

Supplementary Information for

Ni-Catalyzed Asymmetric Hydrophosphinylation of Conjugated Enynes and Mechanistic Studies

Ya-Qian Zhang[†], Xue-Yu Han[†], Yue Wu, Peng-Jia Qi, Qing Zhang & Qing-Wei Zhang*

Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026

*Corresponding Author: qingweiz@ustc.edu.cn

[†]Y.-Q. Z. and X.-Y. H. contributed equally to this work

INDEX

1. General information	3
2. Optimization of reaction conditions.....	4
3. General procedure for the synthesis of racemic products.....	5
4. General procedure for the synthesis of chiral products.....	6
5. Synthetic applications.....	7
6. Mechanism experiments.....	8
7. DFT Computational Studies.....	17
8. X-ray crystal structure of 3ka (ORTEP drawing).....	32
9. Spectroscopic data of products.....	33
10. Supplementary references.....	49

1. General Information

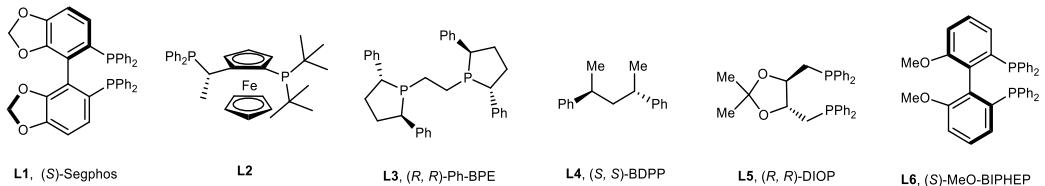
All reagents were obtained commercially unless otherwise noted. All reactions under standard conditions were monitored by thin-layer chromatography (TLC) on gel F₂₅₄ plates. The silica gel (300-400 meshes) was used for column chromatography, and the distillation range of petroleum ether was 60-90 °C. Mesitylene was purchased and used directly. ¹H, ¹³C, ³¹P, ¹¹B and ¹⁹F NMR spectra were recorded in CDCl₃ or C₆D₆ solution on Bruker Aescend™ 400 MHz and 500MHz instruments and spectral data were reported in ppm. The residual solvent peak or tetramethylsilane (TMS) was used as an internal reference: proton (TMS δ 0.0) and carbon (CDCl₃ δ 77.0). High-resolution mass spectral analysis (HRMS) data were measured by means of the ESI technique. Enantiomer excess was determined by HPLC analysis employing Darcel Chiracel columns (AD-H, OD-H, OJ-H, IH-3 and AS-H) and *n*-Hexane/*i*-PrOH as eluents. Optical rotations were measured by Perkin-Elmer-343 polarimeter.

Enynes were prepared according to the reference 1 and phosphine oxides were prepared according to the reference 2 and 3.

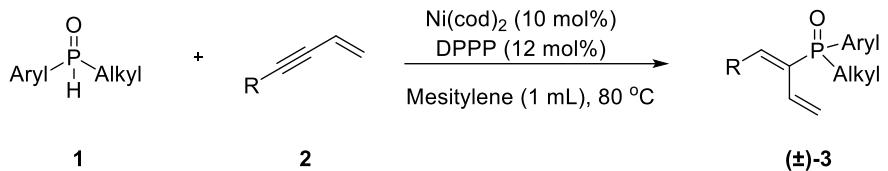
2. Optimization of reaction conditions

Entry ^a	Ligand	Additive	Solvent	Yield (%) ^b	rr ^c	ee (%) ^d 3aa	ee (%) ^d 3aa'
1	L1	KOAc	Mesitylene	trace	--	--	--
2	L2	KOAc	Mesitylene	8%	1:1	3%	nd
3	L3	KOAc	Mesitylene	90%	>20:1	35%	--
4	L4	KOAc	Mesitylene	83%	>20:1	82%	--
5	L5	KOAc	Mesitylene	<5%	>20:1	--	--
6	L6	KOAc	Mesitylene	trace	--	--	--
7	L4	none	Mesitylene	78%	>20:1	54%	--
8	L4	K ₂ HPO ₄	Mesitylene	74%	>20:1	80%	--
9	L4	KH ₂ PO ₄	Mesitylene	78%	>20:1	59%	--
10	L4	Ph ₂ P(O)OH	Mesitylene	<5%	1:1	-14%	nd
				41% ^e		-21% ^e	
11	L4	K ₃ PO ₄	Mesitylene	70%	>20:1	71%	--
12	L4	t-BuCO ₂ K	Mesitylene	66%	>20:1	86%	--
13 ^f	L4	t-BuCO ₂ K	Mesitylene	72%	>20:1	88%	--
14 ^f	L4	t-BuCO ₂ K	DCM	trace	--	--	--
15 ^f	L4	t-BuCO ₂ K	Dioxane	9%	>20:1	69%	--
16 ^f	L4	t-BuCO ₂ K	THF	35%	>20:1	58%	--
17 ^{f-h}	L4	t-BuCO ₂ K	Mesitylene	60%	>20:1	91%	--
18 ^{f-i}	L4	t-BuCO ₂ K	Mesitylene	>95%(89%) ^j	>20:1	91%	--
19 ^{f-i, k}	L4	t-BuCO ₂ K	Mesitylene	41%	>20:1	94%	--

^aReaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), [Ni] (10 mol %), L (12 mol %), Additive (1.5 equiv), solvent (1.0 mL), 3 h. ^bNMR yield and with PO(OMe)₃ as internal standard. ^cDetermined by ¹H NMR analysis of crude reaction mixture. ^dDetermined by chiral HPLC analysis. ^e24 h. ^ft-BuCO₂K 2 equiv. ^g-20 °C. ^h5d. ⁱ**1a** (0.2 mmol), **2a** (0.1 mmol). ^jIsolated yield. ^kNi(stb^F)₃ instead of Ni(cod)₂.

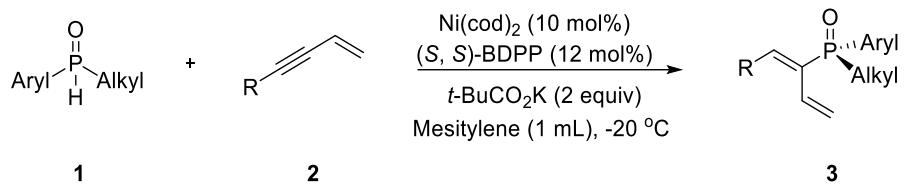


3. General procedure for the synthesis of racemic products.



To a 4 mL vial were added Ni(cod)₂ (2.8 mg, 0.01 mmol), DPPP (4.9 mg, 0.012 mmol), and mesitylene (1 mL) in a N₂ flushed glove box. The mixture was stirred for 10 minutes followed by the addition of enynes (0.12 mmol) and SPOs (0.1 mmol). The vial was capped, removed from the glove box, and the system was stirred at 80 °C overnight. The reaction mixture was cooled to room temperature and subjected to silica gel column chromatography directly for purification.

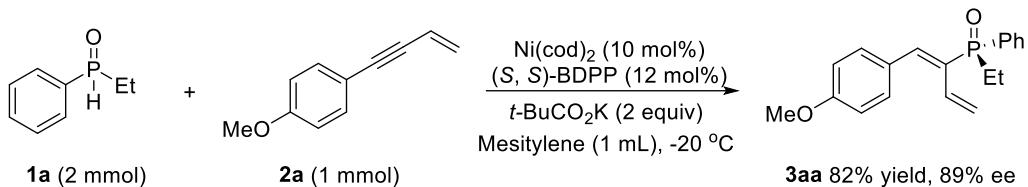
4. General procedure for the synthesis of chiral products.



To a 4 mL vial were added $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol), (*S, S*)-BDPP (5.3 mg, 0.012 mmol) and mesitylene (1 mL) in a N_2 flushed glove box. The mixture was stirred for 10 minutes, cooled to -20°C in the glove box followed by the addition of enynes (0.1 mmol), *t*-BuCO₂K (28.0 mg, 2 mmol) and SPO (0.2 mmol). The vial was rapidly capped, removed from the glove box, and the system was stirred at -20°C for 5 days. The reaction mixture was subjected to silica gelcolumn chromatography directly for purification.

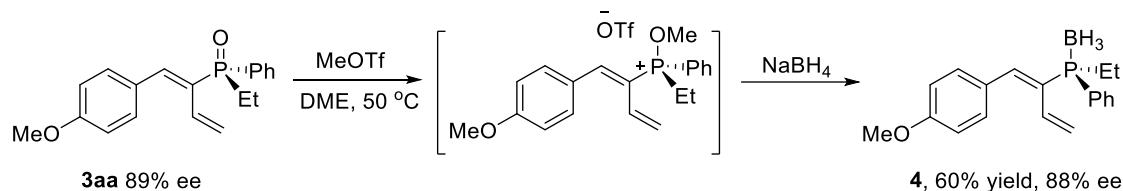
5. Synthetic applications.

5.1 1 mmol-scale synthesis.



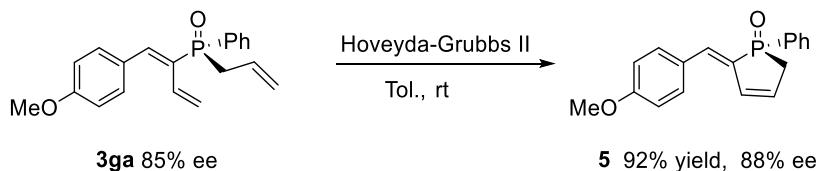
To a 25 mL vial were added $\text{Ni}(\text{cod})_2$ (27.5 mg, 0.01 mmol), (*S, S*)-BDPP (53.0 mg, 0.012 mmol) and mesitylene (10 mL) in a N_2 flushed glove box. The mixture was stirred for 10 minutes, cooled to -20 °C in the glovebox followed by the addition of 2a (158.0 mg, 1 mmol), *t*-BuCO₂K (280.0 mg, 2 mmol) and 1a (308.0 mg, 2 mmol). The vial was rapidly capped, removed from the glove box, and the system was stirred at -20 °C until disappearance of 2a by TLC. The reaction mixture was subjected to silica gel column chromatography directly for purification to afford 3aa (256.8 mg, 89% ee).

