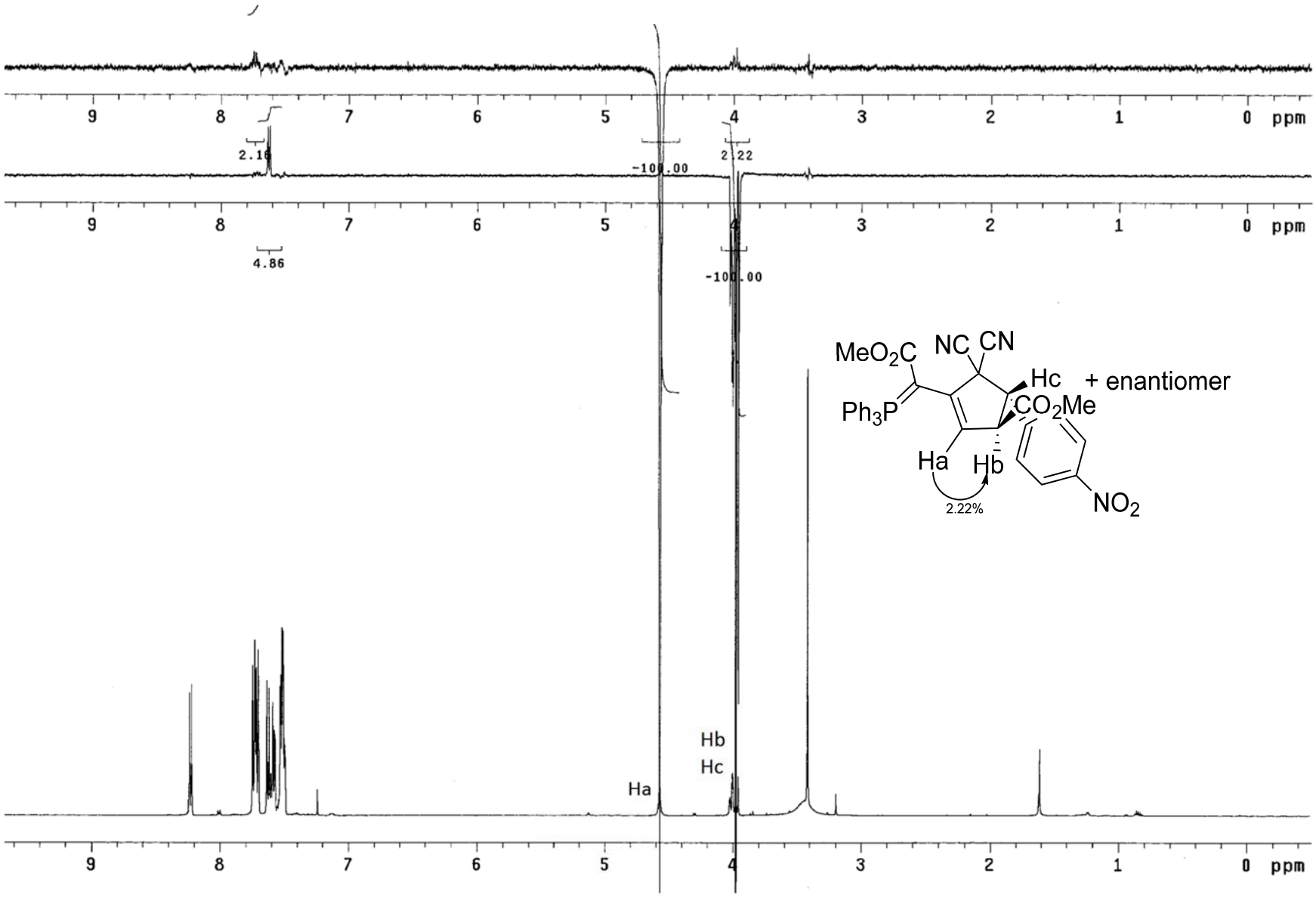


Fig. S82. 2D-HMQC of **4a** (^{1}H NMR δ 6.5–8.5 ppm; ^{13}C NMR δ 115–140 ppm)

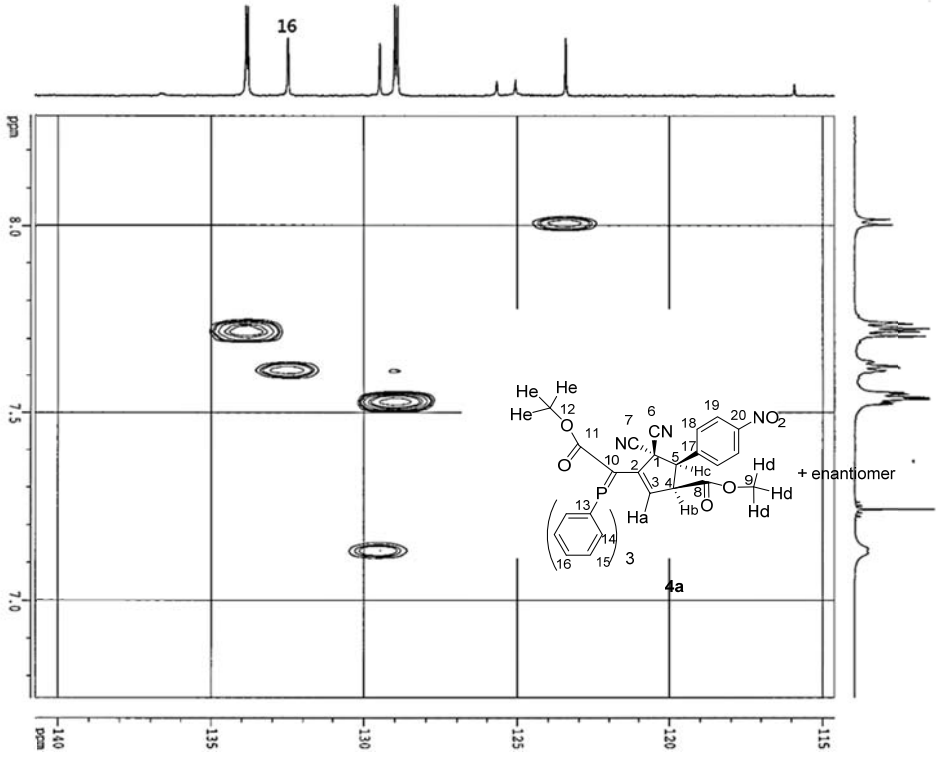


Fig. S83. 2D-HMQC of **4a** (^{1}H NMR δ 3.0–4.5 ppm; ^{13}C NMR δ 46–62 ppm)

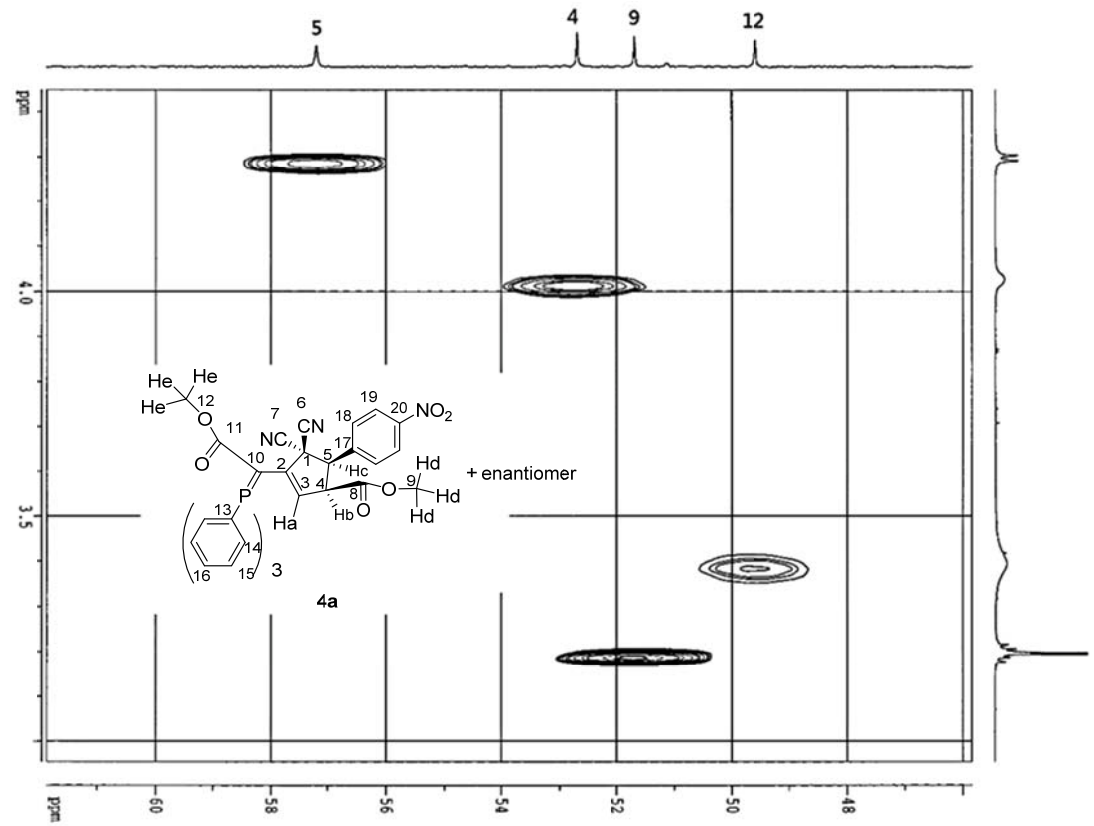


Fig. S84. 2D-HMBC of **4a** (^{1}H NMR δ 2.5–5.5 ppm; ^{13}C NMR δ 40–180 ppm)

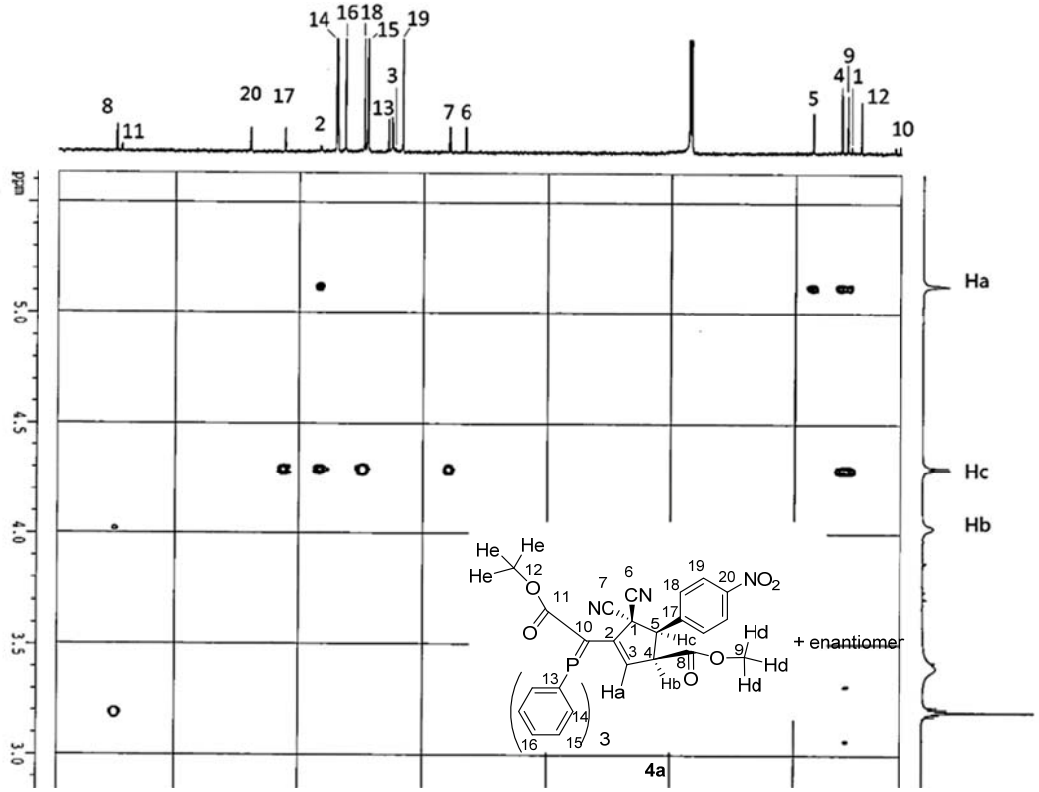


Fig. S85. 2D-HMBC of **4a** (^{1}H NMR δ 7.3–8.2 ppm; ^{13}C NMR δ 120–150 ppm)