5.2 Compound 4.



According to reference 4, to a stirred solution of tertiary phosphine oxide 3aa (31.2 mg, 0.1 mmol) in DME (0.5 mL) was added MeOTf (13.6 μL , 0.12 mmol) dropwise at room temperature under N_2 . The reaction was heated at 50 °C overnight. After cooling to room temperature, a dispersion of NaBH₄ (11.3 mg, 0.3 mmol) in diglyme (0.5 mL) was added dropwise to the vial. The reaction mixture was stirred for additional 3 hours at 50 °C before being cooled to room temperature and diluted with DCM (5 mL). Water was then added dropwise to quench the remaining NaBH₄. The mixture was washed with water (5mL x 3) and the organic layer was dried over anhydrous MgSO₄ and removed in vacuo. The residue was purified by silica gel column chromatography afford the desired product 4 in 60% yield (18.6 mg) with 88% ee.

5.3 Compound 5.

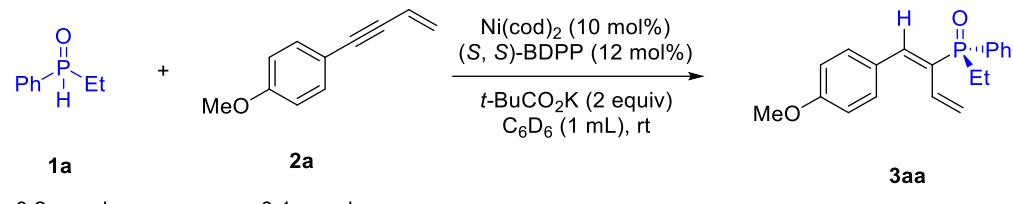


A 4 mL reaction vial equipped with a magnetic stirrer under N_2 was charged with 3ga (85% ee, 32.4 mg, 0.1 mmol) and Hoveyda-Grubbs II (3.1 mg, 0.005 mmol). toluene (1 mL) was added as solvent and the reaction mixture was stirred at rt for 5 min. The resulting mixture was subjected to column chromatography to afford the adduct 5 in 92% yield (27.3 mg) with 88% ee.

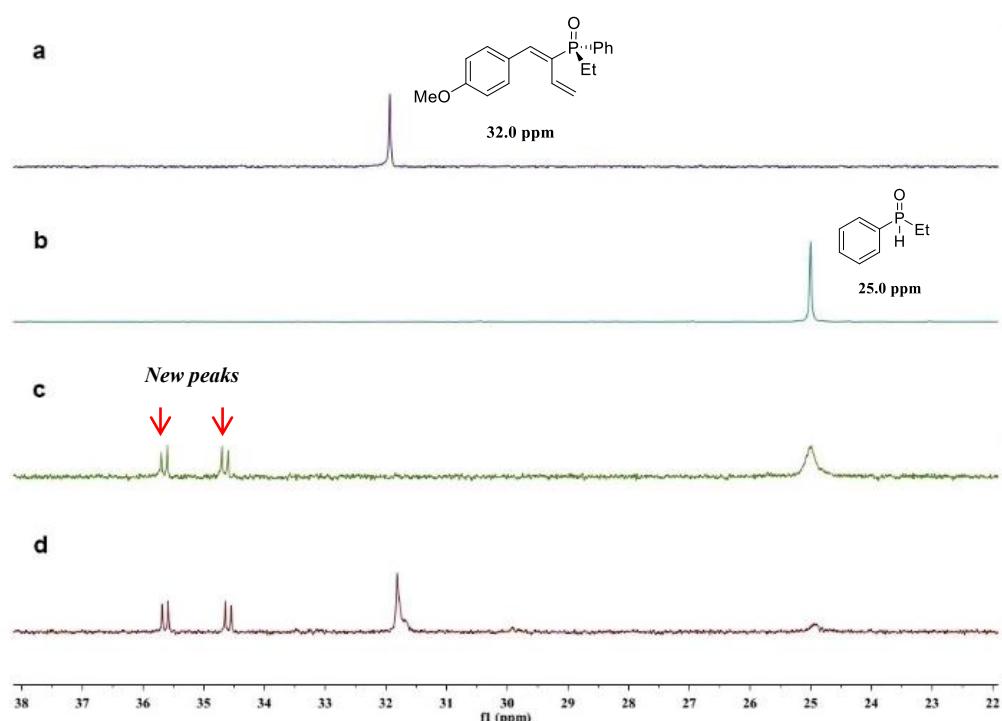
6. Mechanism experiments.

6.1. Identification of the Catalyst Resting State.

6.1.1 The NMR of the reaction mixture.

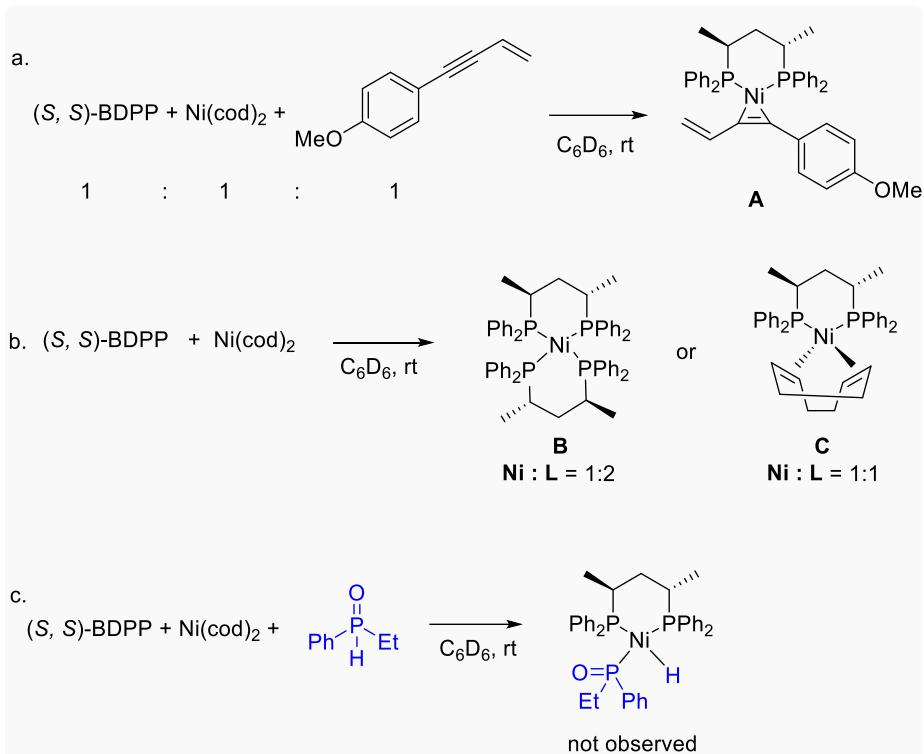


According to standard condition except that the solvent was replaced with C₆D₆ and the temperature is room temperature.



Supplementary Figure 1. (a) ³¹P NMR spectra of **3aa** and (b) **1a**; (c) ³¹P NMR spectra of reaction mixture in 10 minutes and (d) ³¹P NMR spectra of reaction mixture in 6 hours.

6.1.2 Control experiments (Supplementary Figure 2).



Supplementary Figure 2. Three possible pathways can lead to the formation of the catalyst resting state.

6.1.3 The ³¹P NMR of the mixture of the (*S, S*)-BDPP and Ni(cod)₂.

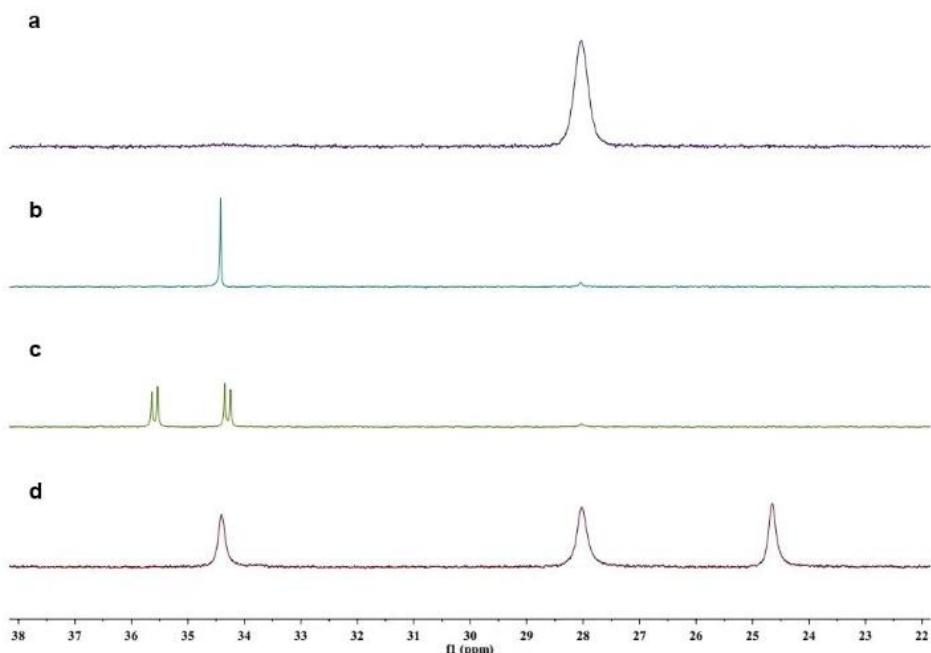
Preparation: To a 4 mL vial were added Ni(cod)₂ (13.8 mg, 0.05 mmol), (*S, S*)-BDPP (44.0 mg, 0.1 mmol) and C₆D₆ (1 mL) in a N₂ flushed glove box, another 4 mL vial were added Ni(cod)₂ (13.8 mg, 0.05 mmol), (*S, S*)-BDPP (22.0 mg, 0.05 mmol) and C₆D₆ (1 mL) in a N₂ flushed glove box. Then the mixture were stirred at rt overnight and tested by NMR. The ³¹P NMR with ¹H-decoupling of the mixture was obtained in **Supplementary Figure 3a** and **b**.

6.1.4 The ³¹P NMR of the mixture of the (*S, S*)-BDPP, Ni(cod)₂ and enyne **2a**.

Preparation: To a 4 mL vial were added Ni(cod)₂ (13.8 mg, 0.05 mmol), (*S, S*)-BDPP (22.0 mg, 0.05 mmol) and C₆D₆ (0.5 mL) in a N₂ flushed glove box. Then the mixture was stirred for 10 minutes. After that, enyne **2a** (7.9 mg, 0.05 mmol) in C₆D₆ (0.5 mL) were added, the mixture was stirred at rt overnight and tested by NMR. The ³¹P NMR with ¹H-decoupling of the mixture was obtained in **Supplementary Figure 3c**.