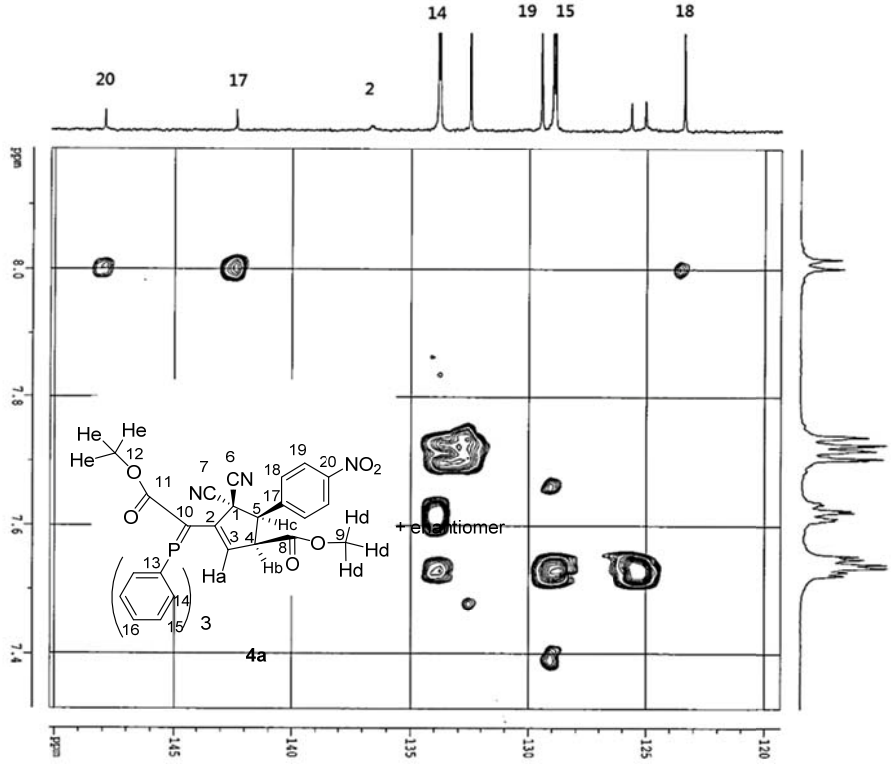


Fig. S86. 2D-HMQC of **4a′**

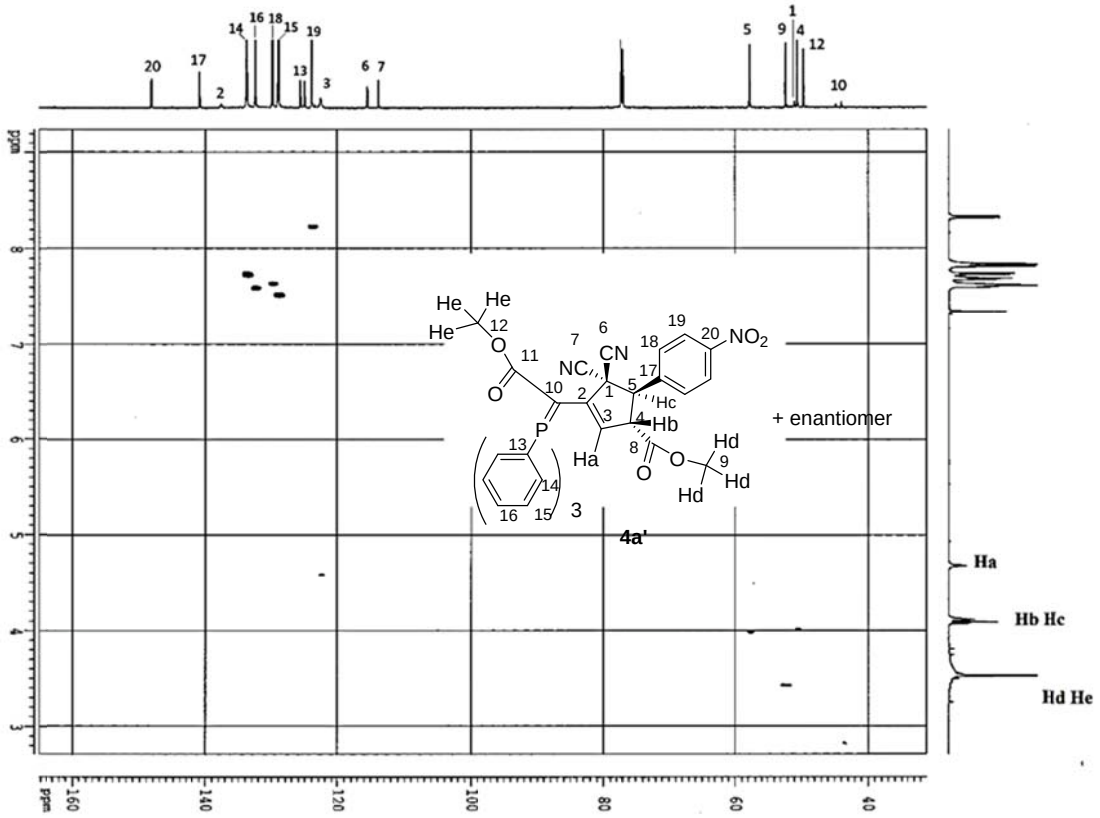


Fig. S87. 2D-HMBC of **4a′**

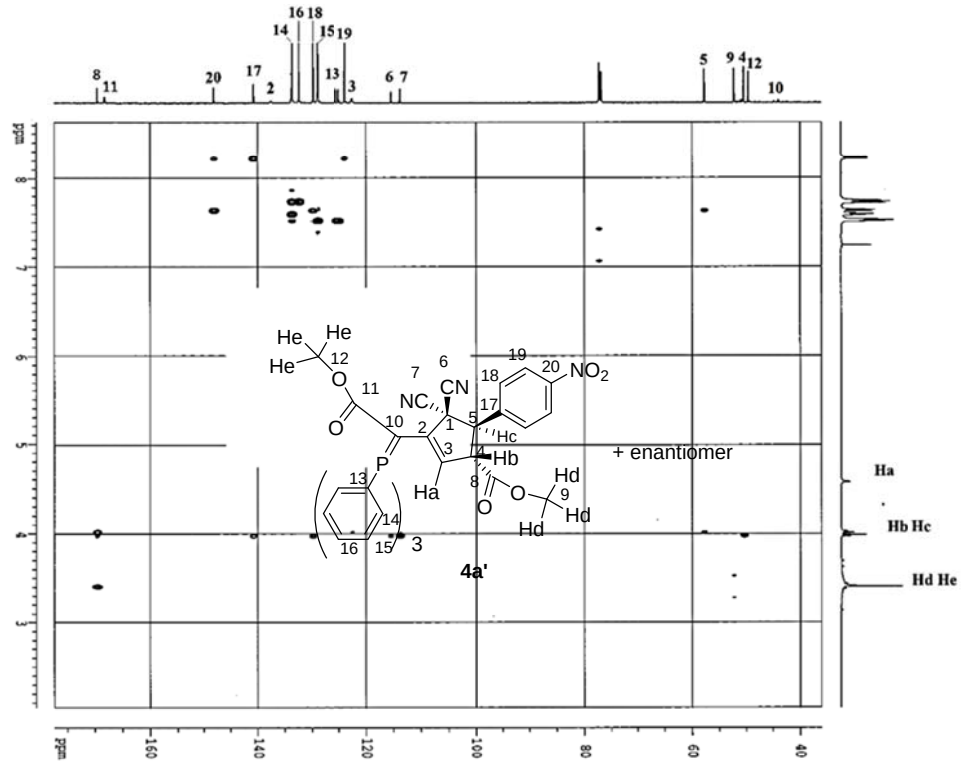


Fig. S88. X-ray crystal structure of **4a**

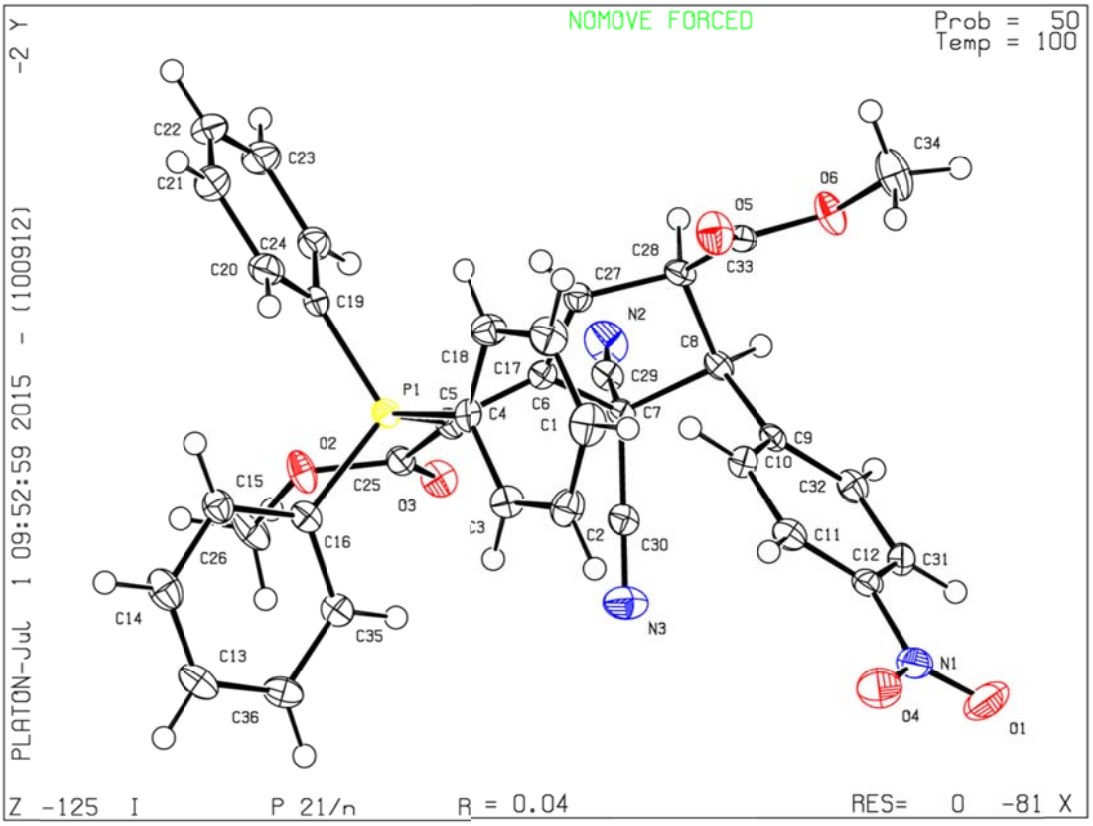


Table S1. Crystallographic data of **4a**

Empirical formula	$C_{36}H_{28}N_3O_6P$	
Formula weight	629.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.4651(7) Å	α= 90°.
	b = 27.3604(18) Å	β= 112.634(2)°.
	c = 11.6914(9) Å	γ = 90°.
Volume	3089.8(4) $Å^3$	
Z	4	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	0.142 mm^{-1}	
F(000)	1312	
Crystal size	0.25 x 0.18 x 0.05 mm^3	
Theta range for data collection	1.489 to 26.439°.	
Index ranges	-13<=h<=11, -34<=k<=31, -14<=l<=14	
Reflections collected	25478	
Independent reflections	6308 [R(int) = 0.0492]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8693	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6308 / 0 / 417	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1242	
R indices (all data)	R1 = 0.0635, wR2 = 0.1620	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.417 and -0.639 $e.Å^{-3}$	

Fig. S89. X-ray crystal structure of **4a′**

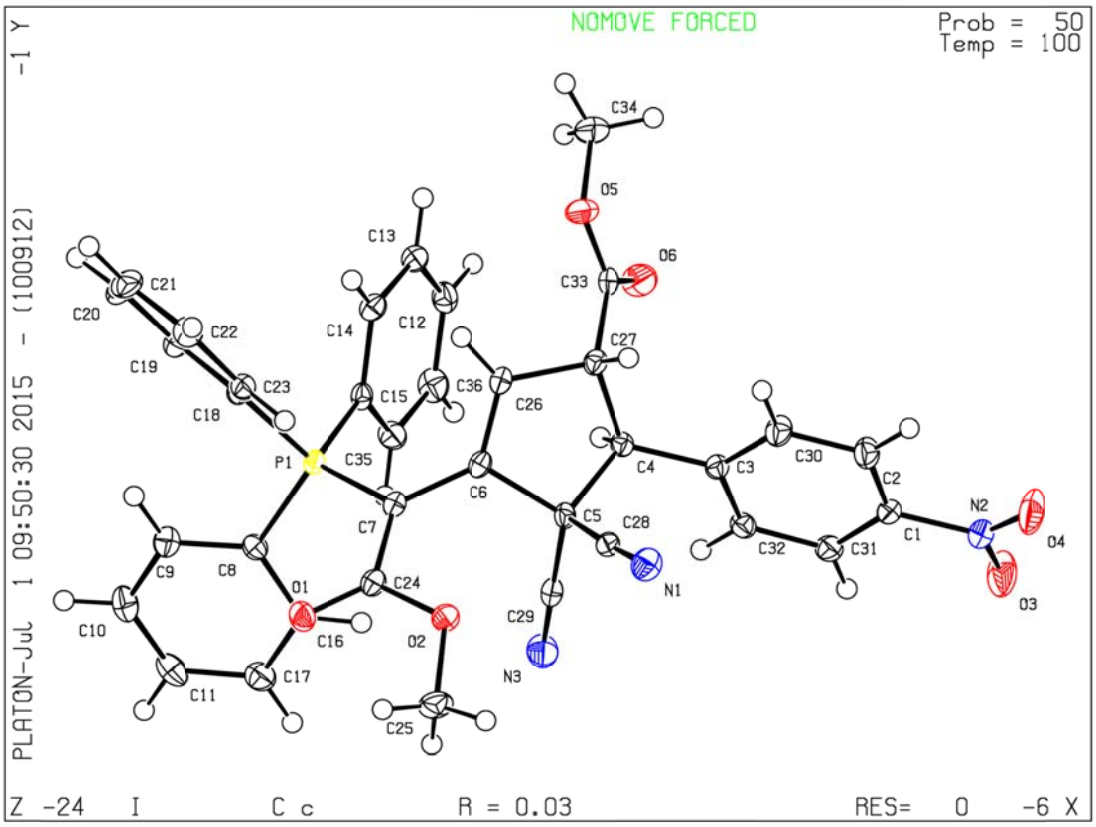
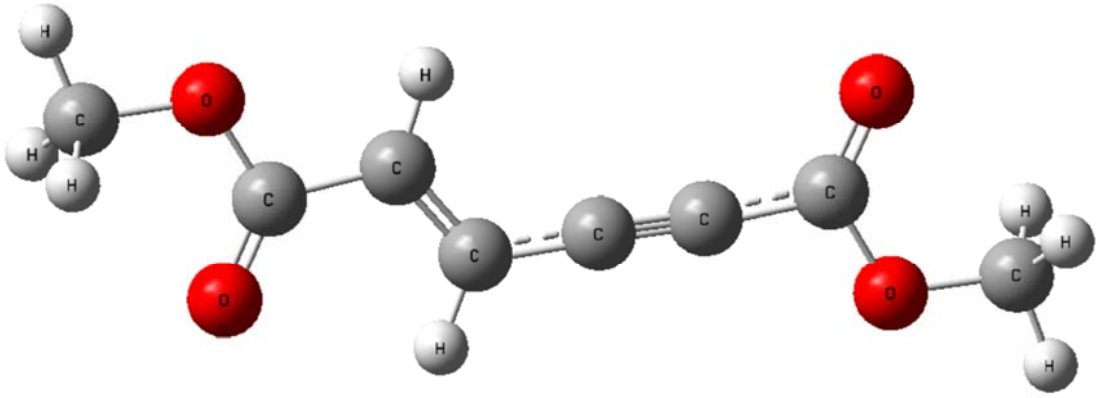


Table S2. Crystallographic data of **4a′**

Empirical formula	$C_{36}H_{28}N_3O_6P$	
Formula weight	629.58	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.4651(7) Å	α= 90°.
	b = 27.3604(18) Å	β= 112.634(2)°.
	c = 11.6914(9) Å	γ = 90°.
Volume	3089.8(4) $Å^3$	
Z	4	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	0.142 mm^{-1}	
F(000)	1312	
Crystal size	0.25 x 0.18 x 0.05 mm^3	
Theta range for data collection	1.489 to 26.439°.	
Index ranges	-13<=h<=11, -34<=k<=31, -14<=l<=14	
Reflections collected	25478	
Independent reflections	6308 [R(int) = 0.0492]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8693	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6308 / 0 / 417	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1242	
R indices (all data)	R1 = 0.0635, wR2 = 0.1620	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.417 and -0.639 $e.Å^{-3}$	

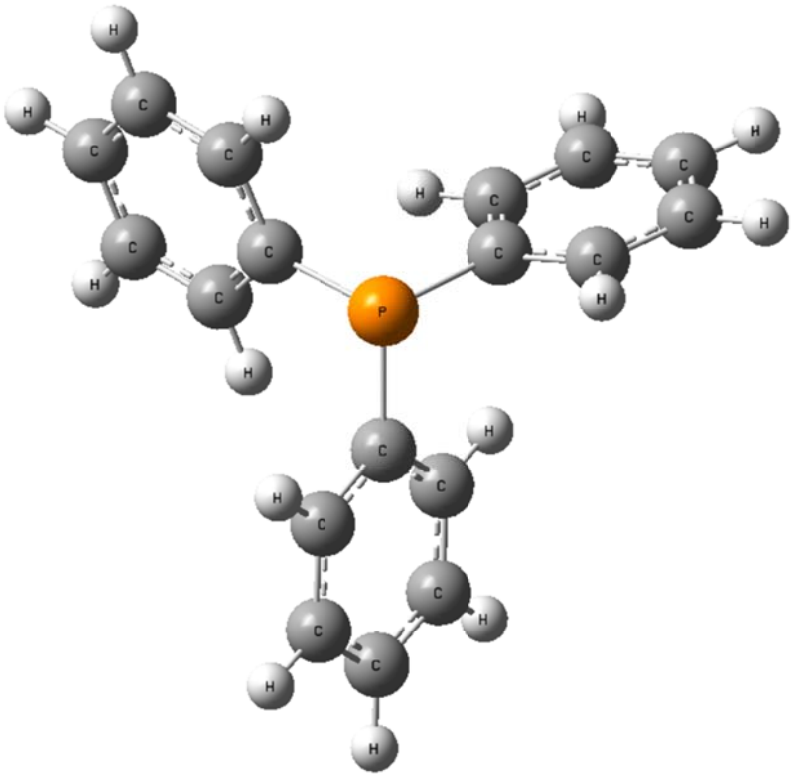
Table S3. Optimized atomic coordinate of **1a** at B3LYP/6-31G(d) level.



N_{imag} = 0

C	0	-3.135124	-0.207670	-0.000124
C	0	-1.727362	0.256013	0.000176
H	0	-1.542991	1.325049	0.001353
C	0	-0.724324	-0.643287	-0.000979
H	0	-0.981760	-1.701839	-0.002124
O	0	-3.494194	-1.368941	-0.001378
O	0	-3.981711	0.845152	0.001188
C	0	-5.378677	0.508488	0.001012
H	0	-5.908742	1.461006	0.002216
H	0	-5.631822	-0.073246	-0.889368
H	0	-5.631542	-0.075345	0.890096
C	0	0.646916	-0.293921	-0.000708
C	0	1.832611	-0.031715	-0.000471
C	0	3.219779	0.377018	-0.000307
O	0	3.593026	1.531929	-0.002056
O	0	4.039930	-0.693964	0.001424
C	0	5.444581	-0.381003	0.001417
H	0	5.953862	-1.344640	0.002951
H	0	5.708378	0.194765	-0.889563
H	0	5.707822	0.197307	0.890915

Table S4. Optimized atomic coordinate of **2a** at B3LYP/6-31G(d) level.

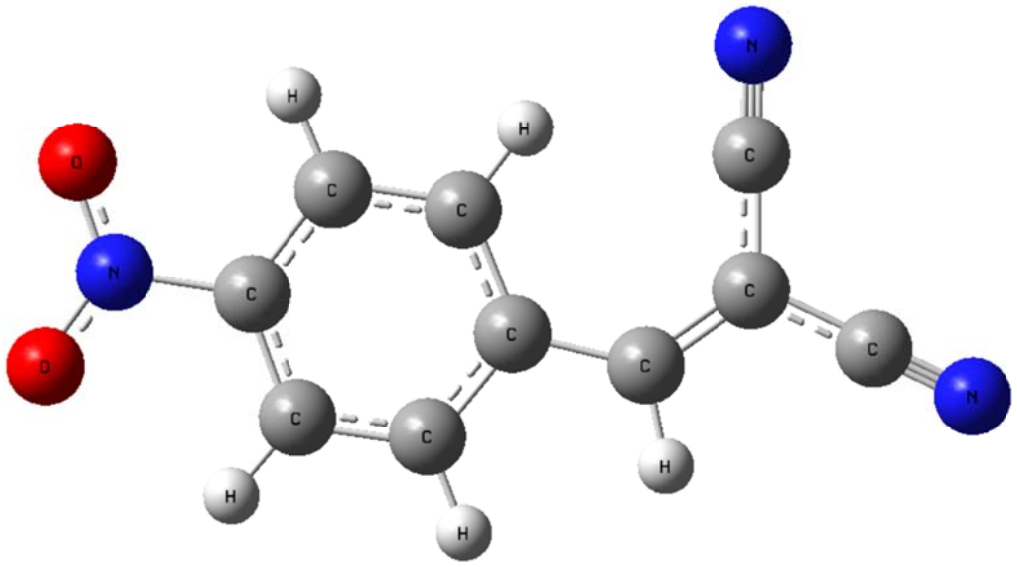


N_{imag} = 0

P	0	-0.000030	0.000133	1.206472
C	0	-1.407097	0.900930	0.402461
C	0	-1.851370	2.075628	1.032865
C	0	-2.067960	0.473326	-0.759251
C	0	-2.910976	2.814035	0.506452
H	0	-1.364898	2.410276	1.946369
C	0	-3.136561	1.206310	-1.280239
H	0	-1.749917	-0.437790	-1.257056
C	0	-3.558359	2.379104	-0.651967
H	0	-3.237896	3.722219	1.006303
H	0	-3.639103	0.859334	-2.179693
H	0	-4.390831	2.947468	-1.058473
C	0	-0.076699	-1.668899	0.402693
C	0	0.625565	-2.028145	-0.757865
C	0	-0.873566	-2.640303	1.032061
C	0	0.524957	-3.320106	-1.278756

H	0	1.256841	-1.297677	-1.254852
C	0	-0.983385	-3.927158	0.505706
H	0	-1.407844	-2.385772	1.944694
C	0	-0.281493	-4.271077	-0.651572
H	0	1.077890	-3.582389	-2.177327
H	0	-1.607758	-4.663819	1.004718
H	0	-0.357612	-5.276208	-1.058034
C	0	1.483807	0.768103	0.402585
C	0	2.723257	0.564834	1.032792
C	0	1.444096	1.554753	-0.758778
C	0	3.892678	1.113092	0.506503
H	0	2.769724	-0.024223	1.946020
C	0	2.613318	2.113567	-1.279600
H	0	0.496063	1.735413	-1.256447
C	0	3.839869	1.891760	-0.651552
H	0	4.842642	0.941559	1.006174
H	0	2.564216	2.722701	-2.178768
H	0	4.748432	2.328403	-1.057937

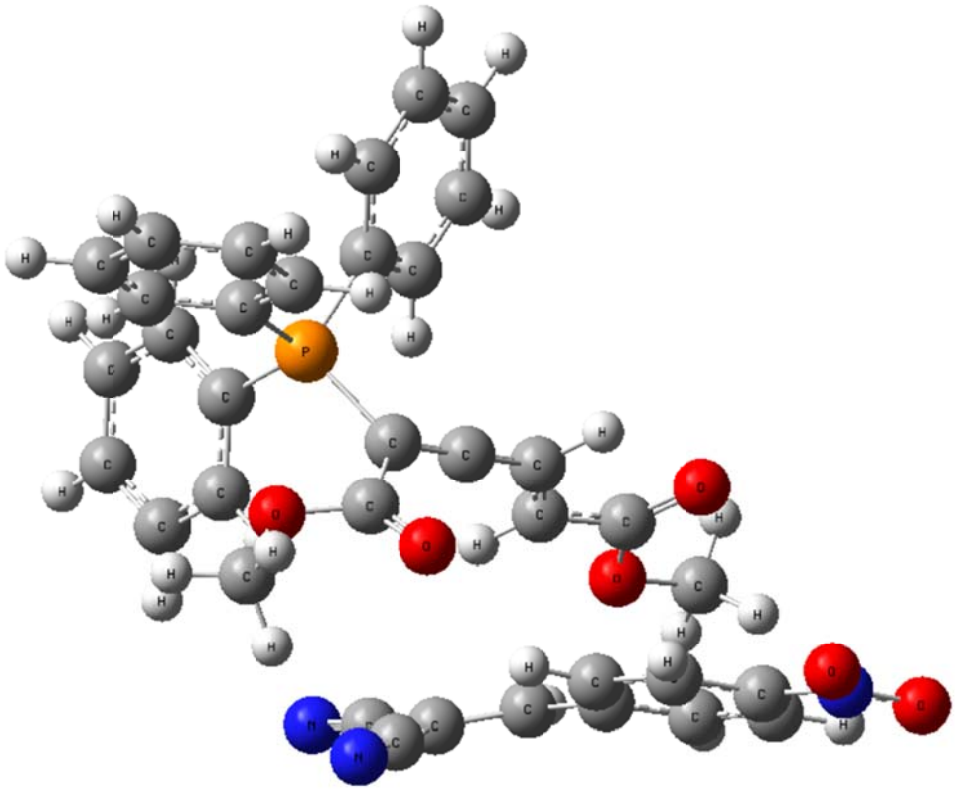
Table S5. Optimized atomic coordinate of **3a** at B3LYP/6-31G(d) level.