6.1.5 The ³¹P NMR of the mixture of the (*S, S*)-BDPP, Ni(cod)₂ and SPO **1a**.

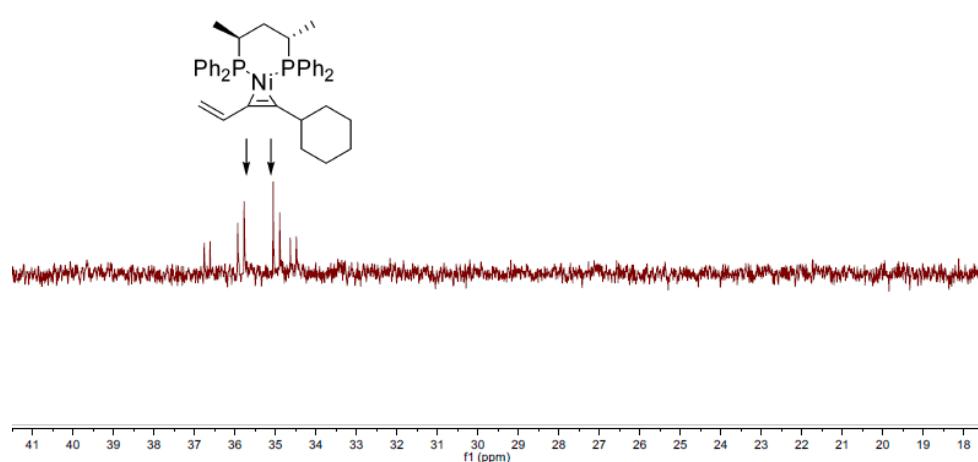
Preparation: To a 4 mL vial were added Ni(cod)₂ (13.8 mg, 0.05 mmol), (*S, S*)-BDPP (22.0 mg, 0.05 mmol) and C₆D₆ (0.5 mL) in a N₂ flushed glove box. Then the mixture was stirred for 10 minutes. After that, SPO **1a** (7.7 mg, 0.05 mmol) in C₆D₆ (0.5 mL) were added, the mixture was stirred at rt overnight and tested by NMR. The ³¹P NMR of the mixture was obtained in **Supplementary Figure 3d**.



Supplementary Figure 3. ^{31}P NMR spectra of (a) (*S, S*)-BDPP : Ni(cod)₂ = 2:1; (b) (*S, S*)-BDPP : Ni(cod)₂ = 1:1; (c) (*S, S*)-BDPP : Ni(cod)₂ : **2a** = 1:1:1; (d) (*S, S*)-BDPP : Ni(cod)₂ : **1a** = 1:1:1.

6.1.6 The ^{31}P NMR of the mixture of the (*S, S*)-BDPP, Ni(cod)₂ and enyne **2u**.

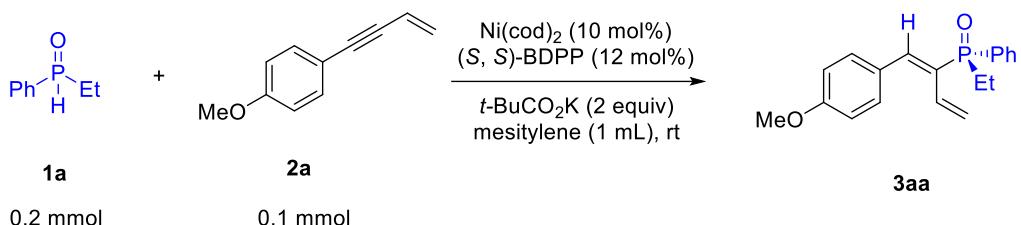
Preparation: To a 4 mL vial were added Ni(cod)₂ (13.8 mg, 0.05 mmol), (*S, S*)-BDPP (22.0 mg, 0.05 mmol) and C₆D₆ (0.5 mL) in a N₂ flushed glove box. Then the mixture was stirred for 10 minutes. After that, enyne **2u** (6.7 mg, 0.05 mmol) in C₆D₆ (0.5 mL) were added, the mixture was stirred at rt overnight and tested by NMR. The ^{31}P NMR with ^1H -decoupling of the mixture was obtained in **Supplementary Figure 4**.



Supplementary Figure 4. ^{31}P NMR spectra of (*S, S*)-BDPP : Ni(cod)₂ : **2u** = 1:1:1

6.2. Kinetic Studies.

General procedure of kinetic experiments



To a 4 mL vial were added Ni(cod)₂ (2.8 mg, 0.01 mmol), (S, S)-BDPP (5.3 mg, 0.012 mmol) and mesitylene (1 mL) in a N₂ flushed glove box. The mixture was stirred for 10 minutes followed by the addition of enynes (0.1 mmol), *t*-BuCO₂K (28.0 mg, 0.2 mmol) and SPO (0.2 mmol). The vial was capped, removed from the glove box, and the system was stirred at room temeperature and the aliquots were analyzed by HPLC.

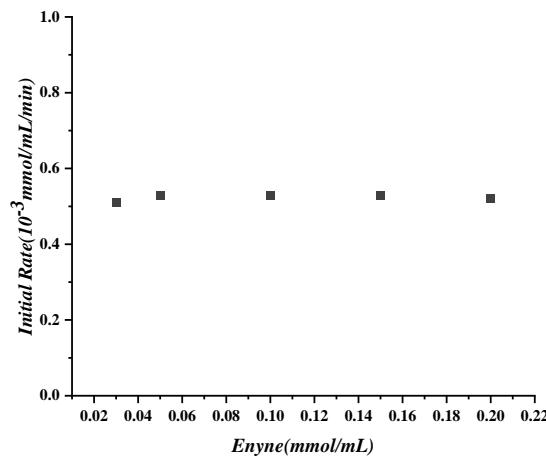
Note: The conversion of the product was detected by HPLC with Inertsil® SIL-100A column. Calibration factors are obtained at 228 nm using triphenyl phosphine oxide as the standard. 10 uL mixture was withdrawn at each time point; The wavelength was detected by HPLC, triphenoxyphosphine was used as the internal standard, and the concentration curve was made to ensure a linear relationship within the tested concentration range. The slope of integral of area/concentration between the product and the internal standard is determined to be 1.75. The concentration of the product and the initial rate were thus obtained. For each kinetic experiment we took samples every 5 minutes or 10 minutes, with three samples per experiment. The conversion of the reaction is controlled less than 15% at the end of the sampling to ensure the accuracy of the initial rate.

6.2.1 Reaction order in enyne.

According to procedure above except for the varied concentration of enyne **2a**. Kinetic data is shown in **Supplementary Table 1**. Kinetic plots for the reaction order in enyne is shown in **Supplementary Figure 5**.

Supplementary Table 1. Initial rate for the formation of **3aa** with varying concentrations of **2a** at rt.

Conc. of enyne (mmol/mL)	Initial rate (10 ⁻³ mmol/mL/min)
0.03	0.51
0.05	0.53
0.1	0.53
0.15	0.53
0.2	0.52



Supplementary Figure 5. Dependence of the initial rate on enyne **2a**

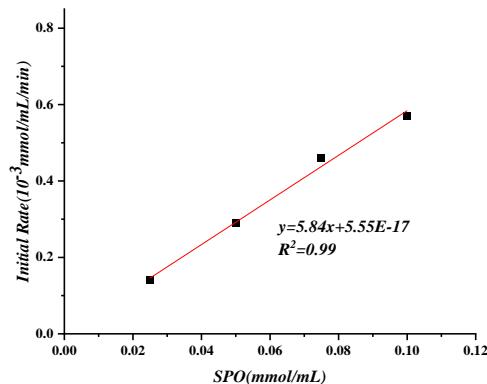
6.2.2 Reaction order in SPO

According to procedure above except for the varied concentration of **1a**. Kinetic data is shown in **Supplementary Table 2**. Kinetic plots for the reaction order in enyne is shown in **Supplementary Figure 6**.

Supplementary Table 2. Initial Rate for the formation of **3aa** with varying concentrations of **1a** at rt.

Conc. of SPO (mmol/mL) ^a	Initial rate (10 ⁻³ mmol/mL/min)
0.025	0.14
0.05	0.29
0.075	0.46
0.1	0.57

^aReferred to the concentration of (*R*)-**1a**.



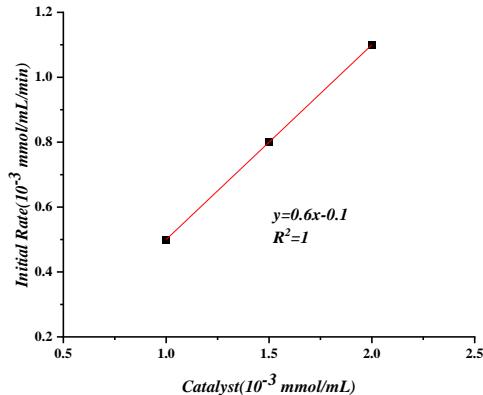
Supplementary Figure 6. Dependence of the initial rate on SPO **1a**.

6.2.3 Reaction order in catalyst

According to procedure above except for the varied concentration of Ni(cod)₂ and (S, S)-BDPP. Kinetic data is shown in **Supplementary Table 3**. Kinetic plots for the reaction order in catalyst is shown in **Supplementary Figure 7**.

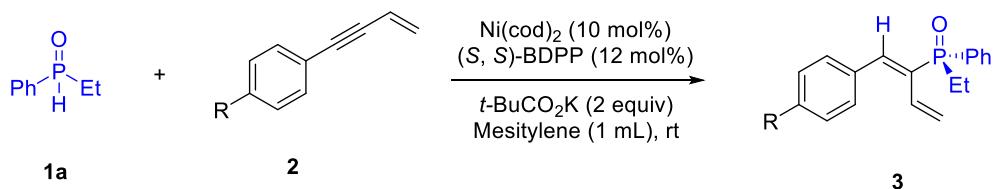
Supplementary Table 3. Initial rate for the formation of **3aa** with varying concentrations of catalyst at rt.

Conc. of catalyst (10 ⁻³ mmol/mL)	Initial rate (10 ⁻³ mmol/mL/min)
1	0.5
1.5	0.8
2	1.1



Supplementary Figure 7. Dependence of the initial rate on catalyst.

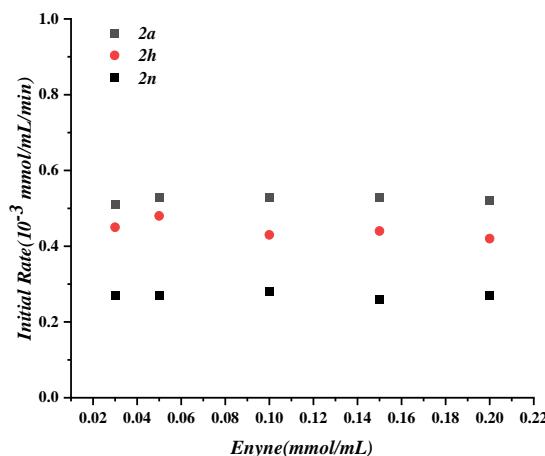
6.2.4 The electronic effects of substituent on enyne.



According to the general procedure of the kinetic experiments. Kinetic data is shown in **Supplementary Table 4**. Kinetic plot is shown in **Supplementary Figure 8**.

Supplementary Table 4. Initial rate for the formation of **3** with varying concentrations and varying substituent of enyne at rt.

Conc. of enyne (mmol/mL)	Initial rate _{2a} (10 ⁻³ mmol/mL/min)	Initial rate _{2n} (10 ⁻³ mmol/mL/min)	Initial rate _{2h} (10 ⁻³ mmol/mL/min)
0.03	0.51	0.45	0.27
0.05	0.53	0.48	0.27
0.1	0.53	0.43	0.28
0.15	0.53	0.44	0.26
0.2	0.52	0.42	0.27



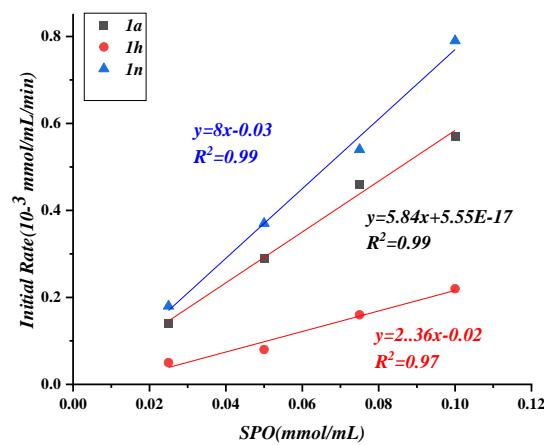
Supplementary Figure 8. Dependence of the initial rate on enynes.

6.2.5 The electronic effects of substituent on SPO.

According to the general procedure of the kinetic experiments. Kinetic data is shown in **Supplementary Table 5**. Kinetic plot is shown in **Supplementary Figure 9**.

Supplementary Table 5. Initial rate for the formation of **3** with varying concentrations and varying substituent of SPO at rt.

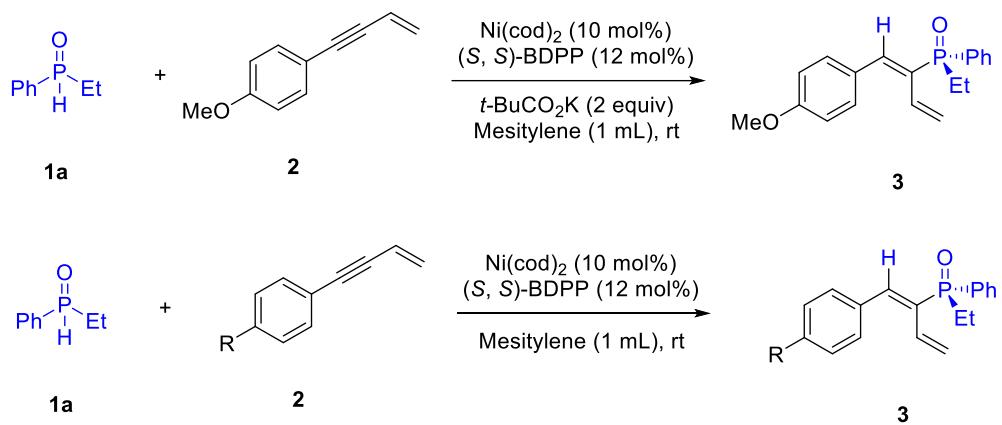
Conc. of SPO (mmol/mL)	Initial rate _{Ia} (10 ⁻³ min ⁻¹)	Initial rate _{Ih} (10 ⁻³ min ⁻¹)	Initial rate _{In} (10 ⁻³ min ⁻¹)
0.025	0.14	0.05	0.18
0.05	0.29	0.08	0.37
0.075	0.46	0.16	0.54
0.1	0.57	0.22	0.79



Supplementary Figure 9. Dependence of the initial rate on SPO.

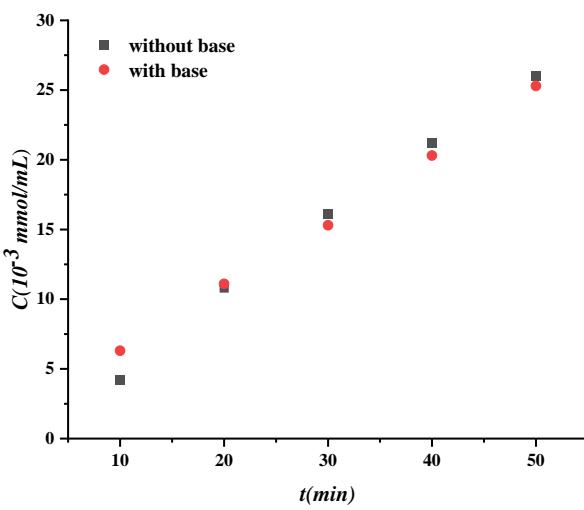
6.2.6 The deuteration experiment.

According to the general procedure of the kinetic experiment except *t*-BuCO₂K was not added in eq. 2. Kinetic Data is shown in **Supplementary Table 6**, Kinetic plots is shown in **Supplementary Figure 10**.



Supplementary Table 6. Kinetic data of time-course for the reaction with or without base.

<i>t</i> (min)	<i>C</i> with base (10^{-3} mmol/mL)	<i>C</i> without base (10^{-3} mmol/ml)
10	6.3	4.2
20	11.1	10.8
30	15.3	16.1
40	20.3	21.2
50	25.3	26.0

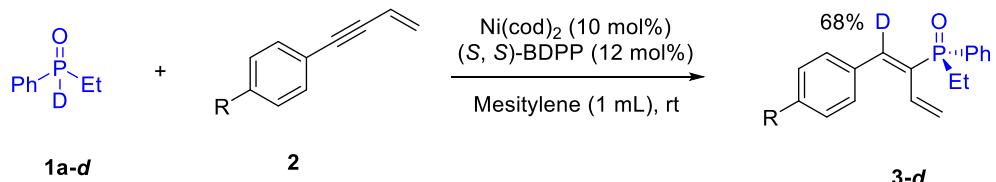


Supplementary Figure 10. Time-course for the reaction with or without base.

Synthesis of deuterated SPO

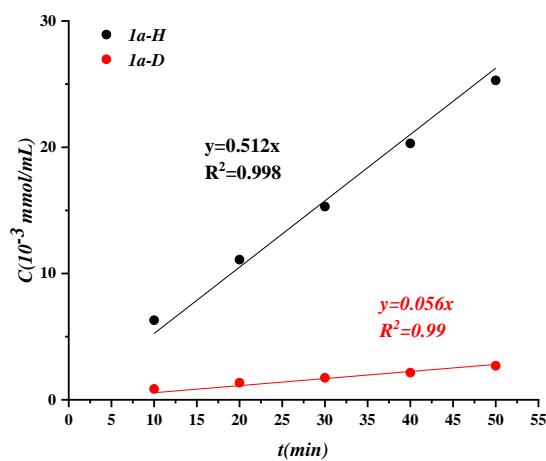
Dissolve SPO in 1 mL of D₂O under argon atmosphere and stir at 60 °C for 12 h. After completion of the reaction, the solvent was removed through the vacuum oven to obtain the deuterated SPO (\pm) in quantitative yield (96% D).

The deuteration experiment is conducted following the general procedure of the kinetic experiment without *t*-BuCO₂K. Kinetic data is shown in **Supplementary Table 7**, Kinetic plots is shown in **Supplementary Figure 11**.



Supplementary Table 7. Kinetic datas of time-course for the deuterated reaction.

t (min)	10	20	30	40	50
C (10^{-3} mmol/mL)	0.86	1.35	1.74	2.15	2.69

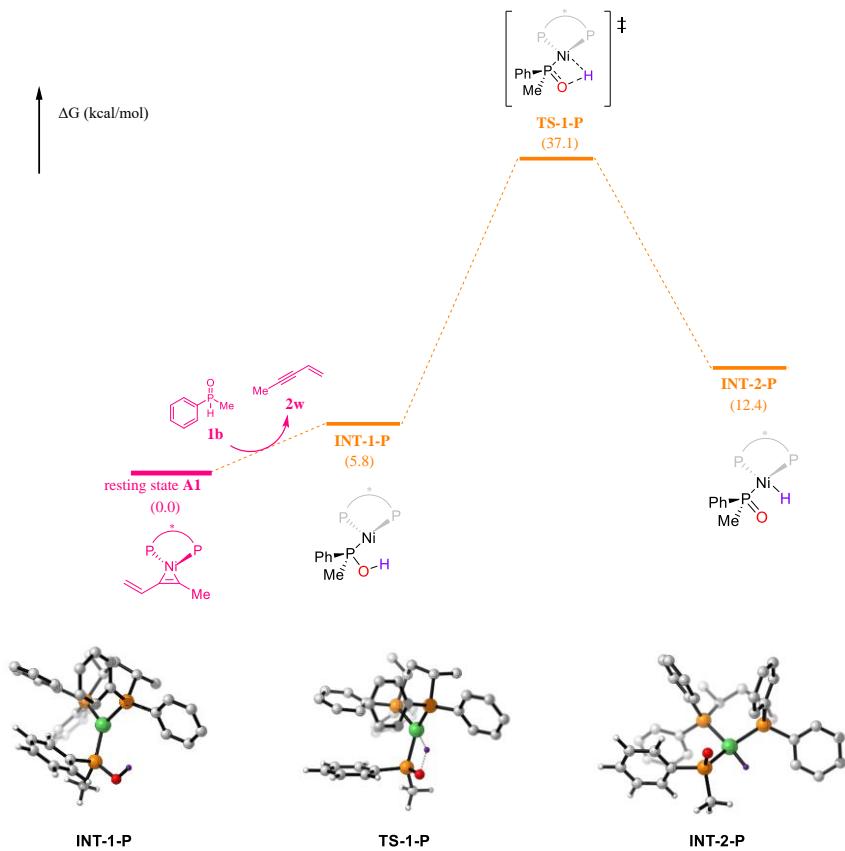


Supplementary Figure 11. Time-course for the deuterated reaction.