N_{imag} = 0

C	0	1.870187	-0.837354	0.000070
C	0	2.981821	-0.045487	-0.000001
C	0	2.982576	1.386917	-0.000129
C	0	4.278590	-0.660922	0.000046
N	0	3.004005	2.550211	-0.000267
N	0	5.327034	-1.164541	0.000090
H	0	2.079495	-1.904348	0.000139
C	0	0.452198	-0.503693	0.000057
C	0	-0.071985	0.807744	0.000135
C	0	-0.449675	-1.590840	-0.000028
C	0	-1.444703	1.018617	0.000122
H	0	0.585904	1.667046	0.000213
C	0	-1.823403	-1.390358	-0.000062
H	0	-0.061210	-2.605312	-0.000070
C	0	-2.300293	-0.082095	0.000015
H	0	-1.860551	2.018491	0.000197
H	0	-2.521866	-2.217721	-0.000147
N	0	-3.758184	0.145172	-0.000013
O	0	-4.485413	-0.846219	-0.000266
O	0	-4.150042	1.310064	0.000220

Table S6. Optimized atomic coordinate of [**Ib** + **3a**] at B3LYP/6-31G(d) level.



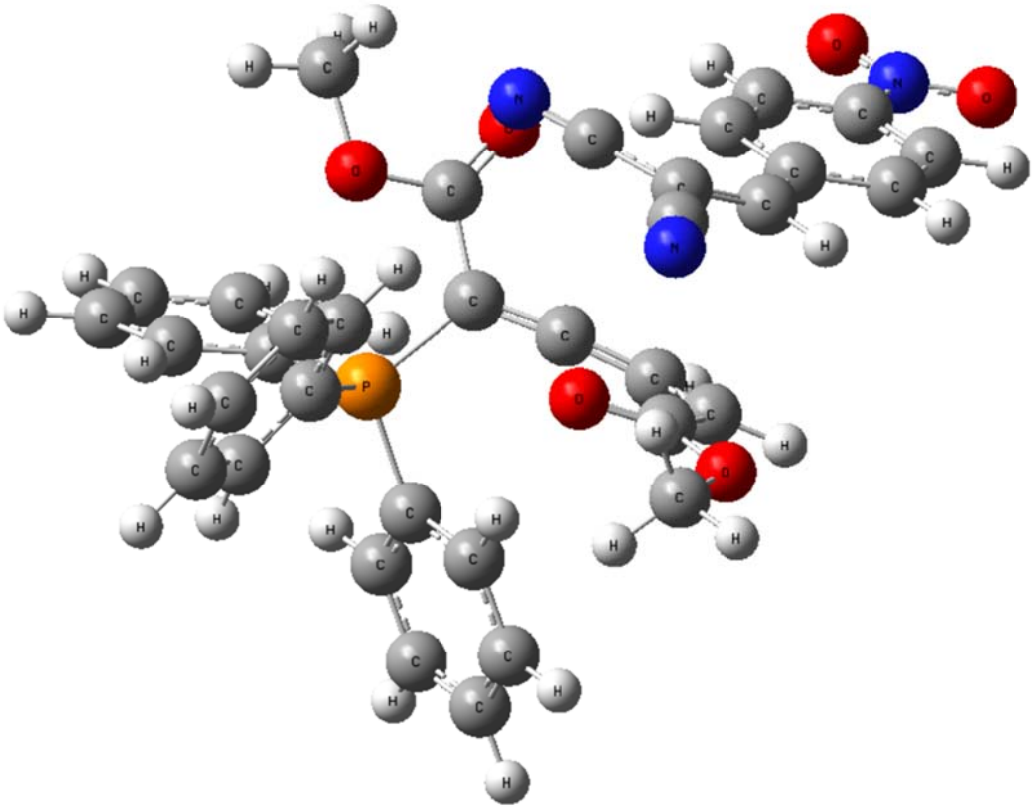
N_{imag} = 0

C	0	-3.074196	0.748851	1.829996
C	0	-2.151535	0.414761	2.794453
C	0	-0.056447	0.054510	-0.638302
C	0	-1.013511	0.899289	-1.044483
C	0	-1.563057	1.989114	-0.353142
H	0	-1.453510	0.696306	-2.025394
C	0	0.934710	-0.700038	-0.222681
P	0	2.668707	-0.081339	-0.416987
C	0	0.714101	-1.973420	0.544977
O	0	1.709955	-2.182766	1.435740
O	0	-0.237191	-2.709403	0.409198
C	0	1.577868	-3.365784	2.254407
H	0	1.545957	-4.256894	1.622562
H	0	2.464003	-3.375133	2.889298
H	0	0.666164	-3.301250	2.851312
C	0	2.770004	0.905194	-1.941324

C	0	2.033277	2.100668	-2.023216
C	0	3.542095	0.489178	-3.037153
C	0	2.063904	2.856442	-3.194117
H	0	1.436520	2.444290	-1.185790
C	0	3.570923	1.256242	-4.201681
H	0	4.121638	-0.425968	-2.985239
C	0	2.829961	2.436139	-4.282926
H	0	1.484573	3.772918	-3.252553
H	0	4.173040	0.928876	-5.044360
H	0	2.850879	3.029129	-5.192981
C	0	3.869593	-1.444424	-0.541321
C	0	5.052407	-1.465190	0.210080
C	0	3.569423	-2.519424	-1.396034
C	0	5.932365	-2.541762	0.093846
H	0	5.283383	-0.650978	0.888955
C	0	4.454514	-3.590319	-1.507860
H	0	2.644123	-2.525552	-1.966386
C	0	5.637322	-3.601875	-0.764618
H	0	6.847576	-2.551721	0.678858
H	0	4.215886	-4.417872	-2.169565
H	0	6.323819	-4.439414	-0.850134
C	0	3.102421	1.036190	0.952046
C	0	4.217286	1.885674	0.836767
C	0	2.297479	1.096139	2.098545
C	0	4.525484	2.770347	1.868230
H	0	4.829920	1.870026	-0.060378
C	0	2.599499	1.999807	3.118120
H	0	1.431396	0.451565	2.192003
C	0	3.714567	2.830804	3.005135
H	0	5.387101	3.425353	1.775563
H	0	1.944740	2.064772	3.981479
H	0	3.945917	3.536768	3.797774
C	0	-1.752797	-0.907012	3.163822

C	0	-1.474833	1.446286	3.521834
N	0	-1.389483	-1.952170	3.529204
N	0	-0.880753	2.260846	4.106361
H	0	-3.322671	1.803143	1.762058
H	0	-1.149805	2.333926	0.585953
C	0	-3.837931	-0.130289	0.955699
C	0	-3.453233	-1.450604	0.636483
C	0	-5.020142	0.389880	0.383810
C	0	-4.241012	-2.228339	-0.202708
H	0	-2.523277	-1.866136	1.003030
C	0	-5.818364	-0.383711	-0.444962
H	0	-5.307149	1.414801	0.598295
C	0	-5.417793	-1.690810	-0.722898
H	0	-3.950778	-3.237995	-0.464459
H	0	-6.729263	0.003549	-0.883296
N	0	-6.254251	-2.519230	-1.602060
O	0	-7.294440	-2.022878	-2.036949
O	0	-5.868637	-3.662166	-1.850734
C	0	-2.659951	2.703991	-0.941332
O	0	-3.187032	2.499596	-2.030975
O	0	-3.122653	3.695001	-0.092709
C	0	-4.173995	4.498991	-0.629120
H	0	-5.044798	3.891566	-0.895342
H	0	-4.433602	5.211611	0.156620
H	0	-3.843427	5.032216	-1.526404

Table S7. Optimized atomic coordinate of [**Ib** + **3a**]' at B3LYP/6-31G(d) level.



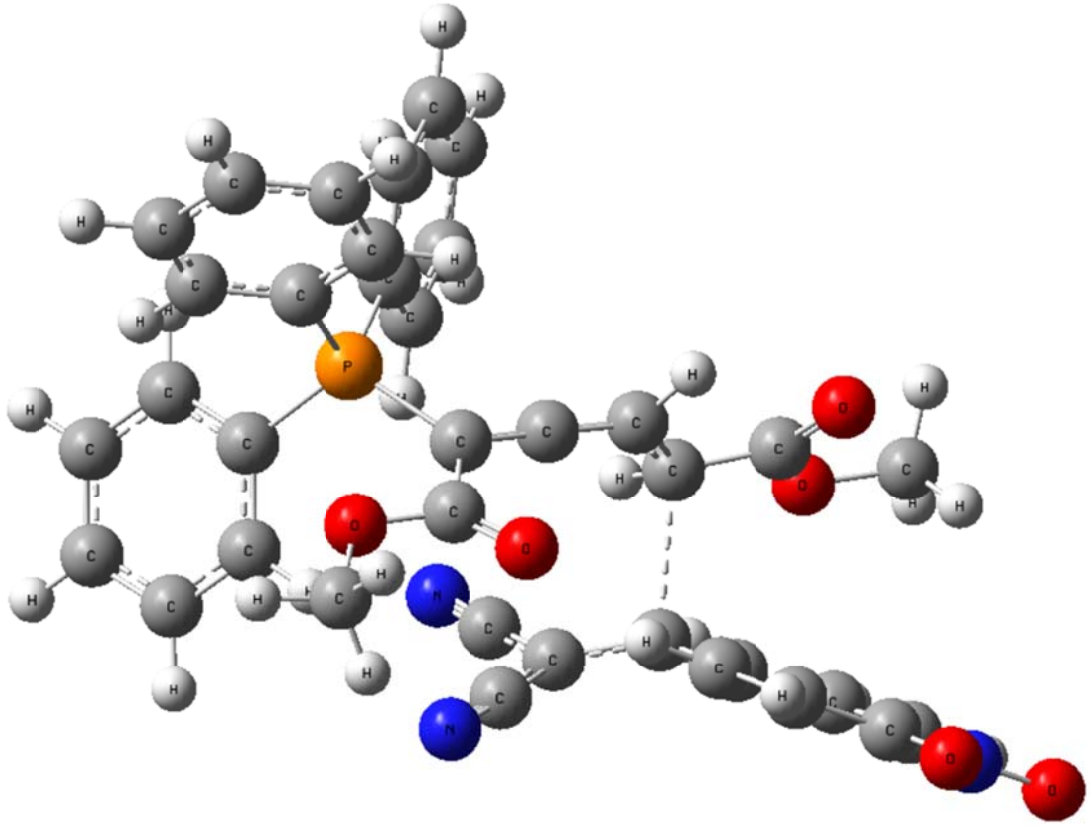
N_{imag} = 0

C	0	3.647231	1.815168	-0.707103
C	0	2.737195	2.247134	-1.638310
C	0	0.357374	-0.313259	0.699454
C	0	1.209212	0.113008	1.641925
C	0	1.729717	1.397505	1.891617
H	0	1.551920	-0.690889	2.299538
H	0	2.443938	1.530440	2.693668
C	0	-0.555740	-0.790196	-0.124180
P	0	-2.332940	-0.477251	0.217237
C	0	-0.214720	-1.487751	-1.406588
O	0	-1.236633	-1.409911	-2.289142
O	0	0.825769	-2.064243	-1.639759
C	0	-0.989652	-1.989926	-3.584248
H	0	-0.720938	-3.044153	-3.483385
H	0	-1.924846	-1.879781	-4.133670
H	0	-0.181403	-1.445992	-4.077088

C	0	1.159036	2.536947	1.261440
O	0	0.275701	2.516132	0.388468
O	0	1.667716	3.719973	1.737473
C	0	1.015284	4.907361	1.277917
H	0	1.497370	5.728902	1.812200
H	0	1.134882	5.041617	0.200333
H	0	-0.053868	4.883428	1.515421
C	0	-2.539511	-0.088498	1.981971
C	0	-1.990364	1.113290	2.462449
C	0	-3.228253	-0.944073	2.854337
C	0	-2.125815	1.440158	3.810669
H	0	-1.453169	1.777726	1.791273
C	0	-3.361263	-0.602884	4.200721
H	0	-3.663188	-1.868653	2.490298
C	0	-2.809061	0.586022	4.679200
H	0	-1.692213	2.364376	4.181023
H	0	-3.897910	-1.266942	4.872395
H	0	-2.912765	0.848157	5.728663
C	0	-3.318007	-1.967241	-0.157895
C	0	-4.506183	-1.917277	-0.899266
C	0	-2.834152	-3.207637	0.292309
C	0	-5.209231	-3.091664	-1.170554
H	0	-4.877162	-0.969427	-1.274143
C	0	-3.543075	-4.376600	0.019782
H	0	-1.900202	-3.262351	0.845292
C	0	-4.732455	-4.319842	-0.710175
H	0	-6.128743	-3.044718	-1.747117
H	0	-3.161193	-5.330959	0.370672
H	0	-5.281550	-5.232096	-0.925806
C	0	-2.974700	0.958126	-0.697635
C	0	-4.249575	1.462042	-0.383147
C	0	-2.189971	1.595239	-1.667688
C	0	-4.744636	2.573847	-1.060796

H	0	-4.847436	0.999055	0.397344
C	0	-2.691464	2.714325	-2.333694
H	0	-1.192229	1.240130	-1.892367
C	0	-3.965341	3.198884	-2.038274
H	0	-5.730586	2.959099	-0.816689
H	0	-2.074420	3.210347	-3.076614
H	0	-4.348496	4.072092	-2.559156
C	0	1.926906	1.429680	-2.486186
C	0	2.550264	3.654438	-1.830631
N	0	1.242070	0.826897	-3.210656
N	0	2.417017	4.796914	-2.012153
H	0	4.147098	2.614682	-0.167250
C	0	4.118346	0.478758	-0.383431
C	0	3.541740	-0.710613	-0.874315
C	0	5.242427	0.381864	0.470571
C	0	4.059670	-1.948846	-0.514936
H	0	2.672622	-0.693010	-1.515435
C	0	5.775863	-0.846624	0.823067
H	0	5.693639	1.290505	0.859566
C	0	5.171067	-2.003644	0.324168
H	0	3.599926	-2.861541	-0.871695
H	0	6.637864	-0.929812	1.472883
N	0	5.719053	-3.310889	0.704220
O	0	5.166920	-4.317866	0.258599
O	0	6.700675	-3.325993	1.450129

Table S8. Optimized atomic coordinate of **4a-TS** at B3LYP/6-31G(d) **l**evel.



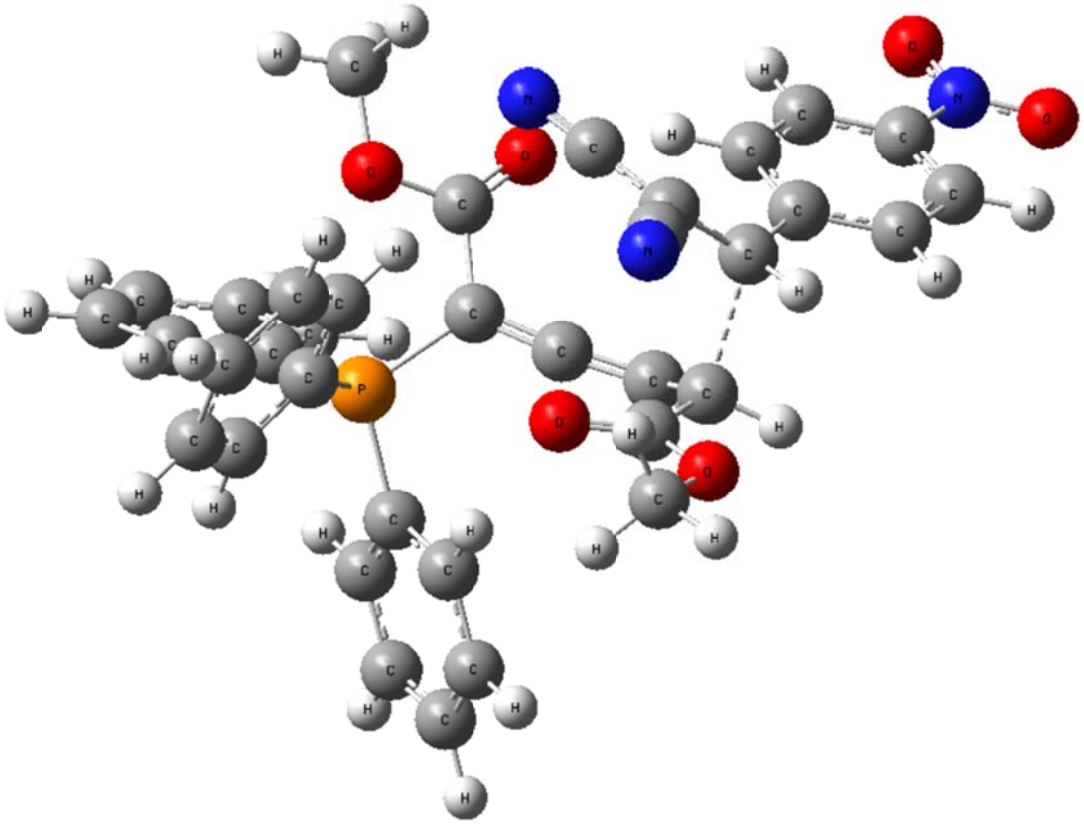
N_{imag} = 1, (-245.8497)

C	0	-2.665431	0.906006	1.425893
C	0	-1.573978	0.439278	2.205630
C	0	0.005745	0.228288	-0.743902
C	0	-0.985082	1.018953	-1.112121
C	0	-1.742801	1.947481	-0.317453
H	0	-1.295154	0.938809	-2.159439
C	0	0.949229	-0.638818	-0.421667
P	0	2.683122	-0.081473	-0.305361
C	0	0.617069	-2.087327	-0.183331
O	0	1.660491	-2.742815	0.367478
O	0	-0.427607	-2.611011	-0.492670
C	0	1.403808	-4.117477	0.725991
H	0	1.119162	-4.691478	-0.158723
H	0	2.340923	-4.486269	1.143020
H	0	0.602558	-4.149540	1.467022

C	0	2.750871	1.640770	-0.882355
C	0	2.210967	2.640631	-0.052598
C	0	3.300219	1.980513	-2.126395
C	0	2.217967	3.966488	-0.480396
H	0	1.786376	2.396811	0.918306
C	0	3.305100	3.312754	-2.541631
H	0	3.725084	1.215600	-2.768042
C	0	2.763297	4.303286	-1.721948
H	0	1.795598	4.734368	0.160596
H	0	3.733481	3.573230	-3.505139
H	0	2.766852	5.339239	-2.049214
C	0	3.730145	-1.121482	-1.374553
C	0	4.998424	-1.560815	-0.970655
C	0	3.233303	-1.493304	-2.635259
C	0	5.765957	-2.351037	-1.826643
H	0	5.381638	-1.300493	0.010159
C	0	4.008011	-2.280090	-3.486109
H	0	2.240746	-1.180262	-2.947188
C	0	5.274964	-2.708130	-3.083318
H	0	6.746339	-2.691817	-1.506538
H	0	3.617186	-2.565344	-4.458392
H	0	5.874804	-3.325948	-3.745527
C	0	3.318979	-0.059793	1.398557
C	0	4.519902	0.629190	1.652341
C	0	2.618509	-0.655928	2.456427
C	0	5.025492	0.692175	2.948421
H	0	5.049093	1.130593	0.846717
C	0	3.128090	-0.573628	3.753091
H	0	1.682293	-1.173055	2.287398
C	0	4.328943	0.090392	3.999769
H	0	5.952895	1.224491	3.138846
H	0	2.571436	-1.024586	4.568724
H	0	4.717476	0.152680	5.012348

C	0	-1.180284	-0.903333	2.414135
C	0	-0.674052	1.404910	2.729576
N	0	-0.773252	-1.975976	2.649069
N	0	0.092828	2.215214	3.083251
H	0	-3.023117	1.893057	1.699246
H	0	-1.216210	2.520703	0.435216
C	0	-3.707320	0.042472	0.843052
C	0	-3.446572	-1.236669	0.314198
C	0	-5.026995	0.535874	0.796863
C	0	-4.474629	-2.001099	-0.225510
H	0	-2.439387	-1.634314	0.294810
C	0	-6.062557	-0.220911	0.265479
H	0	-5.237227	1.526212	1.190422
C	0	-5.771047	-1.487991	-0.238199
H	0	-4.283408	-2.983482	-0.638855
H	0	-7.080441	0.147086	0.234451
N	0	-6.857311	-2.297119	-0.802355
O	0	-7.992600	-1.816831	-0.800438
O	0	-6.574869	-3.411303	-1.245837
C	0	-2.823607	2.628733	-1.017688
O	0	-3.262387	2.350288	-2.124760
O	0	-3.363807	3.622034	-0.244572
C	0	-4.460598	4.322807	-0.842356
H	0	-5.277891	3.637237	-1.083553
H	0	-4.781697	5.055719	-0.100162
H	0	-4.146092	4.826123	-1.761484

Table S9. Optimized atomic coordinate of **4a'-TS** at B3LYP/6-31G(d) level.