7. DFT Computational Studies.

All DFT calculations were performed using Gaussian 16.⁵ Geometry optimizations were carried out with the B3LYP-D3(BJ) functional. The Lanl2dz basis set with ECP was used for Ni, and the 6-31G(d) basis set was used for other atoms. Frequency calculations and the intrinsic reaction coordinate (IRC) calculations at the same level as the geometry optimizations were performed to ensure each stationary point to be either a minimum or a transition state which were correctly connected. Conformational search has been performed for all starting materials, intermediates and products by crest-xTB 6.4.0.⁶⁻⁸

The single-point energies were calculated at the level of M06/SDD with ECP for Ni, and M06/6-311++g(d,p) for other atoms. Solvent effects (solvent=mesitylene) are calculated using the SMD implicit solvation model based on the optimized geometries. All of the enthalpies and Gibbs energies were calculated at standard conditions and relative energies were shown in kcal/mol (1 atm and 298.15 K). Quasi-harmonic corrected Gibbs free energy at 253.15 K (-20 °C) of **TS-1a** and **TS-1a-S** were performed with GoodVibes-3.0.1 program.⁹⁻¹⁰ 3D models of optimized structures were displayed with CYLview.



Supplementary Figure 12. Free energy profile for the P-H oxidative addition pathway. Computed at the SMD(mesitylene)/M06/6-311++G(d,p)/SDD//B3LYP-D3(BJ)/6-31G(d)/LANL2DZ level.

Energy Data for all Reported Structures

Supplementary Table 8. Single-Point Energies (SPEs) and Gibbs free energies (G)

Structures	SPE(a.u.) ^a	G(a.u.) ^b
resting state A1	-2170.267979	-2,169.734147
resting state A2	-2170.268161	-2169.734073
1b	-688.598969	-688.490004
INT-1	-2858.893780	-2,858.220589
TS-1a	-2858.860894	-2858.191233
TS-1b	-2858.846037	-2858.180201
TS-1-regio	-2858.846647	-2858.180093
INT-2	-2858.896556	-2858.224544
TS-2	-2858.875785	-2858.202871
2w	-193.955914	-193.896397
3bw	-882.613494	-882.416582
TS-1a-S	-2858.855436	-2858.187252
INT-1-P	-2664.900122	-2,664.318439
TS-1-P	-2664.845354	-2,664.268558
INT-2-P	-2664.890759	-2,664.308012

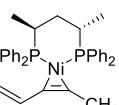
[a] Single point energy computed at the levels of M06/SDD and M06/6-311++g(d,p).

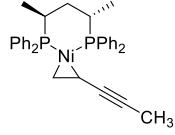
[b] A standard state at 1 atm and 298K was used.

Structure	SP	ZPE	T*S	G(253.15K) ^c
TS-1a	-2858.860894	0.730931	0.089911	-2858.184201
TS-1a-S	-2858.855436	0.730461	0.097212	-2858.179447
ΔAG(253.15k)=3.0 kcal/mol, predicted ee at -20 °C is 99%				

[c] Quasi-harmonic treatment at T = 253.15 K, c = 0.1 M with ZPE scale factor=0.977.

Cartesian Coordinates (Å) of Optimized Structures.

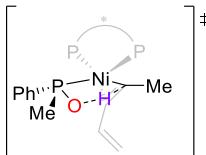
				H	0.17156	1.20422	3.59891
				C	1.43099	0.09019	2.27456
				H	1.27646	-0.93381	2.63152
Resting state A1				C	-1.27222	-1.17195	3.04620
P	-1.61800	-0.04809	0.51339	H	-0.66952	-1.93080	2.53517
P	1.70919	-0.11409	0.42499	H	-2.29794	-1.54536	3.09083
C	-1.20967	0.18392	2.32690	H	-0.89710	-1.07449	4.07260
H	-1.99050	0.82008	2.76338	C	2.60847	0.68963	3.05034
C	0.14282	0.90030	2.54271	H	2.74437	1.74742	2.80560
H	0.17680	1.83154	1.96339	H	3.54377	0.16410	2.83467

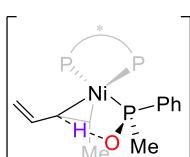
H	2.42102	0.61848	4.12906	H	4.17260	0.09211	-1.22354
C	-2.07483	1.63447	-0.07827	C	0.68118	-1.86709	-2.16101
C	-2.21136	1.79047	-1.46927	C	-0.60391	-1.83734	-2.24687
H	-2.07001	0.92815	-2.11497	Ni	-0.00516	-0.90624	-0.67969
C	-2.49068	3.03903	-2.02044	C	-1.73040	-2.25269	-3.04709
H	-2.59372	3.14092	-3.09721	H	-1.50950	-2.98279	-3.83134
C	-2.62244	4.15811	-1.19298	C	-2.99437	-1.81640	-2.92799
H	-2.82782	5.13452	-1.62281	H	-3.27979	-1.09912	-2.16659
C	-2.48624	4.01509	0.18729	H	-3.77849	-2.17446	-3.58913
H	-2.58469	4.88013	0.83744	C	1.96945	-2.29791	-2.75492
C	-2.21946	2.76062	0.74159	H	1.81874	-2.95577	-3.62228
H	-2.11517	2.67482	1.81787	H	2.55553	-1.43097	-3.08477
C	-3.24898	-0.88698	0.64200	H	2.58869	-2.82667	-2.02162
C	-3.31224	-2.25757	0.35879	 Resting state A2			
H	-2.41872	-2.76254	0.00376	P	1.93166	-0.32861	-0.20994
C	-4.51477	-2.95052	0.50015	P	-1.40685	-0.56807	-0.53096
H	-4.55572	-4.01215	0.27319	C	1.74151	-0.80653	-2.00979
C	-5.66541	-2.27699	0.91367	H	2.59303	-0.38778	-2.56190
H	-6.60406	-2.81475	1.01576	C	0.45441	-0.21975	-2.63925
C	-5.61251	-0.90735	1.18512	H	0.37880	0.85195	-2.41698
H	-6.50917	-0.37897	1.49773	H	0.57920	-0.28790	-3.72959
C	-4.40906	-0.21525	1.05159	C	-0.89261	-0.89928	-2.30795
H	-4.37288	0.85169	1.25373	H	-0.74584	-1.98384	-2.35601
C	2.19534	1.58101	-0.10337	Ni	0.16992	-0.71852	0.97607
C	3.39622	2.20819	0.26915	C	-2.17034	1.41407	2.91860
H	4.13747	1.66204	0.84221	C	-1.52625	0.38433	2.86839
C	3.65340	3.52534	-0.10922	C	-0.80309	-0.84269	2.73140
H	4.58759	3.99705	0.18338	H	-1.40055	-1.75441	2.75619
C	2.71399	4.23825	-0.85961	C	0.60402	-0.92923	2.91906
H	2.91550	5.26679	-1.14640	H	1.15349	-0.08122	3.32321
C	1.52440	3.62158	-1.24652	H	1.04112	-1.90181	3.13823
H	0.78643	4.16063	-1.83350	C	1.82172	-2.33423	-2.13835
C	1.27420	2.29888	-0.87912	H	2.81946	-2.69649	-1.87660
H	0.35874	1.81443	-1.19479	H	1.10597	-2.83244	-1.47501
C	3.27131	-1.07788	0.34854	H	1.60456	-2.64457	-3.16799
C	3.41071	-2.23297	1.13402	C	-1.94959	-0.50091	-3.34555
H	2.63757	-2.50165	1.84825	H	-2.06870	0.58633	-3.38178
C	4.52728	-3.05694	1.00035	H	-1.64932	-0.84265	-4.34404
H	4.61837	-3.94434	1.62070	H	-2.92762	-0.93482	-3.11860
C	5.52161	-2.74692	0.07004	C	-2.93317	2.65785	2.89684