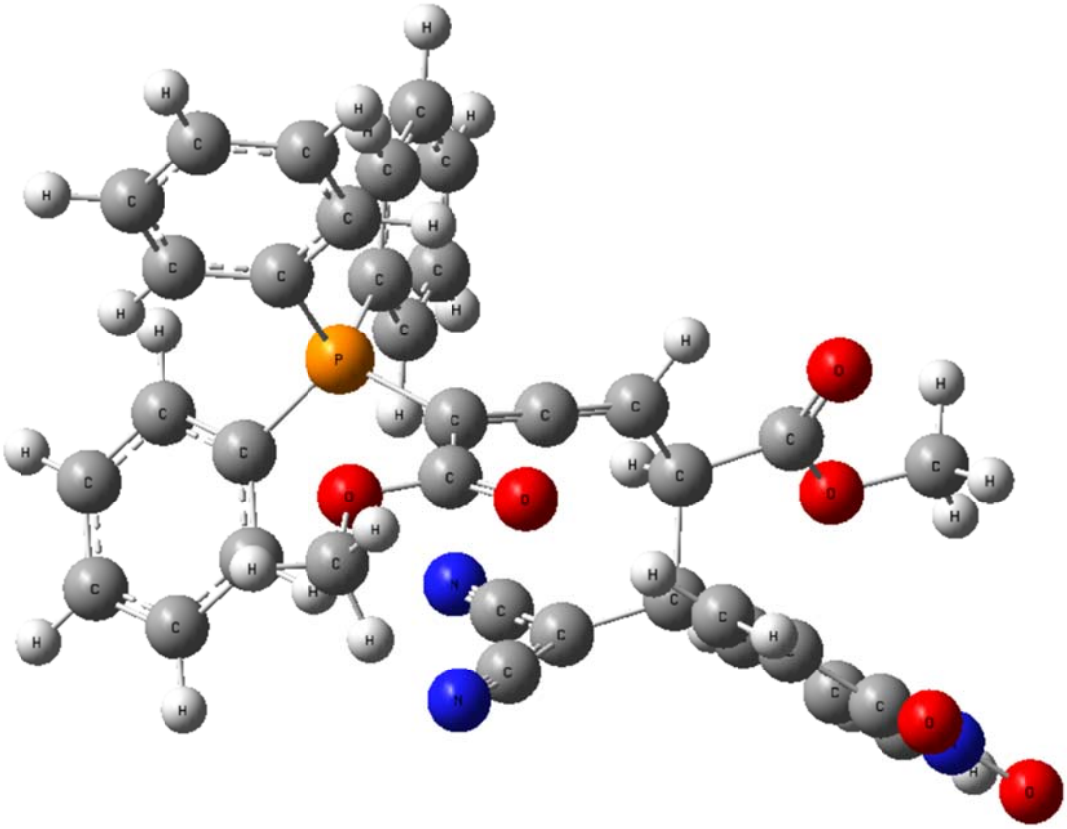
N_{imag} = 1, (-261.1550)

C	0	3.110595	1.735246	-0.420658
C	0	2.374767	1.969898	-1.619730
C	0	0.273333	-0.199204	0.746728
C	0	1.264270	0.326899	1.441856
C	0	1.862472	1.643169	1.303517
H	0	1.687772	-0.332409	2.202430
H	0	2.603199	1.880553	2.060503
C	0	-0.617827	-0.827306	0.003742
P	0	-2.392336	-0.516986	0.264152
C	0	-0.187917	-1.713615	-1.138136
O	0	-1.132214	-1.760466	-2.095112
O	0	0.854164	-2.326823	-1.167483
C	0	-0.778474	-2.498492	-3.285485
H	0	-0.498483	-3.521695	-3.024957
H	0	-1.674295	-2.486679	-3.906410

H	0	0.050665	-1.989105	-3.779029
C	0	0.962295	2.735255	0.957799
O	0	-0.110678	2.604894	0.373795
O	0	1.478652	3.942234	1.289824
C	0	0.729052	5.090019	0.853777
H	0	1.229084	5.947745	1.306056
H	0	0.755011	5.162855	-0.236798
H	0	-0.306956	5.026174	1.197880
C	0	-2.686262	0.009433	1.981085
C	0	-2.274292	1.295204	2.373762
C	0	-3.307982	-0.842425	2.907121
C	0	-2.482451	1.710661	3.688284
H	0	-1.785401	1.956216	1.664322
C	0	-3.511680	-0.413014	4.218464
H	0	-3.638031	-1.832103	2.610713
C	0	-3.098858	0.861370	4.609708
H	0	-2.160442	2.702843	3.990978
H	0	-3.996004	-1.074745	4.930739
H	0	-3.259935	1.193665	5.631589
C	0	-3.311062	-2.066278	-0.016696
C	0	-4.526571	-2.083246	-0.713073
C	0	-2.778569	-3.265831	0.484789
C	0	-5.207884	-3.287432	-0.894251
H	0	-4.933971	-1.166051	-1.125034
C	0	-3.465675	-4.464613	0.300636
H	0	-1.825138	-3.267813	1.006317
C	0	-4.681380	-4.476116	-0.387173
H	0	-6.147857	-3.294911	-1.438438
H	0	-3.046577	-5.389017	0.687094
H	0	-5.212921	-5.412087	-0.533700
C	0	-2.995943	0.803609	-0.823326
C	0	-4.250426	1.384991	-0.564407
C	0	-2.210358	1.267201	-1.888246

C	0	-4.722578	2.407149	-1.384386
H	0	-4.847408	1.056028	0.281874
C	0	-2.690491	2.298791	-2.695655
H	0	-1.232475	0.845412	-2.088560
C	0	-3.941804	2.863705	-2.449903
H	0	-5.691113	2.855640	-1.182659
H	0	-2.071914	2.665123	-3.508984
H	0	-4.306205	3.669695	-3.080765
C	0	1.753941	0.991631	-2.428465
C	0	2.106553	3.313701	-1.994417
N	0	1.200913	0.229901	-3.125696
N	0	1.904860	4.424288	-2.301035
H	0	3.568201	2.648594	-0.049672
C	0	3.958749	0.543777	-0.166522
C	0	3.674426	-0.744059	-0.655900
C	0	5.113009	0.718568	0.624189
C	0	4.509750	-1.817253	-0.362356
H	0	2.795465	-0.927985	-1.258239
C	0	5.958569	-0.341789	0.920464
H	0	5.350695	1.708138	1.005999
C	0	5.642121	-1.605834	0.422104
H	0	4.287893	-2.811168	-0.730410
H	0	6.849874	-0.209618	1.521199
N	0	6.520750	-2.736784	0.737171
O	0	6.218535	-3.844025	0.288993
O	0	7.512056	-2.517433	1.436879

Table S10. Optimized atomic coordinate of **4a-Ic** at B3LYP/6-31G(d) level.



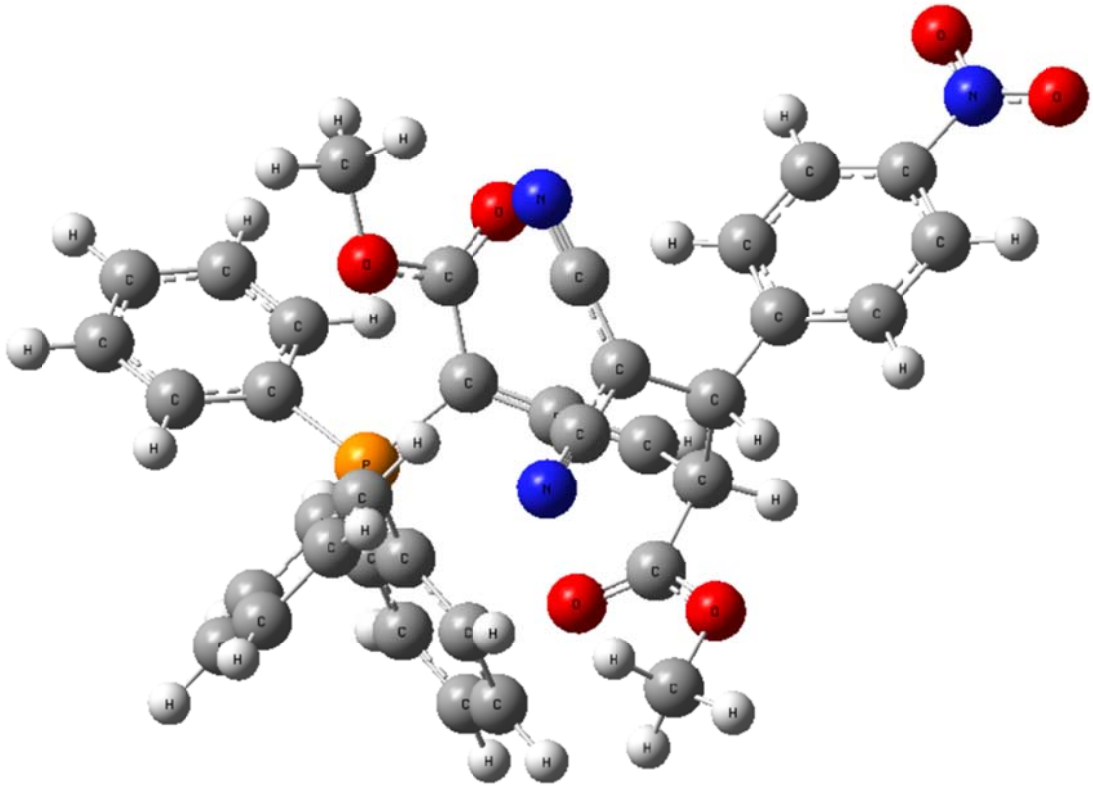
N_{imag} = 0

C	0	-2.511140	1.156687	1.022089
C	0	-1.449569	0.662780	1.994793
C	0	-0.025966	0.227465	-0.776501
C	0	-0.966038	1.059492	-1.125529
C	0	-1.809791	1.917734	-0.208332
H	0	-1.146909	1.207740	-2.191807
C	0	0.917677	-0.663267	-0.498064
P	0	2.625117	-0.104256	-0.242144
C	0	0.558238	-2.115406	-0.379882
O	0	1.545839	-2.812776	0.214237
O	0	-0.463464	-2.601197	-0.809949
C	0	1.218208	-4.179634	0.543122
H	0	0.937375	-4.729907	-0.357436
H	0	2.123702	-4.594059	0.986153
H	0	0.393242	-4.180525	1.258969

C	0	2.739030	1.638903	-0.746965
C	0	2.229643	2.621201	0.122037
C	0	3.300115	2.008094	-1.978686
C	0	2.280126	3.961924	-0.257225
H	0	1.787122	2.364660	1.083318
C	0	3.347638	3.353860	-2.342527
H	0	3.703742	1.255794	-2.648389
C	0	2.837430	4.329393	-1.484163
H	0	1.881957	4.714266	0.417059
H	0	3.786295	3.637351	-3.294903
H	0	2.877086	5.376741	-1.770777
C	0	3.701596	-1.112817	-1.314069
C	0	4.964350	-1.544962	-0.886339
C	0	3.248100	-1.452398	-2.599626
C	0	5.768759	-2.297590	-1.742363
H	0	5.314152	-1.310154	0.113156
C	0	4.058997	-2.202561	-3.449879
H	0	2.260697	-1.144478	-2.931828
C	0	5.320058	-2.624163	-3.022795
H	0	6.744166	-2.633998	-1.403161
H	0	3.700744	-2.464467	-4.441092
H	0	5.948143	-3.213404	-3.684857
C	0	3.178993	-0.178747	1.485067
C	0	4.369224	0.492000	1.826269
C	0	2.436089	-0.840197	2.471957
C	0	4.822548	0.472297	3.142467
H	0	4.928701	1.043693	1.075879
C	0	2.895491	-0.838997	3.790099
H	0	1.498960	-1.332672	2.238551
C	0	4.084988	-0.194038	4.125166
H	0	5.740099	0.991743	3.403130
H	0	2.304113	-1.336282	4.552637
H	0	4.432763	-0.194813	5.154420

C	0	-1.144089	-0.678769	2.234865
C	0	-0.564037	1.624827	2.501899
N	0	-0.811249	-1.790478	2.437582
N	0	0.179159	2.470183	2.846882
H	0	-3.041222	1.979301	1.514052
H	0	-1.160206	2.655926	0.278592
C	0	-3.581125	0.162902	0.603833
C	0	-3.302489	-1.063818	-0.020484
C	0	-4.925271	0.500697	0.840405
C	0	-4.332075	-1.920591	-0.401442
H	0	-2.284289	-1.374384	-0.212660
C	0	-5.966011	-0.342959	0.466956
H	0	-5.158207	1.442326	1.329557
C	0	-5.651621	-1.548632	-0.155836
H	0	-4.120248	-2.868116	-0.880938
H	0	-7.002154	-0.086456	0.649603
N	0	-6.740236	-2.447123	-0.561535
O	0	-7.897030	-2.089532	-0.330745
O	0	-6.437948	-3.506493	-1.112191
C	0	-2.818412	2.690925	-1.053363
O	0	-2.977845	2.573139	-2.251245
O	0	-3.529771	3.545823	-0.291806
C	0	-4.530562	4.310213	-0.988567
H	0	-5.269388	3.645449	-1.442918
H	0	-4.993800	4.941147	-0.229885
H	0	-4.069976	4.920521	-1.769501

Table S11. Optimized atomic coordinate of **4a'-Ic** at B3LYP/6-31G(d) level.



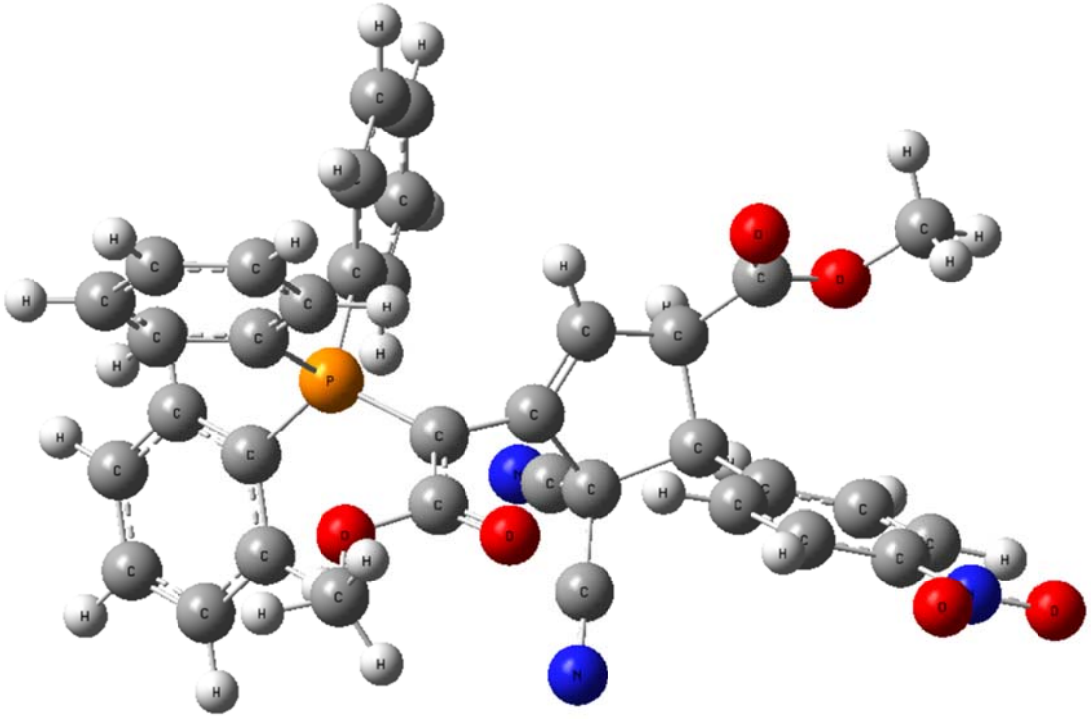
N_{imag} = 0

C	0	-2.794923	-1.481729	-0.359578
C	0	-1.989508	-1.226986	-1.619398
C	0	-0.182541	0.132045	0.745916
C	0	-1.128917	-0.481824	1.404312
C	0	-1.897402	-1.699791	0.956419
H	0	-1.398365	-0.054341	2.370721
H	0	-2.591278	-1.980351	1.757005
C	0	0.741872	0.835775	0.120769
P	0	2.504230	0.434136	0.288475
C	0	0.315512	1.952799	-0.809141
O	0	1.032494	1.929041	-1.937421
O	0	-0.542779	2.756974	-0.528061
C	0	0.641506	2.893087	-2.948427
H	0	0.691912	3.903774	-2.536533
H	0	1.363973	2.763583	-3.754027
H	0	-0.371860	2.651503	-3.275516

C	0	-0.976193	-2.900572	0.734973
O	0	0.237232	-2.870216	0.678512
O	0	-1.698441	-4.021228	0.596637
C	0	-0.966713	-5.190447	0.169339
H	0	-1.701292	-5.995536	0.150249
H	0	-0.558658	-5.010564	-0.828227
H	0	-0.163495	-5.415293	0.875161
C	0	2.880007	-0.077897	1.996090
C	0	2.423124	-1.331678	2.439253
C	0	3.612365	0.749321	2.862181
C	0	2.695292	-1.738204	3.745020
H	0	1.855633	-1.979299	1.778445
C	0	3.879920	0.327830	4.164416
H	0	3.980051	1.712378	2.526030
C	0	3.420926	-0.913536	4.607123
H	0	2.339538	-2.706263	4.085679
H	0	4.450360	0.969961	4.829246
H	0	3.632148	-1.239571	5.621817
C	0	3.438161	1.955860	-0.068072
C	0	4.554159	1.944328	-0.914754
C	0	3.021541	3.161994	0.521901
C	0	5.254596	3.126598	-1.157422
H	0	4.867150	1.024006	-1.395891
C	0	3.726231	4.338322	0.272797
H	0	2.140759	3.190112	1.157644
C	0	4.844724	4.320936	-0.564057
H	0	6.116299	3.112501	-1.818322
H	0	3.395493	5.268161	0.725886
H	0	5.389816	5.239943	-0.759651
C	0	2.976307	-0.916561	-0.817062
C	0	4.259731	-1.485474	-0.707496
C	0	2.048479	-1.435105	-1.729659
C	0	4.611658	-2.548601	-1.533889

H	0	4.970007	-1.114950	0.026930
C	0	2.403608	-2.517725	-2.536419
H	0	1.047329	-1.026825	-1.799451
C	0	3.683022	-3.064244	-2.444922
H	0	5.602148	-2.987494	-1.453501
H	0	1.652417	-2.939931	-3.196167
H	0	3.956524	-3.907897	-3.072676
C	0	-1.992551	-0.025880	-2.342524
C	0	-1.382622	-2.333363	-2.238878
N	0	-1.961267	0.965486	-2.972530
N	0	-0.864292	-3.272149	-2.722897
H	0	-3.276432	-2.459928	-0.464398
C	0	-3.909787	-0.487298	-0.070458
C	0	-3.700989	0.899796	0.026638
C	0	-5.208223	-0.981335	0.140311
C	0	-4.752116	1.760268	0.332109
H	0	-2.722093	1.326937	-0.151353
C	0	-6.269884	-0.136572	0.446836
H	0	-5.391377	-2.049591	0.059147
C	0	-6.023361	1.231060	0.544043
H	0	-4.597937	2.829840	0.402511
H	0	-7.271502	-0.515032	0.609051
N	0	-7.131162	2.134212	0.879797
O	0	-6.884398	3.337133	0.976845
O	0	-8.246075	1.637556	1.051334

Table S12. Optimized atomic coordinate of **4a** at B3LYP/6-31G(d) level.