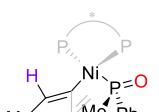
H	-2.26824	3.52952	2.93560	H	2.98812	4.13605	-2.27933
H	-3.52062	2.74270	1.97401	H	2.15851	4.09073	1.94157
H	-3.62465	2.73334	3.74649	H	2.71446	5.35490	-0.13069
C	-2.87647	-1.64341	-0.28662		1b		
C	-3.71083	-1.37311	0.81345				
C	-3.13749	-2.78161	-1.06233				
C	-4.78607	-2.20730	1.10922				
H	-3.50506	-0.51229	1.44257	C	-0.15090	-0.00542	-0.16430
C	-4.21250	-3.62036	-0.75883	C	-0.88843	-1.17941	-0.36539
H	-2.50660	-3.02684	-1.91014	C	-0.80819	1.17954	0.18377
C	-5.04291	-3.33440	0.32374	C	-2.27327	-1.16883	-0.21083
H	-5.42190	-1.97970	1.96051	H	-0.38719	-2.10239	-0.64920
H	-4.39941	-4.49639	-1.37407	C	-2.19475	1.18690	0.33963
H	-5.87995	-3.98601	0.55809	H	-0.22131	2.08247	0.32273
C	-2.12481	1.12261	-0.63484	C	-2.92599	0.01465	0.14414
C	-3.45449	1.37893	-0.99871	H	-2.84395	-2.07963	-0.36833
C	-1.28040	2.20590	-0.35151	H	-2.70417	2.10741	0.60996
C	-3.92269	2.69049	-1.08850	H	-4.00571	0.02156	0.26406
H	-4.12684	0.55240	-1.20349	C	2.27648	-1.19844	0.85979
C	-1.74333	3.51703	-0.45647	H	1.80596	-2.17312	0.69340
H	-0.26301	2.02156	-0.03235	H	2.04873	-0.85999	1.87483
C	-3.06686	3.76309	-0.82458	P	1.65880	0.04164	-0.33155
H	-4.95636	2.87488	-1.36867	O	2.24685	1.41440	-0.20943
H	-1.06877	4.33973	-0.23632	H	1.88022	-0.61210	-1.57569
H	-3.43411	4.78316	-0.89751	H	3.36107	-1.29803	0.75611
C	3.58864	-1.02829	0.17689		INT-1		
C	4.77190	-0.52319	-0.38060				
C	3.65441	-2.13147	1.03746				
C	5.99833	-1.11835	-0.08831				
H	4.73497	0.34559	-1.03198				
C	4.88159	-2.73089	1.32571	P	1.44569	0.63797	-0.55484
H	2.73638	-2.50508	1.48135	P	-1.92010	0.43813	-0.24831
C	6.05434	-2.22530	0.76292	C	0.90010	0.42275	-2.34322
H	6.91132	-0.71768	-0.52055	H	1.59123	1.01782	-2.95564
H	4.92236	-3.58644	1.99427	C	-0.51877	0.96053	-2.63744
H	7.01107	-2.68687	0.99125	H	-0.60909	2.00607	-2.32249
C	2.26326	1.48336	-0.26019	H	-0.61529	0.97561	-3.73291
C	2.58697	2.20492	-1.41730	C	-1.75018	0.19189	-2.10369
C	2.11341	2.18399	0.94898	H	-1.58057	-0.88374	-2.23137
C	2.74706	3.59148	-1.37049	Ni	-0.13745	-0.03124	0.93841
H	2.70573	1.69507	-2.36749	P	-0.07663	-2.19433	1.23858
C	2.28241	3.56640	0.99822	O	1.21492	-2.71697	2.16204
H	1.83478	1.63670	1.84431	H	1.67132	-1.92572	2.51698
C	2.59396	4.27578	-0.16457	C	2.90443	-0.05368	3.25188

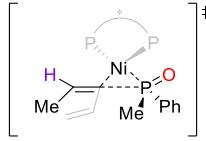
C	1.71630	0.16995	3.10634	H	3.93009	1.44219	-2.01056
C	0.31097	0.36295	2.93679	C	4.72976	-1.81006	-0.06240
H	-0.32606	-0.24440	3.57823	H	2.71240	-1.67256	0.67527
C	-0.24740	1.49029	2.30955	C	5.70602	-1.22476	-0.86901
H	0.38485	2.31498	2.00041	H	6.17046	0.41172	-2.19672
H	-1.27898	1.75129	2.52505	H	4.95085	-2.71730	0.49404
C	1.04853	-1.04240	-2.77232	H	6.69267	-1.67332	-0.94639
H	2.09480	-1.35621	-2.75809	C	1.90169	2.42600	-0.46508
H	0.49547	-1.71704	-2.11740	C	1.64273	3.38117	-1.45802
H	0.66684	-1.17454	-3.79267	C	2.50204	2.85734	0.73265
C	-2.98064	0.62230	-2.91594	C	1.95265	4.72887	-1.25429
H	-3.08194	1.71204	-2.90819	H	1.19538	3.08839	-2.40063
H	-2.87401	0.30093	-3.95965	C	2.81918	4.19866	0.93204
H	-3.91283	0.20596	-2.52644	H	2.71517	2.13051	1.51144
C	4.34138	-0.27037	3.39552	C	2.53754	5.14364	-0.05875
H	4.54912	-1.14005	4.03079	H	1.73830	5.45182	-2.03698
H	4.81368	-0.44745	2.42146	H	3.28206	4.50848	1.86511
H	4.83161	0.59666	3.85602	H	2.77609	6.19156	0.09981
C	-3.39893	-0.54844	0.22481	C	0.05624	-3.37117	-0.16149
C	-3.90445	-0.35199	1.52255	C	-1.05365	-3.58141	-0.99439
C	-3.95424	-1.57239	-0.55476	C	1.27500	-3.97513	-0.49549
C	-4.93235	-1.14734	2.01978	C	-0.94167	-4.35679	-2.14711
H	-3.47696	0.42789	2.14678	H	-2.00915	-3.13546	-0.74181
C	-4.97433	-2.38456	-0.04982	C	1.38744	-4.74811	-1.65214
H	-3.59157	-1.75101	-1.56077	H	2.13059	-3.83912	0.15482
C	-5.46765	-2.17531	1.23680	C	0.28414	-4.93502	-2.48592
H	-5.30963	-0.97491	3.02402	H	-1.81076	-4.50944	-2.78194
H	-5.38369	-3.17818	-0.66897	H	2.34141	-5.20457	-1.90218
H	-6.26056	-2.80565	1.62861	H	0.37589	-5.53180	-3.38905
C	-2.57538	2.16137	-0.18322	C	-1.47961	-2.94325	2.17563
C	-3.93910	2.47670	-0.27910	H	-1.63236	-2.36767	3.09333
C	-1.64742	3.20890	-0.08919	H	-2.39873	-2.88732	1.58665
C	-4.35978	3.80700	-0.28438	H	-1.26430	-3.98625	2.42729
H	-4.67372	1.68097	-0.34720				
C	-2.06537	4.53916	-0.11423	TS-1a			
H	-0.59471	2.97939	0.01238	P	1.52290	0.66545	-0.51213
C	-3.42451	4.84184	-0.20807	P	-1.90624	0.40058	-0.23817
H	-5.41998	4.03568	-0.35369	C	0.97747	0.50970	-2.31022
H	-1.32508	5.33190	-0.05052	H	1.63627	1.18070	-2.87802
H	-3.75551	5.87675	-0.21615	C	-0.46451	0.98353	-2.59294

H	-0.60575	2.01833	-2.26435	H	-0.68626	3.02765	-0.14397
H	-0.55690	1.01367	-3.68820	C	-3.61151	4.73111	-0.38859
C	-1.66657	0.15002	-2.08507	H	-5.56684	3.82223	-0.42685
H	-1.44476	-0.91613	-2.20455	H	-1.53559	5.32900	-0.31936
Ni	-0.10427	0.02420	0.99747	H	-3.99308	5.74677	-0.44534
P	0.08558	-2.22770	1.15690	C	3.23607	-0.01987	-0.63152
O	1.39758	-2.72133	1.92941	C	4.20253	0.57682	-1.45772
H	1.86923	-1.78326	2.57069	C	3.58202	-1.15527	0.10729
C	2.19897	-0.72588	3.37757	C	5.48314	0.03688	-1.55290
C	1.19237	0.02911	3.24460	H	3.95530	1.47424	-2.01789
C	-0.03668	0.61962	3.02718	C	4.86853	-1.69383	0.01519
H	-0.87961	0.24075	3.60566	H	2.85032	-1.62070	0.75399
C	-0.24833	1.69428	2.11575	C	5.81936	-1.10271	-0.81533
H	0.57487	2.35754	1.87476	H	6.22191	0.50715	-2.19650
H	-1.21880	2.17911	2.15145	H	5.12131	-2.57612	0.59723
C	1.20599	-0.91073	-2.83996	H	6.81999	-1.52057	-0.88641
H	2.26184	-1.18668	-2.80232	C	1.98247	2.44666	-0.36814
H	0.65143	-1.65460	-2.26938	C	1.63789	3.45131	-1.28168
H	0.87393	-0.97182	-3.88404	C	2.68681	2.81488	0.79347
C	-2.89298	0.52852	-2.93176	C	1.97573	4.78641	-1.03853
H	-3.02047	1.61522	-2.95309	H	1.10752	3.20747	-2.19484
H	-2.75318	0.18452	-3.96400	C	3.03040	4.14265	1.03199
H	-3.82495	0.10184	-2.55507	H	2.96325	2.04681	1.51187
C	3.42647	-0.84016	4.21704	C	2.66998	5.13723	0.11773
H	3.43167	-1.79955	4.74811	H	1.69869	5.54885	-1.76180
H	4.31934	-0.82845	3.57971	H	3.57674	4.40351	1.93418
H	3.51754	-0.03510	4.95548	H	2.93188	6.17448	0.30602
C	-3.35717	-0.62235	0.23725	C	0.13131	-3.25109	-0.36612
C	-3.81386	-0.46325	1.55812	C	-1.01652	-3.43916	-1.14872
C	-3.94835	-1.61433	-0.55598	C	1.34189	-3.80997	-0.79605
C	-4.83403	-1.26241	2.06433	C	-0.95093	-4.14018	-2.35250
H	-3.35124	0.28785	2.19295	H	-1.96666	-3.04246	-0.81219
C	-4.95907	-2.43215	-0.04162	C	1.40846	-4.50957	-2.00174
H	-3.61957	-1.76725	-1.57725	H	2.22430	-3.69073	-0.17894
C	-5.40661	-2.25839	1.26669	C	0.26654	-4.66851	-2.78880
H	-5.17347	-1.12081	3.08658	H	-1.84990	-4.27730	-2.94839
H	-5.39592	-3.20330	-0.67005	H	2.35595	-4.93033	-2.32773
H	-6.19186	-2.89396	1.66527	H	0.32161	-5.20835	-3.73006
C	-2.62988	2.09902	-0.23484	C	-1.31822	-3.00336	2.07398
C	-4.00901	2.34365	-0.30664	H	-1.41805	-2.49268	3.03645
C	-1.75272	3.19469	-0.23159	H	-2.25831	-2.88814	1.52888
C	-4.49507	3.65001	-0.37656	H	-1.11566	-4.06528	2.24392
H	-4.70580	1.51216	-0.30845				
C	-2.23689	4.49905	-0.31890				