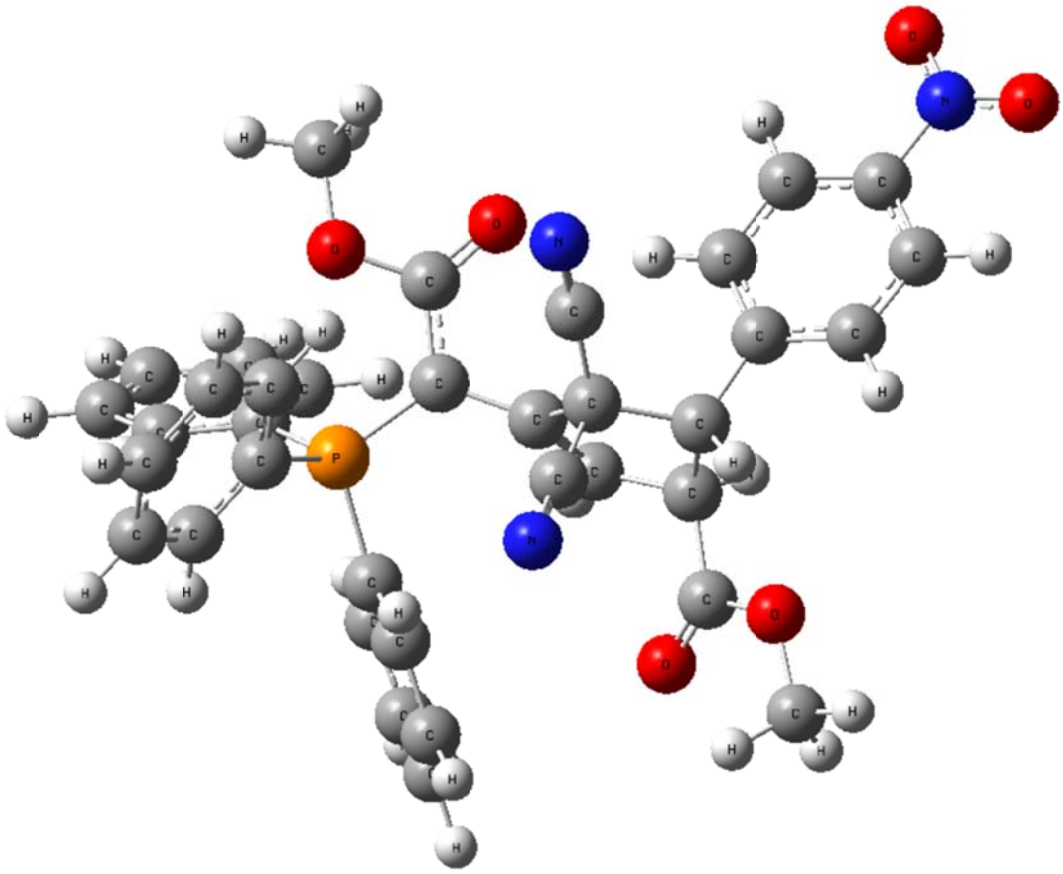
N_{imag} = 0

C	0	2.359502	1.077024	-1.138527
C	0	1.033019	0.304659	-1.518895
C	0	0.216795	0.278370	-0.170763
C	0	0.704870	1.247431	0.615124
C	0	1.835127	2.024507	0.003398
H	0	0.319762	1.483841	1.599635
C	0	-0.917198	-0.629219	0.040455
P	0	-2.568776	-0.086815	0.158215
C	0	-0.599821	-2.028219	0.191993
O	0	-1.708808	-2.840097	0.142350
O	0	0.522231	-2.495549	0.361619
C	0	-1.468103	-4.227594	0.405342
H	0	-1.056042	-4.368396	1.408936
H	0	-2.441761	-4.713609	0.324084
H	0	-0.768577	-4.642768	-0.324517
C	0	-2.635755	1.725212	0.422654
C	0	-2.503972	2.597691	-0.669802

C	0	-2.782785	2.255601	1.713438
C	0	-2.505623	3.977809	-0.466688
H	0	-2.391125	2.210225	-1.676304
C	0	-2.788839	3.637019	1.908679
H	0	-2.897569	1.594834	2.566294
C	0	-2.648416	4.499536	0.820337
H	0	-2.396218	4.642044	-1.319146
H	0	-2.906651	4.036695	2.911988
H	0	-2.654016	5.575181	0.974433
C	0	-3.426800	-0.853099	1.591349
C	0	-4.794630	-1.155377	1.571766
C	0	-2.682822	-1.107103	2.754167
C	0	-5.410677	-1.691695	2.703650
H	0	-5.379744	-0.990280	0.673622
C	0	-3.303241	-1.639940	3.883550
H	0	-1.616039	-0.903166	2.764603
C	0	-4.668824	-1.931415	3.860798
H	0	-6.470827	-1.927914	2.676071
H	0	-2.716986	-1.835327	4.777102
H	0	-5.150712	-2.351240	4.739519
C	0	-3.614308	-0.378023	-1.325785
C	0	-4.819093	0.319141	-1.519927
C	0	-3.185297	-1.294791	-2.294764
C	0	-5.587790	0.087338	-2.660191
H	0	-5.149938	1.055807	-0.793237
C	0	-3.957901	-1.521981	-3.434229
H	0	-2.249373	-1.824491	-2.157145
C	0	-5.158500	-0.834954	-3.617279
H	0	-6.515287	0.634349	-2.805290
H	0	-3.614593	-2.231270	-4.181798
H	0	-5.755040	-1.009552	-4.508515
C	0	1.251866	-0.991547	-2.184356
C	0	0.268441	1.135269	-2.478195

N	0	1.393687	-1.967920	-2.794752
N	0	-0.339883	1.825042	-3.187858
H	0	2.683132	1.675074	-1.992808
H	0	1.460306	2.942960	-0.475112
C	0	3.524361	0.189948	-0.727602
C	0	3.381525	-0.937040	0.098145
C	0	4.807159	0.546568	-1.175606
C	0	4.498050	-1.683172	0.469447
H	0	2.403336	-1.266331	0.433874
C	0	5.930249	-0.185762	-0.806712
H	0	4.928041	1.413662	-1.818618
C	0	5.756523	-1.294565	0.018414
H	0	4.399217	-2.559633	1.097537
H	0	6.922747	0.080537	-1.148140
N	0	6.937132	-2.076302	0.417198
O	0	8.036391	-1.703928	0.003870
O	0	6.759972	-3.053834	1.143230
C	0	2.895405	2.464550	1.000536
O	0	2.908688	2.188254	2.178593
O	0	3.821125	3.239321	0.394927
C	0	4.897086	3.689105	1.238889
H	0	5.458732	2.835125	1.625649
H	0	5.529009	4.307512	0.601179
H	0	4.506997	4.271590	2.077181

Table S13. Optimized atomic coordinate of **4a'** at B3LYP/6-31G(d) level.



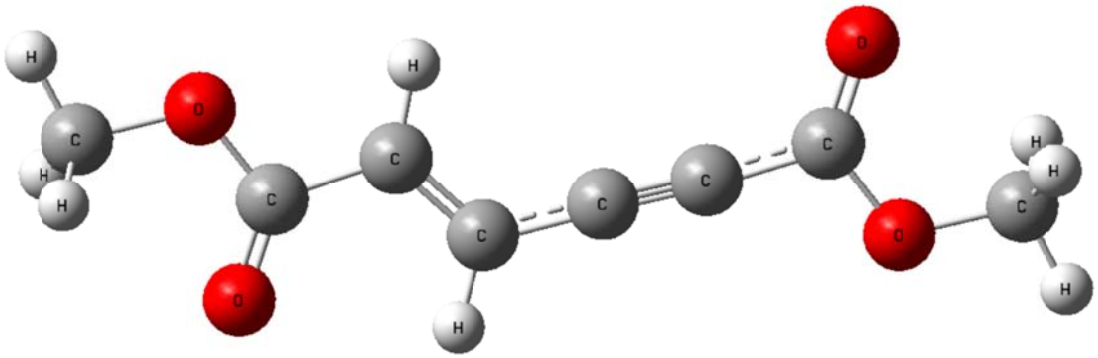
N_{imag} = 0

C	0	-2.559305	1.177268	0.484928
C	0	-1.276569	0.498104	1.110167
C	0	-0.374699	0.167555	-0.137181
C	0	-0.796741	0.921841	-1.160200
C	0	-2.013850	1.756976	-0.865464
H	0	-0.313444	0.944810	-2.129771
H	0	-2.776098	1.624139	-1.646788
C	0	0.743155	-0.783778	-0.057370
P	0	2.420988	-0.317836	-0.114526
C	0	0.373163	-2.173069	0.054277
O	0	1.431494	-2.991057	0.371934
O	0	-0.753461	-2.631740	-0.116619
C	0	1.142271	-4.393711	0.388865
H	0	0.803551	-4.734503	-0.594010
H	0	2.080823	-4.882155	0.656080

H	0	0.367724	-4.619096	1.126285
C	0	-1.710030	3.258606	-0.870597
O	0	-0.817487	3.772329	-1.506766
O	0	-2.602655	3.953349	-0.134026
C	0	-2.414064	5.380551	-0.119118
H	0	-3.216401	5.773863	0.505149
H	0	-1.438512	5.628642	0.305964
H	0	-2.478334	5.784239	-1.132657
C	0	2.603899	1.386115	-0.755490
C	0	2.434746	2.482147	0.105571
C	0	2.879321	1.612045	-2.112975
C	0	2.526309	3.781265	-0.392043
H	0	2.222355	2.330380	1.157995
C	0	2.974148	2.914657	-2.601669
H	0	3.026505	0.775480	-2.788061
C	0	2.795164	3.999997	-1.743421
H	0	2.381917	4.621282	0.280949
H	0	3.188786	3.078953	-3.653904
H	0	2.863220	5.013885	-2.127592
C	0	3.375529	-1.404694	-1.249175
C	0	4.719799	-1.726100	-1.021265
C	0	2.738793	-1.891430	-2.401233
C	0	5.418986	-2.511975	-1.938892
H	0	5.221460	-1.380264	-0.124071
C	0	3.441737	-2.673527	-3.316806
H	0	1.688592	-1.670016	-2.567398
C	0	4.784062	-2.983709	-3.088166
H	0	6.459766	-2.759712	-1.749401
H	0	2.937593	-3.047417	-4.203650
H	0	5.330203	-3.597114	-3.799584
C	0	3.299406	-0.312656	1.500809
C	0	4.511921	0.376852	1.672790
C	0	2.733420	-0.991782	2.587991

C	0	5.153018	0.370476	2.911264
H	0	4.947108	0.934697	0.848463
C	0	3.378589	-0.993831	3.825211
H	0	1.790173	-1.512335	2.465742
C	0	4.587688	-0.316679	3.987898
H	0	6.087357	0.910585	3.037197
H	0	2.929208	-1.519229	4.662977
H	0	5.084913	-0.315092	4.954059
C	0	-1.560906	-0.619549	2.027184
C	0	-0.555091	1.510307	1.915884
N	0	-1.750356	-1.440827	2.824518
N	0	0.017016	2.332946	2.503527
H	0	-2.883999	1.989431	1.135299
C	0	-3.745245	0.253368	0.265988
C	0	-3.617566	-1.046669	-0.250597
C	0	-5.027374	0.755450	0.540358
C	0	-4.750039	-1.821969	-0.488761
H	0	-2.639615	-1.478847	-0.444187
C	0	-6.166192	-0.006457	0.300759
H	0	-5.135384	1.758917	0.943460
C	0	-6.008271	-1.290240	-0.215918
H	0	-4.666010	-2.829418	-0.876946
H	0	-7.159616	0.371044	0.508555
N	0	-7.204803	-2.104757	-0.476324
O	0	-7.041415	-3.231367	-0.944153
O	0	-8.302321	-1.610224	-0.214866

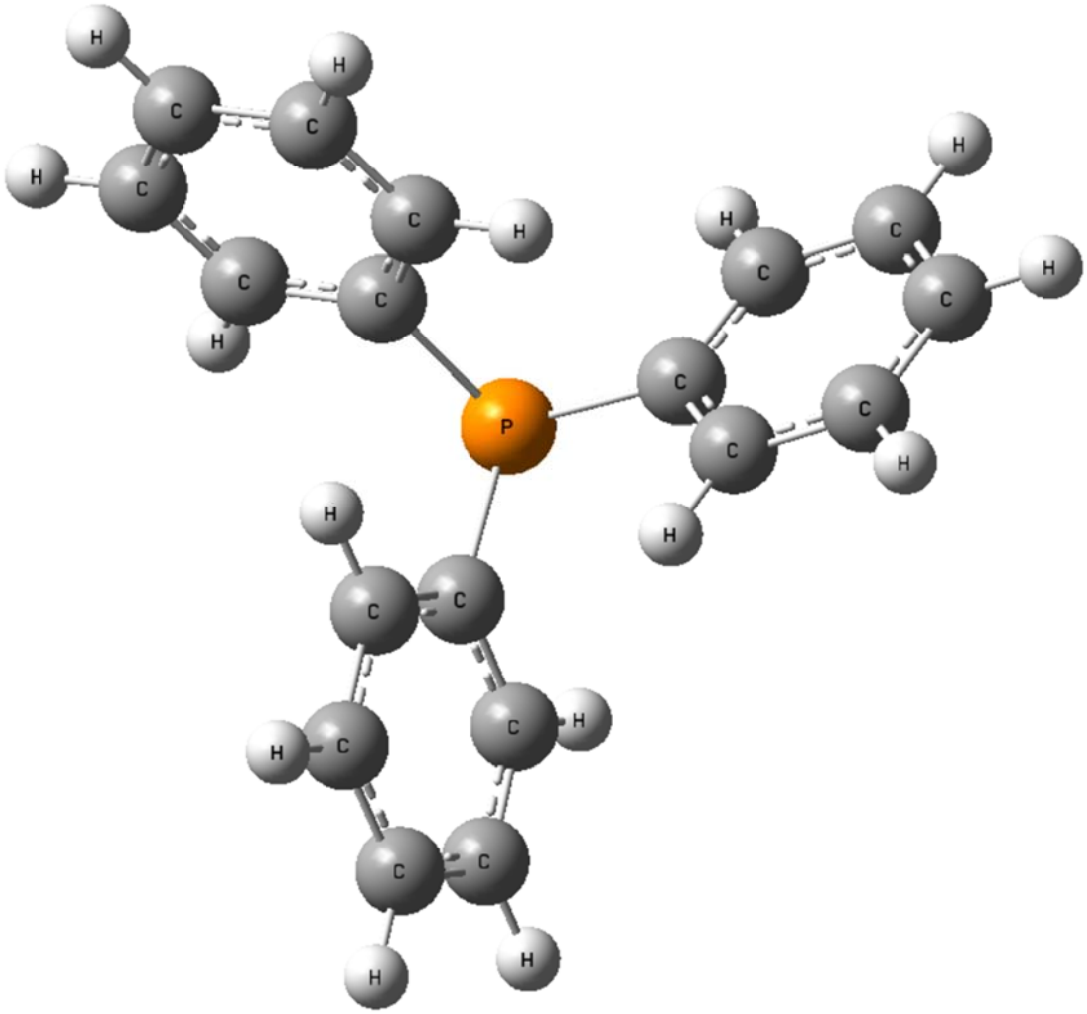
Table S14. Optimized atomic coordinate of **1a** at B3LYP-D3/6-31G(d**)** level.



N_{imag} = 0

C	0	-3.133160	-0.206279	-0.000097
C	0	-1.724518	0.254536	0.000167
H	0	-1.537693	1.323221	0.001327
C	0	-0.724825	-0.648385	-0.001007
H	0	-0.985336	-1.706341	-0.002139
O	0	-3.495099	-1.366929	-0.001327
O	0	-3.977325	0.848455	0.001223
C	0	-5.374995	0.510551	0.001079
H	0	-5.906557	1.462371	0.002260
H	0	-5.627292	-0.072924	-0.889018
H	0	-5.626984	-0.074962	0.889922
C	0	0.646343	-0.300610	-0.000781
C	0	1.830869	-0.034848	-0.000595
C	0	3.217016	0.375928	-0.000507
O	0	3.589557	1.531306	-0.001851
O	0	4.038273	-0.694372	0.001260
C	0	5.442723	-0.375786	0.001492
H	0	5.956467	-1.337189	0.003004
H	0	5.704131	0.202575	-0.889140
H	0	5.703304	0.204932	0.890832

Table S15. Optimized atomic coordinate of **2a** at B3LYP-D3/6-31G(d**)** level.