				C	3.46001	0.51741	-0.57853
				C	4.65491	2.82768	-1.58697
				H	2.66910	3.64770	-1.65957
				C	4.84471	0.56679	-0.75018
TS-1b				H	2.99230	-0.37155	-0.17542
P	0.83773	1.46428	-0.71571	C	5.44290	1.72136	-1.25505
P	-1.97038	-0.34948	-0.62624	H	5.11942	3.73114	-1.97315
C	0.26570	1.44929	-2.49582	H	5.44270	-0.29888	-0.48394
H	0.69752	2.32862	-2.99022	H	6.52090	1.76500	-1.38541
C	-1.27197	1.56886	-2.60659	C	0.39530	3.16595	-0.14235
H	-1.63633	2.36084	-1.94099	C	0.07651	4.23336	-0.99436
H	-1.49573	1.91296	-3.62664	C	0.36515	3.38949	1.24406
C	-2.12545	0.30443	-2.37966	C	-0.26802	5.48395	-0.47728
H	-1.71625	-0.49999	-3.00232	H	0.08834	4.09943	-2.07087
C	0.80129	-0.11643	2.06922	C	0.03247	4.64007	1.76179
C	-0.28471	-0.73507	2.49679	H	0.58255	2.56908	1.91988
Ni	0.01615	-0.28613	0.36200	C	-0.29059	5.69191	0.90165
P	0.69912	-2.47716	0.17011	H	-0.51920	6.29514	-1.15527
O	0.07003	-3.10949	1.49403	H	0.01802	4.78975	2.83795
H	-0.28707	-2.05670	2.03866	H	-0.56059	6.66452	1.30315
C	-2.81888	-1.97638	-0.68462	C	0.82729	0.20507	-3.19549
C	-3.20560	-2.63175	-1.86133	H	0.44787	0.13519	-4.22256
C	-2.98720	-2.63741	0.54315	H	1.91961	0.24281	-3.23629
C	-3.75468	-3.91525	-1.81165	H	0.54956	-0.70731	-2.65820
H	-3.06764	-2.16009	-2.82759	C	-3.56763	0.59270	-2.81985
C	-3.53911	-3.91404	0.59215	H	-3.97483	1.44732	-2.27112
H	-2.65438	-2.15656	1.45635	H	-3.59216	0.83463	-3.88966
C	-3.92418	-4.55868	-0.58611	H	-4.23496	-0.25561	-2.65001
H	-4.04465	-4.41098	-2.73400	C	0.19660	-3.58473	-1.21937
H	-3.64886	-4.41434	1.54967	H	-0.88675	-3.70094	-1.19188
H	-4.34447	-5.55962	-0.54878	H	0.47284	-3.14704	-2.18469
C	-3.17086	0.66995	0.32583	H	0.66790	-4.56748	-1.12208
C	-4.55324	0.42950	0.32218	C	2.49902	-2.80838	0.26911
C	-2.66938	1.73495	1.08413	C	3.29533	-2.99341	-0.87051
C	-5.41258	1.25377	1.04790	C	3.11988	-2.75585	1.52632
H	-4.95456	-0.40922	-0.23723	C	4.67992	-3.12889	-0.75654
C	-3.52933	2.56793	1.79920	H	2.83831	-3.02587	-1.85560
H	-1.59972	1.88843	1.12776	C	4.50243	-2.88765	1.63977
C	-4.90400	2.32935	1.78141	H	2.50618	-2.61354	2.40900
H	-6.48103	1.05586	1.04232	C	5.28838	-3.07522	0.49906
H	-3.11861	3.39414	2.37285	H	5.28295	-3.27534	-1.64893
H	-5.57745	2.96990	2.34424	H	4.96896	-2.84718	2.62050
C	2.66268	1.61817	-0.91450	H	6.36618	-3.18104	0.58882
C	3.27237	2.77785	-1.41691	C	-1.19436	-0.41673	3.65315

H	-0.80586	0.40205	4.27431	C	-3.49463	3.39915	-0.00814
H	-2.18591	-0.12031	3.28801	H	-1.68604	2.34039	0.49721
H	-1.34061	-1.29554	4.29441	C	-4.76328	3.30336	-0.57978
C	1.98595	0.52303	2.58054	H	-6.19569	2.00098	-1.53347
H	2.51793	1.21005	1.92629	H	-3.14215	4.34018	0.40335
C	2.49203	0.26499	3.80200	H	-5.41416	4.17277	-0.61390
H	2.02007	-0.45343	4.46646	C	2.99342	1.16542	-0.48405
H	3.39468	0.75532	4.15647	C	3.77297	1.84235	-1.43405
				C	3.60875	0.63727	0.65558
TS-1-regio				C	5.14900	1.96857	-1.25642
				H	3.30480	2.28324	-2.30985
				C	4.98731	0.77342	0.83735
				H	3.01424	0.10318	1.38775
P	1.16778	1.02594	-0.65325	C	5.75938	1.43300	-0.11817
P	-1.86557	-0.32208	-0.45933	H	5.74497	2.49039	-2.00026
C	0.92076	0.61444	-2.45231	H	5.45353	0.35511	1.72530
H	1.36281	1.42458	-3.04614	H	6.83206	1.53542	0.02156
C	-0.57671	0.55831	-2.83119	C	0.69969	2.80751	-0.53382
H	-1.07123	1.50546	-2.58673	C	0.32638	3.61184	-1.61741
H	-0.61344	0.47650	-3.92661	C	0.68869	3.36500	0.75553
C	-1.41909	-0.60454	-2.26658	C	-0.08029	4.93315	-1.41538
H	-0.79238	-1.50241	-2.23958	H	0.33872	3.22068	-2.62846
C	0.40150	0.45575	2.90038	C	0.29544	4.68623	0.95449
C	-0.80160	0.05545	2.51852	H	0.97349	2.75597	1.60603
Ni	-0.07108	-0.10395	0.81490	C	-0.10247	5.47329	-0.13022
P	0.99357	-2.09536	1.33440	H	-0.38031	5.53794	-2.26683
O	1.98273	-1.59544	2.49020	H	0.29414	5.09754	1.96024
H	1.39381	-0.51725	2.73606	H	-0.42046	6.50054	0.02527
C	-2.88183	-1.80543	-0.08253	C	1.66546	-0.68014	-2.80482
C	-2.46247	-3.06957	-0.52835	H	1.45801	-0.96200	-3.84464
C	-4.01488	-1.73393	0.74127	H	2.74549	-0.55776	-2.69357
C	-3.15580	-4.22398	-0.16805	H	1.37232	-1.51238	-2.16212
H	-1.58597	-3.15684	-1.16166	C	-2.61653	-0.87167	-3.18624
C	-4.70491	-2.88977	1.10871	H	-3.21395	0.03526	-3.32223
H	-4.36454	-0.76971	1.09313	H	-2.26229	-1.18835	-4.17495
C	-4.27918	-4.13925	0.65660	H	-3.26886	-1.65680	-2.79383
H	-2.81570	-5.19042	-0.53009	C	0.04497	-3.49949	2.07085
H	-5.58025	-2.81062	1.74756	H	-0.52428	-3.09293	2.91225
H	-4.81779	-5.03815	0.94189	H	-0.66705	-3.91974	1.35578
C	-3.08384	1.05459	-0.50521	H	0.71575	-4.28500	2.43312
C	-4.36925	0.96496	-1.06573	C	2.02276	-2.94243	0.08383
C	-2.66536	2.27768	0.03765	C	1.43244	-3.80771	-0.85222
C	-5.20244	2.08219	-1.10025	C	3.38747	-2.64874	-0.03957
H	-4.72482	0.01845	-1.45846	C	2.18170	-4.34623	-1.89759

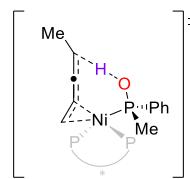
H	0.38032	-4.06378	-0.76422	H	3.12794	-3.49349	1.09283
C	4.13462	-3.18046	-1.09042	C	4.63530	-0.01886	1.92913
H	3.85590	-2.00375	0.69291	H	2.73526	0.77972	1.31494
C	3.53496	-4.02464	-2.02730	C	5.40712	-1.17134	2.08908
H	1.70942	-5.01511	-2.61259	H	5.46135	-3.31935	1.90297
H	5.19019	-2.93581	-1.17492	H	5.05764	0.96052	2.13385
H	4.11793	-4.43575	-2.84670	H	6.43371	-1.09569	2.43666
C	-2.17404	-0.01125	3.08079	C	0.87298	-3.01889	-0.27637
H	-2.53790	-1.04611	3.07942	C	0.38390	-4.21937	0.25922
H	-2.20431	0.35911	4.11464	C	1.24188	-2.98007	-1.63270
H	-2.87890	0.57086	2.47558	C	0.23126	-5.34827	-0.54836
C	0.75869	1.52587	3.82518	H	0.11897	-4.29430	1.30720
H	-0.06210	2.01169	4.36183	C	1.09123	-4.11221	-2.43199
C	2.01185	1.95585	4.04664	H	1.67897	-2.06434	-2.02712
H	2.85819	1.51740	3.52461	C	0.57442	-5.29542	-1.89857
H	2.22240	2.76102	4.74481	H	-0.15483	-6.26779	-0.11707
 INT-2							
P	1.00500	-1.45874	0.69191	C	-4.11490	1.76437	-0.14115
P	-2.06783	-0.02015	0.64517	C	-4.09250	3.17039	2.26536
C	0.23831	-1.88395	2.34989	H	-2.57945	1.78947	2.89350
H	0.73517	-2.80405	2.68176	C	-4.95061	2.86713	0.03145
C	-1.27835	-2.17547	2.28906	H	-4.11693	1.23320	-1.08595
H	-1.51610	-2.83139	1.44461	C	-4.94319	3.57339	1.23528
H	-1.52703	-2.74853	3.19372	H	-4.07300	3.71759	3.20362
C	-2.22940	-0.96829	2.25593	H	-5.60343	3.17739	-0.77953
H	-1.90387	-0.24844	3.01417	H	-5.59285	4.43370	1.36839
C	-1.38892	2.48648	-1.76747	C	-2.84627	-1.11566	-0.60468
C	-0.68590	2.22303	-0.64543	C	-2.00872	-1.70084	-1.56569
Ni	0.06115	0.46201	-0.18594	C	-4.21493	-1.43430	-0.61790
C	-0.60164	3.17038	0.47040	C	-2.51132	-2.61382	-2.49269
H	-1.29124	4.01618	0.47272	H	-0.95644	-1.44173	-1.58540
C	0.23621	3.04649	1.51400	C	-4.72039	-2.33499	-1.55400
H	0.96184	2.23823	1.55530	H	-4.88741	-0.96656	0.09229
P	1.78101	0.84283	-1.58998	C	-3.86839	-2.93459	-2.48594
O	2.70307	-0.37603	-1.73195	H	-1.83587	-3.07304	-3.20784
H	-1.44898	1.70758	-2.52745	H	-5.78079	-2.57156	-1.55452
C	1.18534	1.30704	-3.27981	H	-4.26551	-3.64349	-3.20708
C	2.76763	-1.36841	1.17742	C	0.57605	-0.78759	3.37171
C	3.54455	-2.52122	1.33793	H	0.05577	-0.97908	4.31834
C	3.32258	-0.11844	1.47314	H	1.64852	-0.75565	3.57380
C	4.86059	-2.42098	1.79038	H	0.27786	0.20478	3.01514