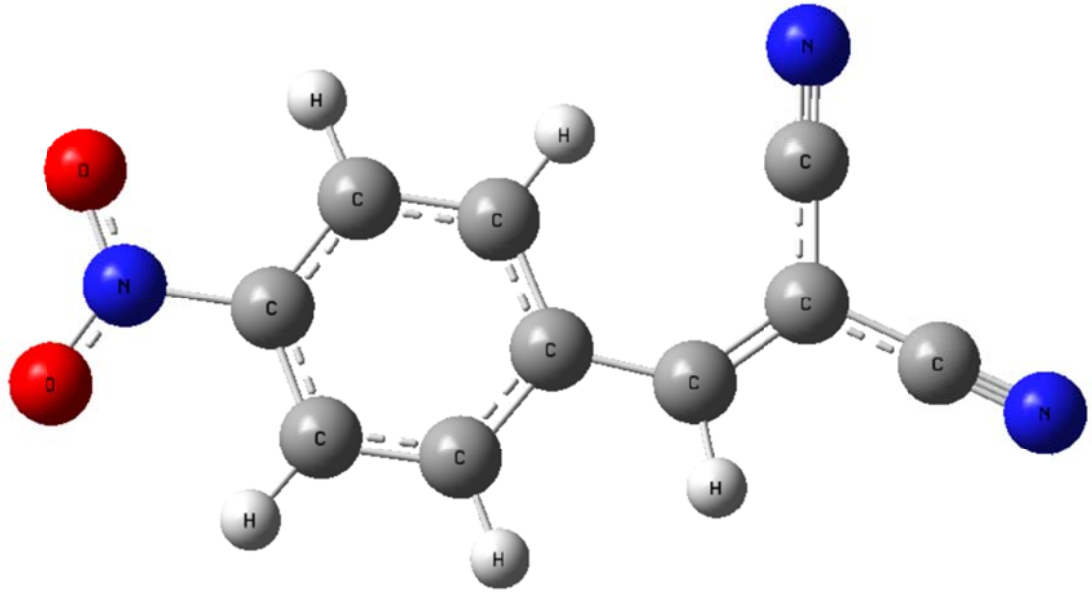


N_{imag} = 0

P	0	-0.000384	0.000388	-1.261249
C	0	-1.605140	0.420990	-0.437415
C	0	-2.776335	-0.087867	-1.022667
C	0	-1.717734	1.206159	0.720098
C	0	-4.025900	0.165892	-0.457447
H	0	-2.707817	-0.686759	-1.928173
C	0	-2.969878	1.469755	1.279251
H	0	-0.825386	1.612762	1.186230
C	0	-4.125745	0.948435	0.695184
H	0	-4.921464	-0.239450	-0.921252
H	0	-3.040840	2.081637	2.175042
H	0	-5.099186	1.154532	1.132402
C	0	1.166727	1.179290	-0.437269
C	0	1.902071	0.883829	0.720744

C	0	1.312822	2.447842	-1.022535
C	0	2.756730	1.835865	1.280358
H	0	1.806936	-0.092188	1.186819
C	0	2.157729	3.402561	-0.456910
H	0	0.760600	2.688256	-1.928378
C	0	2.884440	3.097368	0.696194
H	0	3.321352	1.591104	2.176558
H	0	2.255464	4.380702	-0.920743
H	0	3.549909	3.836922	1.133730
C	0	0.437830	-1.599923	-0.437950
C	0	1.468204	-2.356710	-1.020035
C	0	-0.189525	-2.093059	0.716250
C	0	1.873589	-3.565591	-0.454825
H	0	1.955658	-1.995578	-1.922967
C	0	0.208630	-3.309194	1.275321
H	0	-0.990862	-1.525887	1.179959
C	0	1.242109	-4.046401	0.694534
H	0	2.675656	-4.136023	-0.916072
H	0	-0.288676	-3.678913	2.168562
H	0	1.550680	-4.992374	1.131733

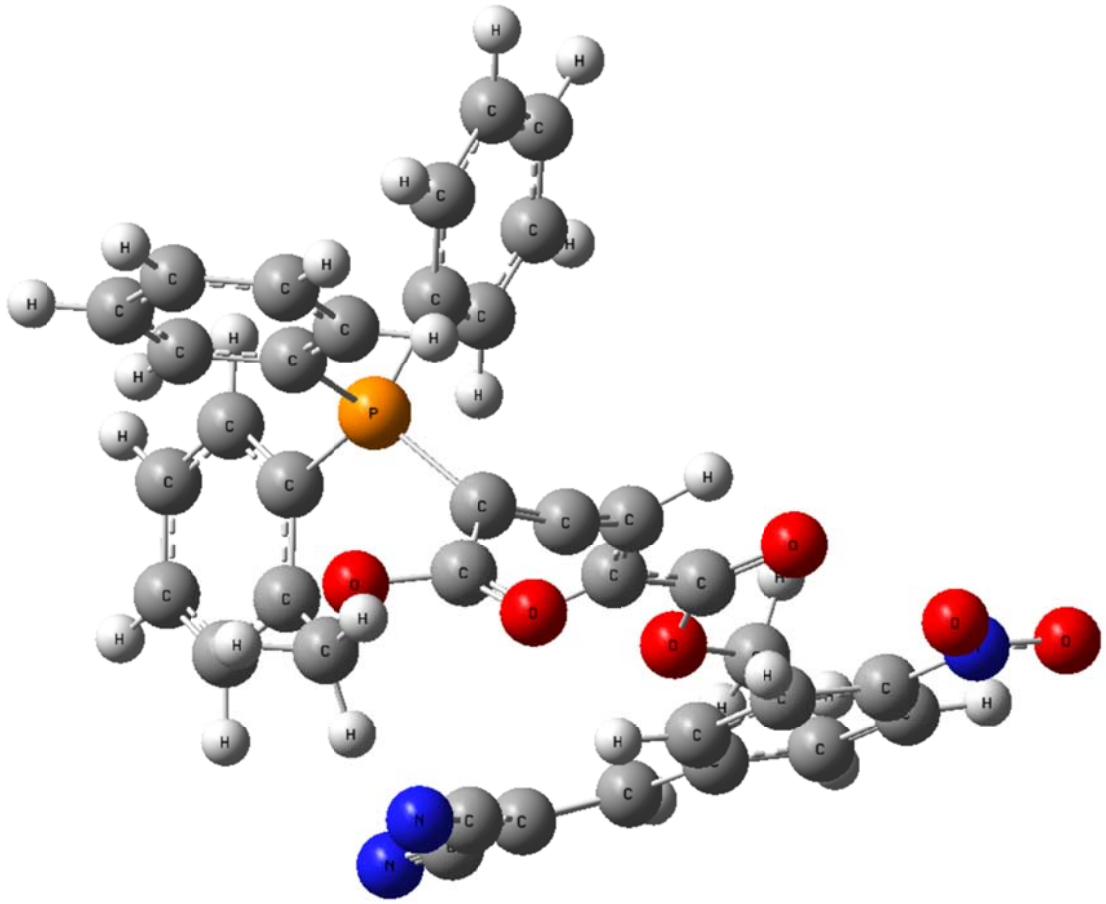
Table S16. Optimized atomic coordinate of **3a** at B3LYP-D3/6-31G(d**)** level.



N_{imag} = 0

C	0	1.870850	-0.839453	0.000044
C	0	2.981052	-0.045933	0.000003
C	0	2.982257	1.386117	-0.000064
C	0	4.278935	-0.658252	0.000016
N	0	3.000941	2.549334	-0.000117
N	0	5.328329	-1.159630	0.000026
H	0	2.082633	-1.906132	0.000077
C	0	0.452834	-0.506708	0.000039
C	0	-0.070460	0.805162	0.000101
C	0	-0.450115	-1.593132	-0.000029
C	0	-1.442684	1.017651	0.000088
H	0	0.587404	1.663961	0.000164
C	0	-1.823552	-1.391017	-0.000049
H	0	-0.064655	-2.608786	-0.000072
C	0	-2.299718	-0.082223	0.000010
H	0	-1.856526	2.018328	0.000138
H	0	-2.522132	-2.218259	-0.000107
N	0	-3.758675	0.146592	-0.000010
O	0	-4.487319	-0.843941	-0.000113
O	0	-4.149842	1.311882	0.000057

Table S17. Optimized atomic coordinate of [**Ib** + **3a**] at B3LYP-D3/6-31G(d) level.



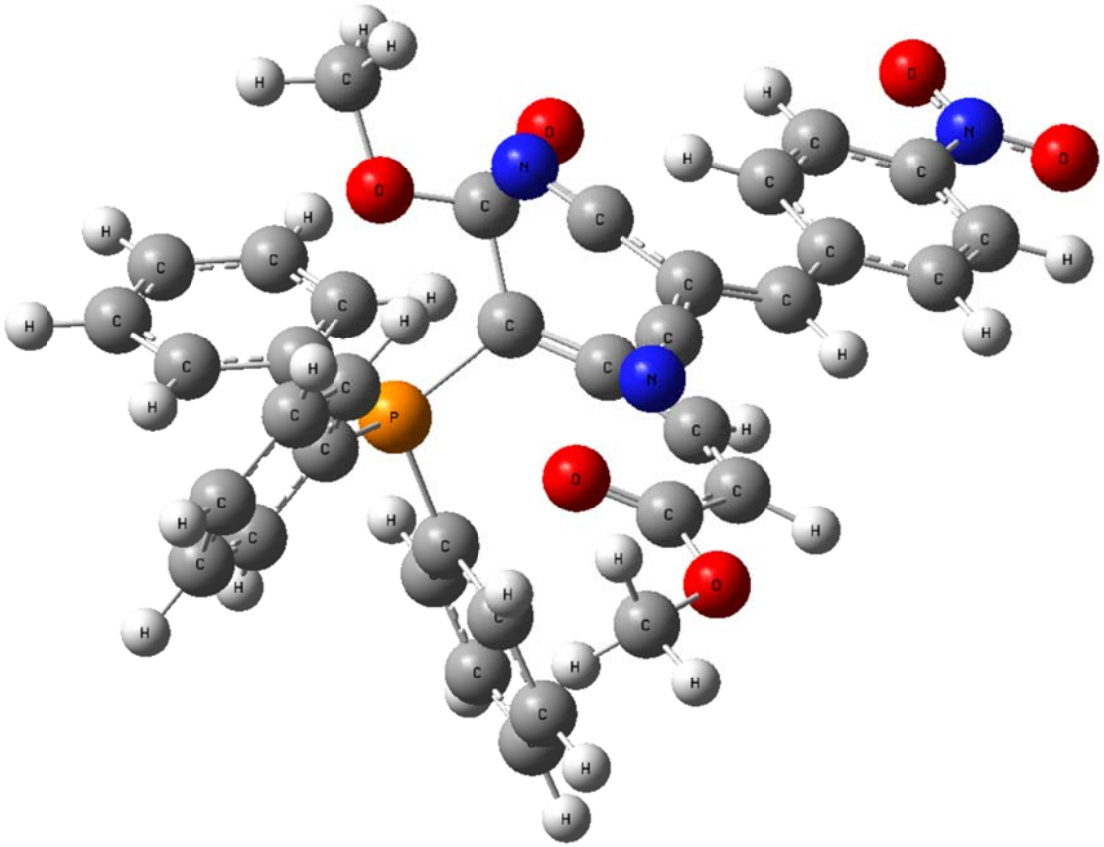
N_{imag} = 0

C	0	-3.002766	1.222100	1.628400
C	0	-2.023677	1.455466	2.571905
C	0	-0.361247	-0.450689	-0.415109
C	0	-1.222214	0.306060	-1.117020
C	0	-1.642128	1.604629	-0.800031
H	0	-1.741370	-0.177144	-1.948637
C	0	0.758570	-0.908451	0.107081
P	0	2.331187	-0.125895	-0.434368
C	0	0.782021	-1.847950	1.274996
O	0	1.864436	-1.611802	2.048195
O	0	-0.048891	-2.696220	1.511859
C	0	1.986115	-2.429070	3.229724
H	0	1.976710	-3.487397	2.956519
H	0	2.943073	-2.151359	3.672091
H	0	1.161103	-2.207334	3.908300
C	0	2.243952	0.222393	-2.212916
C	0	1.411317	1.261178	-2.664175

C	0	2.952969	-0.557605	-3.139939
C	0	1.282924	1.502083	-4.030755
H	0	0.857365	1.873342	-1.961496
C	0	2.821868	-0.303994	-4.504616
H	0	3.607202	-1.354575	-2.802933
C	0	1.985368	0.721257	-4.950791
H	0	0.627306	2.297403	-4.372157
H	0	3.374242	-0.908666	-5.217978
H	0	1.881845	0.912175	-6.015234
C	0	3.773935	-1.188497	-0.140415
C	0	4.975062	-0.666649	0.355050
C	0	3.659846	-2.563256	-0.403930
C	0	6.060708	-1.515979	0.572590
H	0	5.059967	0.392058	0.579387
C	0	4.749117	-3.404110	-0.186126
H	0	2.720670	-2.975796	-0.763923
C	0	5.950048	-2.880845	0.301414
H	0	6.991279	-1.110067	0.958657
H	0	4.657559	-4.467273	-0.388124
H	0	6.796418	-3.539074	0.475794
C	0	2.522575	1.465205	0.413792
C	0	3.309836	2.479504	-0.156748
C	0	1.845739	1.693594	1.621858
C	0	3.411723	3.715193	0.480228
H	0	3.815875	2.314246	-1.103582
C	0	1.940858	2.938815	2.242471
H	0	1.246237	0.911342	2.072282
C	0	2.720634	3.947049	1.672417
H	0	4.013467	4.502116	0.034755
H	0	1.383869	3.127179	3.154079
H	0	2.780245	4.919216	2.153069
C	0	-1.217772	0.478436	3.226108
C	0	-1.663644	2.800540	2.899005
N	0	-0.506729	-0.257721	3.785089
N	0	-1.323694	3.882196	3.168326
H	0	-3.497586	2.116527	1.261444
H	0	-1.129794	2.202252	-0.057932
C	0	-3.505627	-0.027532	1.092124

C	0	-2.892161	-1.279337	1.313335
C	0	-4.626741	0.033881	0.230537
C	0	-3.376935	-2.425610	0.695420
H	0	-2.023844	-1.376869	1.946788
C	0	-5.122793	-1.102912	-0.382624
H	0	-5.084734	0.994256	0.017842
C	0	-4.487115	-2.324829	-0.139047
H	0	-2.885484	-3.378666	0.841611
H	0	-5.970953	-1.061778	-1.053499
N	0	-4.997260	-3.535119	-0.798136
O	0	-5.995041	-3.422448	-1.512861
O	0	-4.399921	-4.594357	-0.599050
C	0	-2.785030	2.150967	-1.475641
O	0	-3.470890	1.599821	-2.332989
O	0	-3.096112	3.407141	-0.999197
C	0	-4.222519	4.023782	-1.626787
H	0	-5.128717	3.422647	-1.495420
H	0	-4.338025	4.994471	-1.140680
H	0	-4.053483	4.153729	-2.700825

Table S18. Optimized atomic coordinate of [**Ib** + **3a**]' at B3LYP-D3/6-31G(d) level.



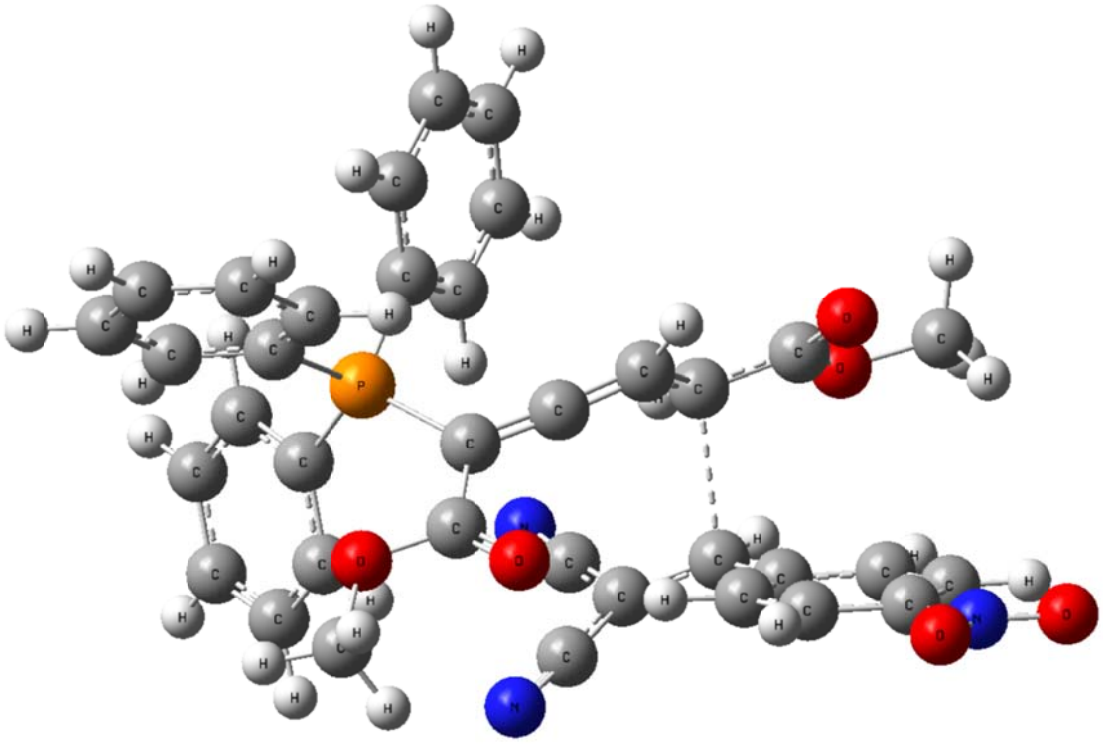
N_{imag} = 0

C	0	3.418759	1.884281	-0.743155
C	0	2.469368	2.338509	-1.626382
C	0	0.572517	-0.401006	0.503097
C	0	1.354152	0.050556	1.493081
C	0	1.768265	1.364967	1.782138
H	0	1.769761	-0.747329	2.113630
H	0	2.488237	1.531224	2.572607
C	0	-0.407258	-0.835363	-0.265734
P	0	-2.129297	-0.506585	0.242899
C	0	-0.193217	-1.442652	-1.616209
O	0	-1.278040	-1.246969	-2.397809
O	0	0.793455	-2.048074	-1.975439
C	0	-1.168701	-1.719376	-3.752953
H	0	-0.937429	-2.787616	-3.764692
H	0	-2.142367	-1.527806	-4.204463
H	0	-0.382587	-1.160910	-4.265257
C	0	1.089001	2.475708	1.211149
O	0	0.193713	2.413026	0.353107

O	0	1.505790	3.676333	1.722240
C	0	0.725979	4.813640	1.333310
H	0	1.156131	5.659289	1.873696
H	0	0.780876	4.988248	0.257003
H	0	-0.324153	4.680007	1.617636
C	0	-2.177908	-0.313060	2.045241
C	0	-1.686556	0.883931	2.591649
C	0	-2.650980	-1.331726	2.884733
C	0	-1.661013	1.048419	3.974751
H	0	-1.315524	1.664855	1.936161
C	0	-2.626300	-1.152895	4.267907
H	0	-3.040089	-2.254626	2.467157
C	0	-2.129805	0.033419	4.812298
H	0	-1.267490	1.969100	4.395141
H	0	-2.996228	-1.940310	4.918319
H	0	-2.109217	0.166845	5.890487
C	0	-3.188812	-1.914175	-0.211154
C	0	-4.479801	-1.736780	-0.724347
C	0	-2.670714	-3.209977	-0.053022
C	0	-5.250858	-2.849553	-1.061738
H	0	-4.876546	-0.737896	-0.873322
C	0	-3.447822	-4.316787	-0.390116
H	0	-1.658678	-3.351772	0.317353
C	0	-4.738927	-4.137410	-0.892963
H	0	-6.250681	-2.708233	-1.462198
H	0	-3.041529	-5.316697	-0.268847
H	0	-5.341629	-5.000782	-1.160350
C	0	-2.774223	1.031733	-0.461164
C	0	-3.942078	1.597705	0.078800
C	0	-2.086836	1.680101	-1.493962
C	0	-4.431168	2.795976	-0.436424
H	0	-4.453642	1.116669	0.908260
C	0	-2.578342	2.885161	-1.993708
H	0	-1.169317	1.268004	-1.890727
C	0	-3.747720	3.439594	-1.472488
H	0	-5.333861	3.233891	-0.020060
H	0	-2.031525	3.394381	-2.781341
H	0	-4.122545	4.381623	-1.863324

C	0	1.631300	1.547394	-2.468749
C	0	2.241344	3.745645	-1.748192
N	0	0.925413	0.966954	-3.191651
N	0	2.065948	4.889986	-1.874142
H	0	3.922449	2.668037	-0.184497
C	0	3.893869	0.539450	-0.480100
C	0	3.338443	-0.616699	-1.062422
C	0	4.959443	0.385886	0.439554
C	0	3.800656	-1.881360	-0.715645
H	0	2.531927	-0.554393	-1.775355
C	0	5.437981	-0.865438	0.781939
H	0	5.394990	1.268466	0.900014
C	0	4.841019	-1.992511	0.201797
H	0	3.340249	-2.764569	-1.138669
H	0	6.248955	-0.992856	1.487729
N	0	5.322184	-3.325681	0.582041
O	0	4.773243	-4.304368	0.072617
O	0	6.247810	-3.392039	1.394759

Table S19. Optimized atomic coordinate of **4a-TS** at B3LYP-D3/6-31G(d) level.



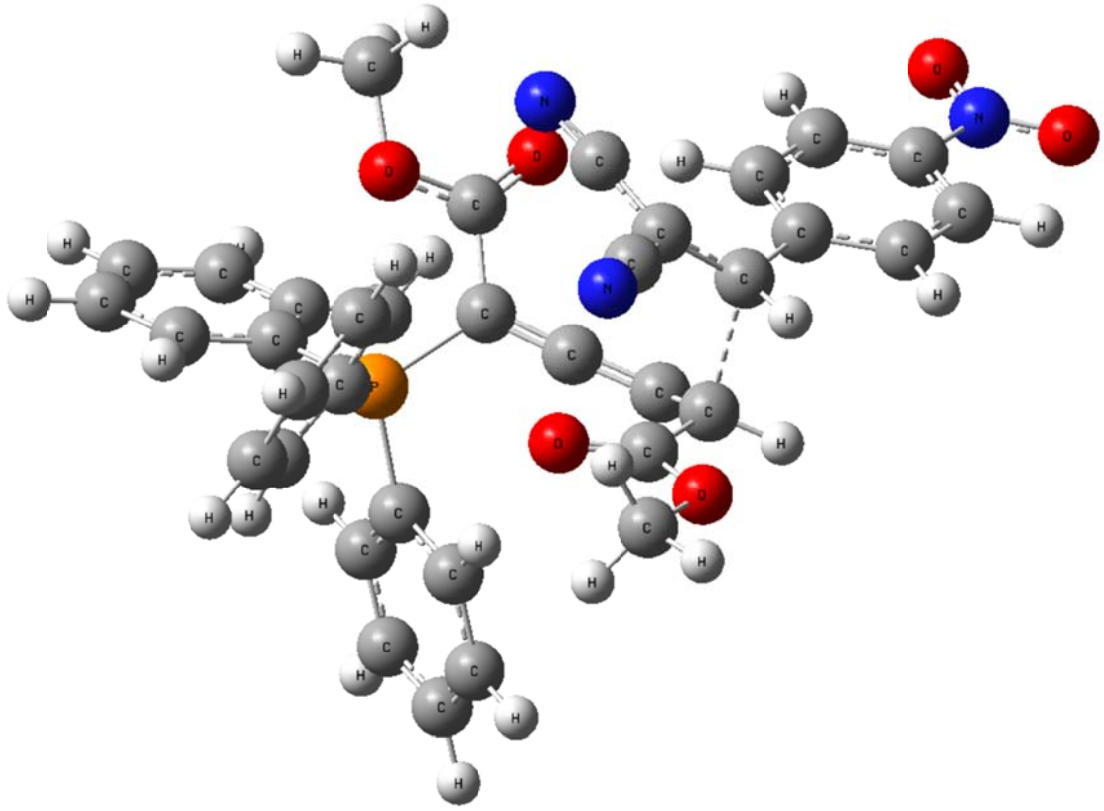
N_{imag} = 1, (-153.1849)

C	0	-2.521695	0.865234	1.562111
C	0	-1.374702	0.459636	2.272753
C	0	-0.110168	0.017008	-0.741706
C	0	-1.061476	0.842819	-1.143680
C	0	-1.692130	1.869314	-0.379801
H	0	-1.456876	0.676624	-2.150380
C	0	0.890289	-0.760714	-0.376613
P	0	2.572169	-0.060479	-0.355768
C	0	0.677764	-2.190052	0.026133
O	0	1.794409	-2.698287	0.591285
O	0	-0.333154	-2.822962	-0.171859
C	0	1.663722	-4.033769	1.121549
H	0	1.395764	-4.731429	0.324216
H	0	2.642102	-4.275153	1.537270
H	0	0.892779	-4.035553	1.895191
C	0	2.464269	1.567394	-1.142063
C	0	1.889248	2.618486	-0.405869
C	0	2.856182	1.764310	-2.472661
C	0	1.700159	3.856630	-1.014725
H	0	1.585055	2.475512	0.628193

C	0	2.667728	3.011632	-3.068586
H	0	3.303682	0.954447	-3.040395
C	0	2.087278	4.053528	-2.343024
H	0	1.245738	4.664332	-0.449158
H	0	2.972852	3.166791	-4.099324
H	0	1.935795	5.021076	-2.813247
C	0	3.703765	-1.123052	-1.297146
C	0	5.037774	-1.303441	-0.908259
C	0	3.211814	-1.770551	-2.441784
C	0	5.876265	-2.116980	-1.670170
H	0	5.416298	-0.823955	-0.011367
C	0	4.057428	-2.578985	-3.199406
H	0	2.170932	-1.652970	-2.730987
C	0	5.389403	-2.751412	-2.814835
H	0	6.908949	-2.258980	-1.365078
H	0	3.673505	-3.080440	-4.082877
H	0	6.045319	-3.386590	-3.403342
C	0	3.203201	0.229371	1.318637
C	0	4.272075	1.129904	1.479589
C	0	2.617526	-0.372869	2.439679
C	0	4.760934	1.404101	2.754245
H	0	4.703557	1.631451	0.617838
C	0	3.106077	-0.078704	3.712163
H	0	1.782509	-1.051657	2.334732
C	0	4.176024	0.801336	3.871301
H	0	5.584479	2.101531	2.876262
H	0	2.632729	-0.532240	4.577439
H	0	4.547261	1.030951	4.866030
C	0	-0.951231	-0.863656	2.545445
C	0	-0.442524	1.461113	2.657606
N	0	-0.520316	-1.913033	2.830351
N	0	0.349574	2.291721	2.880117
H	0	-2.858244	1.876759	1.760520
H	0	-1.110064	2.438617	0.331474
C	0	-3.531969	-0.014916	0.975199
C	0	-3.245990	-1.318978	0.523254
C	0	-4.833754	0.496519	0.791340
C	0	-4.234142	-2.089129	-0.076693

H	0	-2.248516	-1.729853	0.603045
C	0	-5.828897	-0.266505	0.199547
H	0	-5.054711	1.510733	1.110542
C	0	-5.515340	-1.558279	-0.225334
H	0	-4.021001	-3.088178	-0.435577
H	0	-6.831301	0.116593	0.056261
N	0	-6.560595	-2.373774	-0.855605
O	0	-7.685625	-1.881735	-0.966915
O	0	-6.256732	-3.505372	-1.237587
C	0	-2.870988	2.481388	-0.949369
O	0	-3.468891	2.122416	-1.955541
O	0	-3.325758	3.507948	-0.156272
C	0	-4.530348	4.129100	-0.617980
H	0	-5.343644	3.399948	-0.688841
H	0	-4.768429	4.898246	0.119146
H	0	-4.385143	4.579112	-1.605083

Table S20. Optimized atomic coordinate of **4a'-TS** at B3LYP-D3/6-31G(d) level.



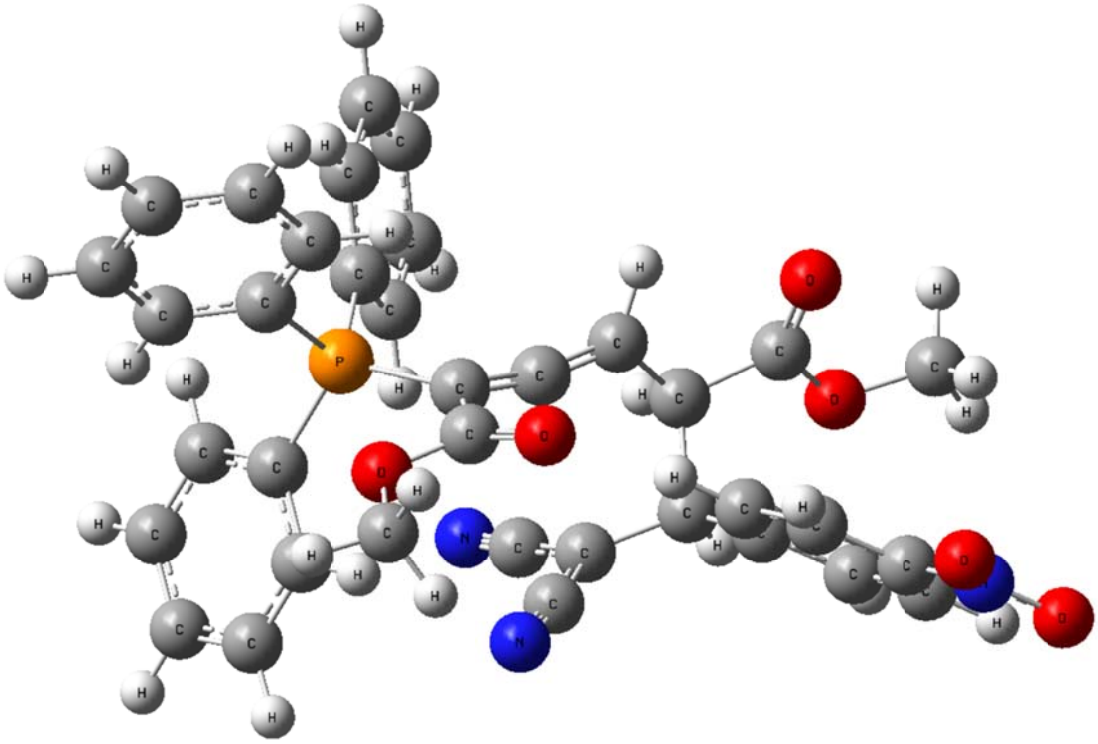
N_{imag} = 1, (-232.6053)

C	0	2.901050	1.688694	-0.542942
C	0	2.068405	1.734251	-1.701514
C	0	0.329099	-0.299944	0.790844
C	0	1.270416	0.301235	1.488480
C	0	1.804636	1.634718	1.257105
H	0	1.705486	-0.286427	2.298264
H	0	2.578454	1.942253	1.953366
C	0	-0.568504	-0.944221	0.074616
P	0	-2.320648	-0.514150	0.289674
C	0	-0.166210	-1.888302	-1.026236
O	0	-1.106484	-1.924217	-1.984766
O	0	0.844171	-2.554131	-1.017151
C	0	-0.817411	-2.769289	-3.119103
H	0	-0.633236	-3.793394	-2.784262
H	0	-1.708389	-2.719095	-3.745031
H	0	0.055469	-2.372335	-3.638788
C	0	0.841361	2.666883	0.903780
O	0	-0.258159	2.458045	0.397345

O	0	1.328270	3.913250	1.105266
C	0	0.479317	4.985676	0.654070
H	0	1.011377	5.901535	0.914944
H	0	0.327746	4.918825	-0.426111
H	0	-0.488251	4.947104	1.164232
C	0	-2.632378	-0.056350	2.018973
C	0	-2.234347	1.213976	2.469223
C	0	-3.232086	-0.963689	2.906350
C	0	-2.433557	1.560745	3.804676
H	0	-1.767208	1.911969	1.782773
C	0	-3.425732	-0.603117	4.239215
H	0	-3.553771	-1.941277	2.563446
C	0	-3.025921	0.656803	4.689237
H	0	-2.123321	2.541869	4.152541
H	0	-3.892836	-1.305858	4.923079
H	0	-3.179646	0.934801	5.728311
C	0	-3.353308	-1.958001	-0.097281
C	0	-4.567751	-1.809443	-0.777510
C	0	-2.921271	-3.233285	0.300461
C	0	-5.351544	-2.932100	-1.047089
H	0	-4.892272	-0.827947	-1.108386
C	0	-3.709630	-4.349213	0.027760
H	0	-1.966447	-3.355829	0.805308
C	0	-4.925781	-4.198874	-0.644430
H	0	-6.291482	-2.815528	-1.578645
H	0	-3.370491	-5.335210	0.331484
H	0	-5.536481	-5.070832	-0.860630
C	0	-2.739857	0.894470	-0.758685
C	0	-3.881257	1.660037	-0.466135
C	0	-1.881481	1.267869	-1.801462
C	0	-4.160750	2.793350	-1.226411
H	0	-4.528744	1.390963	0.364062
C	0	-2.157506	2.417513	-2.538812
H	0	-0.994459	0.689479	-2.025700
C	0	-3.293576	3.175998	-2.254114
H	0	-5.040392	3.389517	-1.001044
H	0	-1.460129	2.734936	-3.306910
H	0	-3.497456	4.077700	-2.824748

C	0	1.626390	0.631280	-2.461996
C	0	1.551860	2.980597	-2.142035
N	0	1.212792	-0.231550	-3.136732
N	0	1.123227	3.999702	-2.524568
H	0	3.297007	2.667991	-0.284952
C	0	3.850425	0.587495	-0.248844
C	0	3.581212	-0.764647	-0.530107
C	0	5.061271	0.910777	0.394426
C	0	4.489183	-1.757942	-0.180406
H	0	2.658626	-1.061106	-1.007801
C	0	5.979858	-0.069922	0.744031
H	0	5.282671	1.950364	0.621561
C	0	5.678606	-1.400926	0.452915
H	0	4.278451	-2.799634	-0.387794
H	0	6.914736	0.173981	1.233120
N	0	6.635270	-2.448092	0.830841
O	0	6.343151	-3.616645	0.571323
O	0	7.677338	-2.100751	1.391251

Table S21. Optimized atomic coordinate of **4a-Ic** at B3LYP-D3/6-31G(d) level.



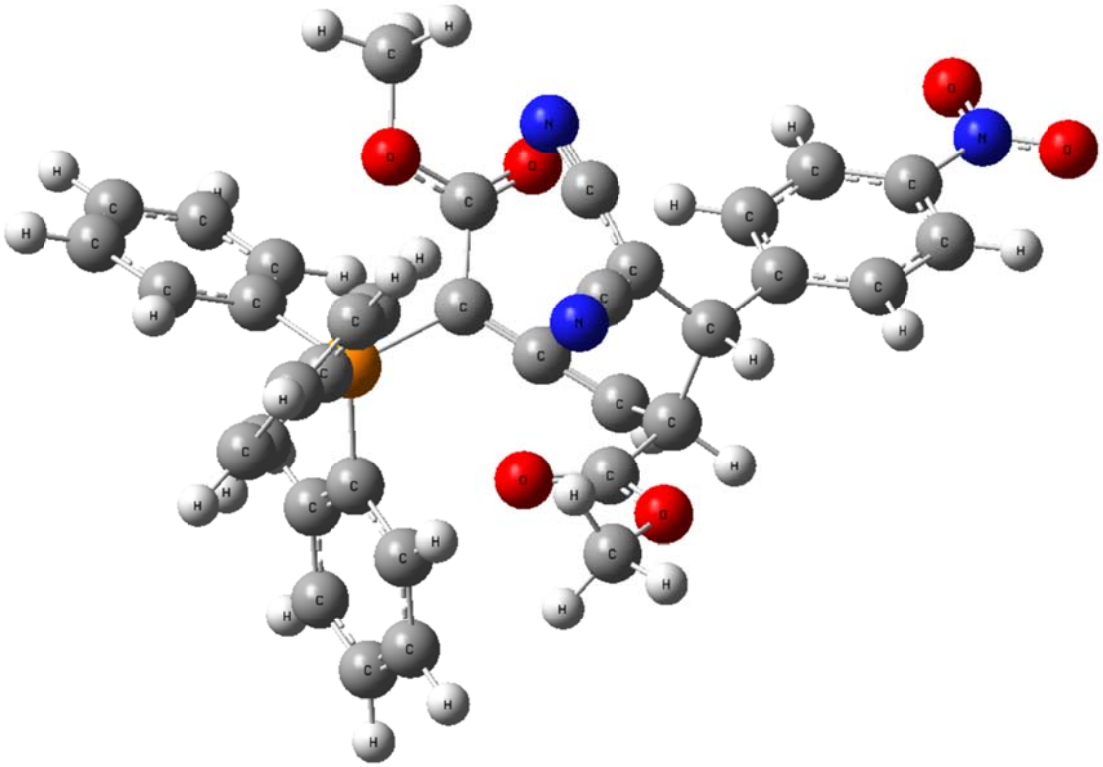
N_{imag} = 1, (-28.3517)

C	0	-2.382153	1.154512	1.068144
C	0	-1.194123	0.537026	1.785081
C	0	-0.031917	0.320345	-0.637684
C	0	-0.891914	1.216647	-1.034753
C	0	-1.850046	1.989937	-0.166064
H	0	-0.934970	1.430542	-2.103637
C	0	0.931137	-0.600277	-0.521597
P	0	2.615702	-0.050822	-0.219842
C	0	0.568977	-2.044546	-0.509502
O	0	1.547552	-2.787127	0.054746
O	0	-0.453070	-2.502753	-0.974318
C	0	1.196168	-4.160535	0.315300
H	0	0.913971	-4.665264	-0.611830
H	0	2.090984	-4.610011	0.746475
H	0	0.363341	-4.181237	1.022982
C	0	2.756541	1.657661	-0.816553
C	0	2.295313	2.705262	-0.000741
C	0	3.247331	1.925181	-2.103493
C	0	2.324440	4.011957	-0.486680
H	0	1.907388	2.512274	0.997205

C	0	3.272318	3.237174	-2.574948
H	0	3.611163	1.119594	-2.733199
C	0	2.809673	4.279564	-1.768722
H	0	1.965281	4.819198	0.144958
H	0	3.655578	3.443457	-3.570093
H	0	2.830468	5.300649	-2.139718
C	0	3.742123	-1.095132	-1.192851
C	0	5.032499	-1.380133	-0.728167
C	0	3.318058	-1.590636	-2.435657
C	0	5.895681	-2.149030	-1.509007
H	0	5.357432	-1.017123	0.241671
C	0	4.186853	-2.357178	-3.210185
H	0	2.310420	-1.389659	-2.788529
C	0	5.475716	-2.635549	-2.748276
H	0	6.893942	-2.372897	-1.144292
H	0	3.853875	-2.743437	-4.169040
H	0	6.149430	-3.237455	-3.351547
C	0	3.103232	-0.069188	1.522715
C	0	4.159650	0.755652	1.946871
C	0	2.424006	-0.879154	2.442163
C	0	4.534434	0.760265	3.288141
H	0	4.667790	1.407399	1.242090
C	0	2.802290	-0.856857	3.783620
H	0	1.594593	-1.500318	2.129339
C	0	3.853636	-0.043229	4.206633
H	0	5.344575	1.403900	3.618244
H	0	2.256485	-1.467443	4.496256
H	0	4.136920	-0.023485	5.255267
C	0	-1.030075	-0.823174	2.068351
C	0	-0.252745	1.422215	2.337932
N	0	-0.779327	-1.952505	2.272922
N	0	0.535083	2.199962	2.730544
H	0	-2.843843	1.905495	1.718425
H	0	-1.303069	2.839199	0.268740
C	0	-3.483810	0.188196	0.664597
C	0	-3.242321	-0.968759	-0.092564
C	0	-4.806983	0.495075	1.021708
C	0	-4.292563	-1.794442	-0.483413

H	0	-2.237848	-1.245645	-0.382526
C	0	-5.868386	-0.316945	0.636641
H	0	-5.006804	1.388551	1.605590
C	0	-5.593372	-1.456373	-0.117148
H	0	-4.110265	-2.689960	-1.064122
H	0	-6.890748	-0.086648	0.909434
N	0	-6.706991	-2.320523	-0.535265
O	0	-7.847444	-1.988902	-0.204908
O	0	-6.439955	-3.325708	-1.194561
C	0	-2.989079	2.562445	-0.996021
O	0	-3.157788	2.392727	-2.184354
O	0	-3.818740	3.286681	-0.216743
C	0	-5.004646	3.775623	-0.870739
H	0	-5.613249	2.936020	-1.217878
H	0	-5.538380	4.350907	-0.113913
H	0	-4.741437	4.406223	-1.723804

Table S22. Optimized atomic coordinate of **4a'-Ic** at B3LYP-D3/6-31G(d) level.



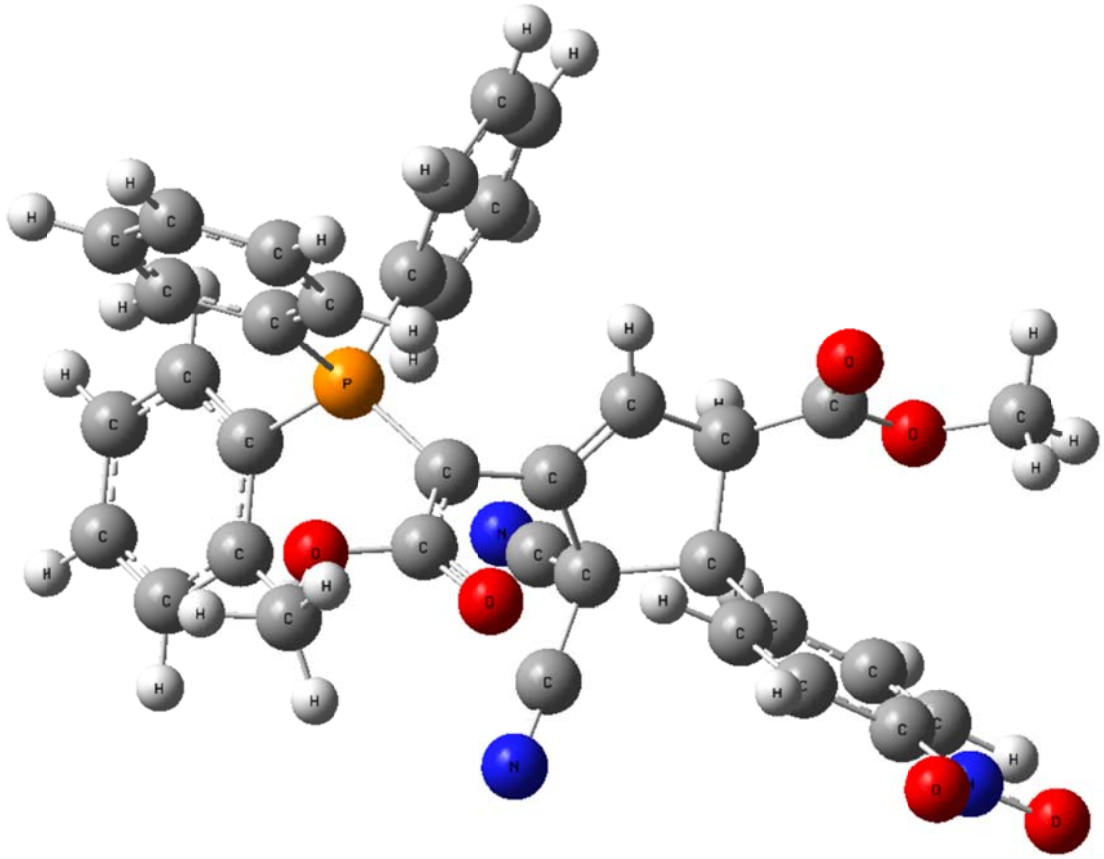
N_{imag} = 0

C	0	2.745532	1.547017	-0.284033
C	0	1.962406	1.420158	-1.571685
C	0	0.227266	-0.227788	0.821622
C	0	1.124564	0.448256	1.482881
C	0	1.830180	1.703070	1.030198
H	0	1.389634	0.061922	2.467261
H	0	2.496091	2.030061	1.835634
C	0	-0.661125	-0.963166	0.183536
P	0	-2.402376	-0.454319	0.262507
C	0	-0.212725	-2.101773	-0.698410
O	0	-1.063381	-2.272944	-1.718165
O	0	0.754201	-2.788775	-0.459311
C	0	-0.675574	-3.262157	-2.696480
H	0	-0.513194	-4.227290	-2.209836
H	0	-1.511234	-3.313353	-3.394523
H	0	0.235411	-2.916845	-3.187546
C	0	0.843921	2.832686	0.754412
O	0	-0.342044	2.698879	0.525937
O	0	1.479520	4.010283	0.733806

C	0	0.702206	5.128483	0.245736
H	0	1.361344	5.992250	0.331951
H	0	0.431526	4.944526	-0.797080
H	0	-0.194287	5.260157	0.857445
C	0	-2.816420	0.066296	1.955279
C	0	-2.386329	1.325604	2.406906
C	0	-3.533019	-0.782401	2.814337
C	0	-2.669916	1.719216	3.714044
H	0	-1.836149	1.984293	1.744722
C	0	-3.808799	-0.375810	4.119103
H	0	-3.883518	-1.749485	2.471176
C	0	-3.376937	0.872826	4.570561
H	0	-2.336967	2.693352	4.060619
H	0	-4.365981	-1.034036	4.779336
H	0	-3.595976	1.187225	5.587257
C	0	-3.465024	-1.867531	-0.146237
C	0	-4.596681	-1.685444	-0.949021
C	0	-3.158997	-3.139621	0.363735
C	0	-5.424801	-2.772782	-1.232676
H	0	-4.822392	-0.707187	-1.361711
C	0	-3.990493	-4.218922	0.076126
H	0	-2.267060	-3.290450	0.966325
C	0	-5.124401	-4.035605	-0.721206
H	0	-6.299861	-2.631487	-1.860145
H	0	-3.748707	-5.203455	0.465427
H	0	-5.768319	-4.880377	-0.948526
C	0	-2.671704	0.926883	-0.860775
C	0	-3.753581	1.798343	-0.648450
C	0	-1.757503	1.156967	-1.899291
C	0	-3.914923	2.901416	-1.482801
H	0	-4.443451	1.632943	0.174409
C	0	-1.919035	2.277481	-2.713053
H	0	-0.920032	0.488206	-2.065716
C	0	-2.992295	3.144536	-2.504855
H	0	-4.745679	3.582274	-1.320664
H	0	-1.178576	2.490760	-3.475182
H	0	-3.102615	4.023560	-3.133557
C	0	1.633356	0.225107	-2.209310

C	0	1.524433	2.600919	-2.193582
N	0	1.305283	-0.755044	-2.771380
N	0	1.149490	3.599426	-2.687988
H	0	3.248092	2.518721	-0.322717
C	0	3.824828	0.505195	-0.040530
C	0	3.577547	-0.877839	-0.080210
C	0	5.121569	0.943302	0.275086
C	0	4.592177	-1.791670	0.188101
H	0	2.598265	-1.261467	-0.330743
C	0	6.147387	0.044351	0.547385
H	0	5.332572	2.009187	0.304739
C	0	5.865018	-1.319739	0.503574
H	0	4.404508	-2.857637	0.154411
H	0	7.148616	0.378474	0.789619
N	0	6.935895	-2.280658	0.800703
O	0	6.658715	-3.480629	0.768461
O	0	8.052523	-1.833225	1.070592

Table S23. Optimized atomic coordinate of **4a** at B3LYP-D3/6-31G(d**)** level.



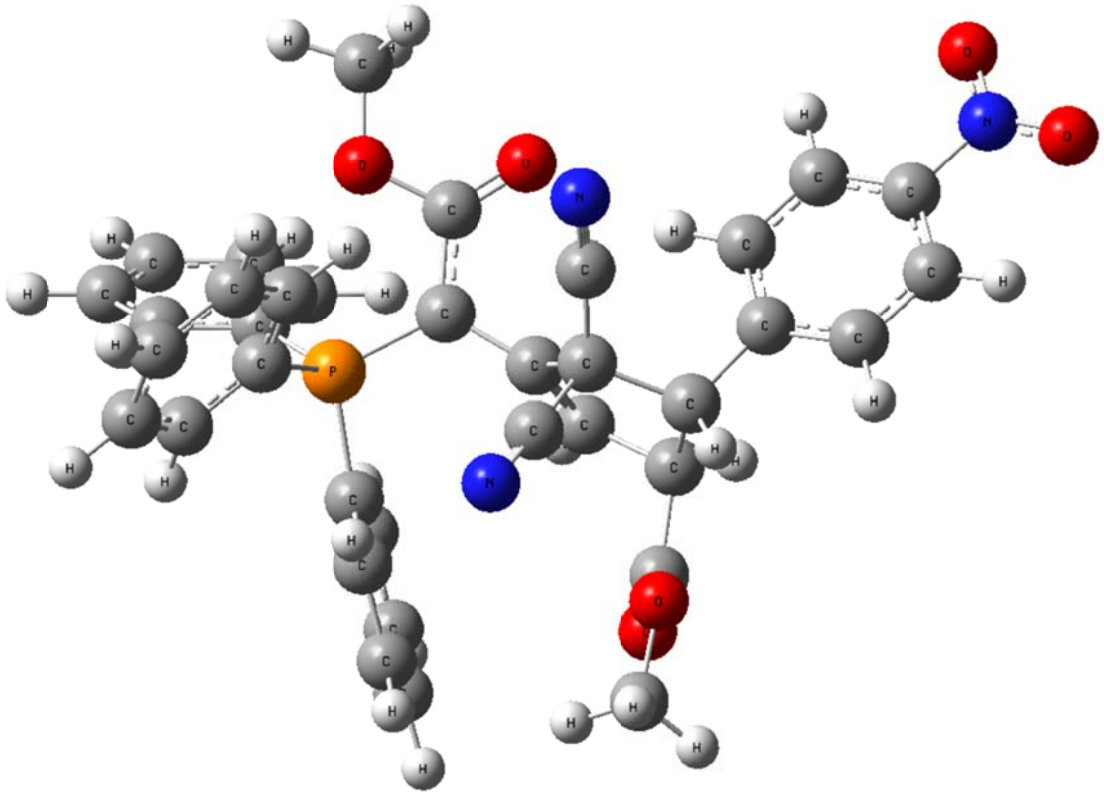
N_{imag} = 0

C	0	-2.288349	1.076636	1.138439
C	0	-0.951894	0.322697	1.489659
C	0	-0.199925	0.249451	0.110590
C	0	-0.709707	1.198663	-0.683619
C	0	-1.811432	1.994706	-0.047555
H	0	-0.355110	1.407842	-1.684944
C	0	0.932919	-0.651518	-0.095507
P	0	2.562199	-0.059130	-0.188809
C	0	0.658006	-2.063824	-0.130998
O	0	1.795124	-2.827633	-0.002696
O	0	-0.446605	-2.579932	-0.269726
C	0	1.612889	-4.236614	-0.181008
H	0	1.229841	-4.455066	-1.182895
H	0	2.601954	-4.678384	-0.048639
H	0	0.910597	-4.631014	0.558297
C	0	2.533998	1.709594	-0.639040
C	0	2.368300	2.684488	0.356262

C	0	2.566389	2.092263	-1.988275
C	0	2.218186	4.024697	-0.000699
H	0	2.340866	2.403928	1.402870
C	0	2.421849	3.434556	-2.337244
H	0	2.701494	1.346221	-2.764966
C	0	2.242407	4.401179	-1.344978
H	0	2.081163	4.771494	0.776089
H	0	2.448975	3.724044	-3.383907
H	0	2.125706	5.445970	-1.619691
C	0	3.514470	-0.924239	-1.489118
C	0	4.897558	-1.119348	-1.391882
C	0	2.829072	-1.366659	-2.630760
C	0	5.589078	-1.740375	-2.433111
H	0	5.435100	-0.805999	-0.503235
C	0	3.524892	-1.984753	-3.668232
H	0	1.751920	-1.240486	-2.690641
C	0	4.906257	-2.170586	-3.571779
H	0	6.661384	-1.893537	-2.349286
H	0	2.986833	-2.328710	-4.547064
H	0	5.447257	-2.656478	-4.379115
C	0	3.519288	-0.154845	1.367174
C	0	4.669784	0.623813	1.573300
C	0	3.061201	-1.003103	2.383876
C	0	5.360840	0.540844	2.781431
H	0	5.011916	1.308846	0.802284
C	0	3.757043	-1.081596	3.590003
H	0	2.163282	-1.592023	2.230414
C	0	4.905380	-0.313171	3.789115
H	0	6.246379	1.149986	2.939871
H	0	3.394303	-1.736505	4.376818
H	0	5.440534	-0.370791	4.732960
C	0	-1.130518	-0.952129	2.203357
C	0	-0.135854	1.181083	2.377473
N	0	-1.226397	-1.918361	2.837498
N	0	0.518883	1.890698	3.022515
H	0	-2.599237	1.691192	1.985453
H	0	-1.423103	2.931553	0.380419
C	0	-3.446111	0.171516	0.754712

C	0	-3.286012	-0.985376	-0.023725
C	0	-4.737579	0.556474	1.149004
C	0	-4.396262	-1.736248	-0.402298
H	0	-2.301961	-1.329635	-0.323783
C	0	-5.854908	-0.178269	0.768789
H	0	-4.869408	1.451784	1.749078
C	0	-5.665050	-1.319000	-0.009047
H	0	-4.284307	-2.635191	-0.995293
H	0	-6.855360	0.110481	1.065765
N	0	-6.841036	-2.102941	-0.421055
O	0	-7.950532	-1.700187	-0.067016
O	0	-6.649996	-3.112445	-1.098262
C	0	-2.935244	2.363166	-0.998131
O	0	-3.021161	2.015312	-2.153475
O	0	-3.847914	3.133174	-0.366541
C	0	-5.031252	3.432231	-1.130748
H	0	-5.571032	2.508624	-1.358229
H	0	-5.633469	4.082267	-0.495541
H	0	-4.769201	3.936047	-2.064506

Table S24. Optimized atomic coordinate of **4a'** at B3LYP-D3/6-31G(d) level.



$N_{imag} = 0$

C	0	-2.496610	1.295623	0.432648
C	0	-1.246779	0.554027	1.048960
C	0	-0.408947	0.139137	-0.210053
C	0	-0.818910	0.871348	-1.251026
C	0	-1.960525	1.808393	-0.943726
H	0	-0.361936	0.839180	-2.232446
H	0	-2.739453	1.738943	-1.712152
C	0	0.668741	-0.848207	-0.125832
P	0	2.340418	-0.387191	-0.122070
C	0	0.276563	-2.224514	0.022858
O	0	1.329932	-3.037667	0.371954
O	0	-0.852838	-2.675635	-0.143827
C	0	1.040409	-4.439255	0.405005
H	0	0.716586	-4.792978	-0.578990
H	0	1.974539	-4.924074	0.693658
H	0	0.252735	-4.653423	1.132504
C	0	-1.451490	3.249935	-1.005174
O	0	-1.031320	3.754837	-2.023237
O	0	-1.495034	3.872489	0.185880

C	0	-0.950045	5.204098	0.217231
H	0	-0.973192	5.501363	1.265350
H	0	0.073295	5.198016	-0.163109
H	0	-1.558304	5.876464	-0.394198
C	0	2.488857	1.301638	-0.797357
C	0	2.462434	2.416822	0.051704
C	0	2.517402	1.488958	-2.188432
C	0	2.455003	3.702755	-0.490428
H	0	2.428411	2.290402	1.126995
C	0	2.497314	2.775638	-2.721909
H	0	2.549655	0.631252	-2.853368
C	0	2.461353	3.884693	-1.873445
H	0	2.437486	4.560149	0.176371
H	0	2.506160	2.912920	-3.799121
H	0	2.436605	4.886591	-2.292010
C	0	3.332388	-1.485293	-1.201799
C	0	4.683641	-1.757044	-0.954492
C	0	2.710989	-2.038148	-2.331785
C	0	5.407676	-2.559842	-1.837215
H	0	5.170537	-1.363255	-0.069063
C	0	3.438783	-2.837673	-3.211362
H	0	1.654192	-1.855209	-2.503374
C	0	4.789364	-3.097504	-2.966995
H	0	6.454386	-2.770099	-1.635826
H	0	2.948407	-3.265132	-4.081462
H	0	5.355335	-3.724394	-3.650543
C	0	3.140106	-0.345922	1.522420
C	0	4.356601	0.323194	1.736504
C	0	2.492312	-0.971185	2.595719
C	0	4.924093	0.349590	3.009664
H	0	4.846513	0.843284	0.917777
C	0	3.065354	-0.941472	3.867041
H	0	1.543173	-1.471003	2.435392
C	0	4.279626	-0.285174	4.074653
H	0	5.861678	0.873919	3.172049
H	0	2.555562	-1.423658	4.695979
H	0	4.719693	-0.257900	5.067714
C	0	-1.575800	-0.547395	1.970366

C	0	-0.420771	1.493685	1.840176
N	0	-1.778433	-1.375740	2.756402
N	0	0.258260	2.224123	2.433922
H	0	-2.772233	2.132418	1.073988
C	0	-3.713229	0.408025	0.243694
C	0	-3.624800	-0.895405	-0.272960
C	0	-4.975927	0.938051	0.547603
C	0	-4.777274	-1.647737	-0.481475
H	0	-2.661842	-1.349109	-0.487076
C	0	-6.135916	0.199604	0.336961
H	0	-5.053828	1.942667	0.955085
C	0	-6.017392	-1.088467	-0.180098
H	0	-4.721956	-2.657992	-0.867247
H	0	-7.115705	0.598481	0.568060
N	0	-7.237729	-1.879283	-0.408726
O	0	-7.109392	-3.009730	-0.878398
O	0	-8.318225	-1.362236	-0.120743

Table S25. Chemical shifts, energetics and geometrical data of **4a** and **4a'** with 6-31G(d), 6-31G(d, p) and 6-311+G(2d, p) basis sets at B3LYP and B3LYP-D3 levels.

		4a			**4a'**		
		6-31G(d)	6-31G(d,p)	6-311+G(2d,p)	6-31G(d)	6-31G(d,p)	6-311+G(2d,p)
	Energy						
B3LYP		-2345.470123	-2345.513059	-2346.113284	-2345.469823	-2345.512877	-2346.112944
B3LYP-D3		-2345.577668	-2345.620648	-2346.220305	-2345.578792	-2345.621842	-2346.220916
	ΔE(**4a**−**4a'**)						
B3LYP		-0.19	-0.11	-0.21			
B3LYP-D3		0.71	0.75	0.38			
	δ of H_a						
B3LYP		5.1768	5.3817	5.4531	5.2153	5.3812	5.6320
B3LYP-D3		4.8324	5.0304	5.0758	5.1872	5.3650	5.3662
	Geom.						
B3LYP							
	φ	-113.481	-113.561	-110.831	-110.547	-110.814	-105.814
	∠H_aC1C2	124.157	124.172	124.132	123.702	123.685	123.645
	R(H_a−C1)	1.08326	1.08259	1.08024	1.08359	1.08286	1.08055
B3LYP-D3							
	φ	-117.310	-117.476	-114.783	-109.809	-110.055	-106.444
	∠H_aC1C2	124.128	124.129	124.119	124.044	124.008	123.821
	R(H_a−C1)	1.08266	1.08196	1.07962	1.08307	1.08233	1.08056