C	-3.65509	-1.41090	2.60436	H	3.12360	0.34751	-1.14068
H	-3.99839	-2.20034	1.92909	C	2.22724	1.67925	-2.47301
H	-3.67826	-1.81209	3.62504	H	1.36998	1.97971	-3.06624
H	-4.36300	-0.57890	2.55221	H	3.05137	2.38389	-2.41202
C	2.82130	2.29900	-1.15946	C	-1.51156	-1.09577	3.29674
C	2.34134	3.61535	-1.13979	H	-2.00914	-2.06331	3.39635
C	4.16494	2.05523	-0.84543	H	-0.48484	-1.28489	2.96808
C	3.18884	4.66812	-0.79657	H	-1.48470	-0.62788	4.28901
H	1.30444	3.81372	-1.38464	C	-0.10840	2.91177	3.29921
C	5.01048	3.10903	-0.49482	H	-0.70773	3.74258	2.91348
H	4.52688	1.03343	-0.88869	H	-0.39000	2.75953	4.34867
C	4.52302	4.41702	-0.46525	H	0.94636	3.20297	3.27157
H	2.80743	5.68598	-0.78400	C	0.38649	-0.36111	-4.12556
H	6.05148	2.90968	-0.25229	H	0.14538	-1.15593	-4.84150
H	5.18018	5.23893	-0.19296	H	-0.37045	0.42708	-4.25385
H	0.24872	3.76501	2.32892	H	1.35339	0.07744	-4.39071
H	0.75360	2.30806	-3.30871	C	2.14593	1.91873	1.12973
H	0.43755	0.58262	-3.61878	C	2.88173	3.00813	0.64599
H	2.05465	1.25585	-3.94317	C	2.81921	0.89845	1.82545
C	-2.10856	3.75591	-2.14177	C	4.25752	3.08806	0.87021
H	-1.67285	4.19627	-3.05050	H	2.38915	3.78274	0.07015
H	-3.16517	3.55543	-2.36537	C	4.19139	0.98544	2.05145
H	-2.07483	4.51525	-1.35697	H	2.27742	0.00799	2.13366
				C	4.91594	2.08149	1.57707
				H	4.81561	3.93684	0.48367
				H	4.69951	0.18383	2.57962
				H	5.98754	2.14269	1.74504
TS-2							
P	-2.03689	-0.81057	0.55883	C	-0.29022	3.11950	-0.03546
P	0.37385	1.60969	0.77182	C	-0.06890	4.44154	0.38529
C	-2.26878	-0.18832	2.31298	C	-1.13420	2.89845	-1.13473
H	-3.33904	-0.26291	2.54669	H	-0.68331	5.50680	-0.27351
C	-1.86783	1.29685	2.47229	C	-1.75989	3.96113	-1.78569
H	-2.36160	1.91395	1.71123	H	-1.30288	1.88039	-1.46725
H	-2.28534	1.62239	3.43571	C	-1.53432	5.26919	-1.35578
C	-0.36055	1.62933	2.49959	H	-0.50072	6.52421	0.06171
H	0.17499	0.81203	2.99406	H	-2.42445	3.76140	-2.62141
Ni	-0.07898	-0.29319	-0.25893	H	-2.01661	6.10175	-1.86070
P	1.36759	-2.02920	-0.21995	C	-2.72831	-2.51262	0.67656
O	1.22909	-2.06746	1.31226	C	-4.04249	-2.83209	0.30864
H	-0.30434	-1.69643	-2.51628	C	-1.88239	-3.53277	1.14664
C	0.39558	-0.88960	-2.71767	C	-4.50454	-4.14579	0.40837
C	1.18299	-0.45942	-1.68876	H	-4.70524	-2.05525	-0.05936
C	2.25958	0.53585	-1.77223	C	-2.35248	-4.84094	1.25553

H	-0.85801	-3.29389	1.41972	H	-3.46814	0.21248	0.00001
C	-3.66269	-5.15219	0.88384				
H	-5.52450	-4.38131	0.11604				
H	-1.69015	-5.62012	1.62324				
H	-4.02399	-6.17403	0.96090				
				3bw			
C	-3.31186	0.09177	-0.41842	P	0.45097	1.03819	-0.38282
C	-4.36500	0.83014	0.13720	O	0.42518	2.36856	0.31916
C	-3.17112	0.07689	-1.81660	C	-3.58482	-1.16179	0.05076
C	-5.23955	1.55107	-0.67917	C	-1.12269	0.13138	-0.21281
H	-4.50967	0.85423	1.21180	C	-1.26942	-1.19445	-0.63926
C	-4.05143	0.78311	-2.63381	H	-0.41856	-1.72743	-1.05626
H	-2.34611	-0.47641	-2.25515	C	2.58251	-0.70721	-0.62900
C	-5.08488	1.53208	-2.06513	H	2.53604	-0.42494	-1.67801
H	-6.04263	2.12789	-0.22874	C	1.70523	-0.14699	0.23070
H	-3.92464	0.75800	-3.71281	C	-2.49816	-1.83867	-0.50919
H	-5.76487	2.09519	-2.69815	H	-2.60890	-2.86831	-0.83794
C	3.17054	-2.21434	-0.56266	C	-3.44065	0.15753	0.48193
C	3.69400	-2.34879	-1.85608	H	-4.28427	0.68147	0.92250
C	4.04068	-2.23799	0.53233	C	-2.21126	0.80455	0.35121
C	5.06528	-2.50241	-2.04961	H	-2.07563	1.82790	0.68796
H	3.02968	-2.30998	-2.71476	C	0.68260	1.18861	-2.19346
C	5.41545	-2.38532	0.33856	H	1.65926	1.62631	-2.41797
H	3.61877	-2.14758	1.52713	H	0.57110	0.23535	-2.71717
C	5.93004	-2.51635	-0.95137	C	1.06221	0.26244	2.61604
H	5.46171	-2.60435	-3.05626	H	0.59075	1.21499	2.39825
H	6.08415	-2.39834	1.19533	H	1.06223	-0.07393	3.64873
H	7.00010	-2.62891	-1.10347	C	1.65240	-0.47379	1.66463
C	0.71679	-3.55684	-1.02834	H	2.13203	-1.40618	1.95614
H	-0.37406	-3.57504	-1.00762	H	-0.09340	1.87484	-2.54450
H	1.07147	-3.64190	-2.05746	H	-4.54180	-1.66581	0.15403
H	1.09823	-4.40509	-0.45115	C	3.67335	-1.68621	-0.30959
				H	3.72891	-1.94225	0.74984
				H	3.54163	-2.61326	-0.88335
				H	4.64666	-1.27248	-0.60507

2w

C	1.13169	-0.06476	0.00000
C	-0.06909	-0.23352	-0.00000
C	2.57225	0.16135	-0.00000
H	2.88535	0.72959	-0.88470
H	2.88542	0.72913	0.88497
H	3.12457	-0.78602	-0.00027
C	-1.47018	-0.48174	-0.00000
H	-1.77329	-1.52901	-0.00002
C	-2.41398	0.47153	0.00001
H	-2.15806	1.52667	0.00002



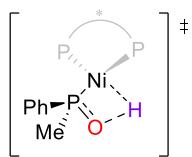
TS-1a-S

C	-0.65492	0.92412	2.66283	H	-3.29150	-0.91414	-1.95737
C	0.72680	1.52783	2.32966	C	-4.70436	2.04118	-2.87811
Ni	0.16372	-0.34518	-0.45372	H	-4.53257	3.88252	-1.77026
P	1.01668	-2.12254	0.60860	H	-4.69137	0.06431	-3.74387
O	0.07383	-3.41583	0.54496	H	-5.31014	2.47501	-3.66851
C	3.04091	1.20963	0.54879	C	-3.10036	1.61389	2.59269
C	3.84173	1.31355	1.69347	H	-2.93009	2.43341	3.30244
C	3.66344	0.97760	-0.68906	H	-3.95757	1.87891	1.96706
C	5.23091	1.18363	1.60260	H	-3.37391	0.72174	3.16377
H	3.39687	1.50190	2.66461	H	-0.87978	1.20366	3.70099
C	5.04719	0.87220	-0.78343	H	-0.58619	-0.16736	2.65823
H	3.04849	0.85855	-1.57655	H	1.45839	0.91028	2.86237
C	5.83715	0.96959	0.36533	C	0.84490	2.96711	2.84409
H	5.83688	1.25947	2.50133	H	1.83275	3.39436	2.65031
H	5.50844	0.68495	-1.74849	H	0.11121	3.62326	2.36525
H	6.91680	0.87195	0.29607	H	0.66832	2.99264	3.92642
C	0.98813	3.00622	-0.20785	H	-0.68624	-3.25765	-0.38358
C	1.95891	4.01236	-0.09129	C	0.20856	-1.01126	-2.43120
C	-0.20148	3.29725	-0.88764	C	-0.09300	0.37837	-2.32488
C	1.73083	5.28171	-0.62301	H	0.65680	1.07588	-2.68908
H	2.89888	3.80154	0.40834	H	-1.11706	0.71235	-2.45025
C	-0.43702	4.56880	-1.40898	H	1.21023	-1.31582	-2.73602
H	-0.93662	2.51717	-1.02954	C	-0.67093	-2.02777	-2.09585
C	0.52960	5.56662	-1.27643	C	-1.28142	-3.04420	-1.64266
H	2.49366	6.04964	-0.52724	C	-2.22301	-4.08609	-2.15034
H	-1.36996	4.76778	-1.92939	H	-1.79477	-5.08479	-2.00140
H	0.35522	6.55636	-1.68920	H	-3.15643	-4.05988	-1.57444
C	-3.16457	-1.13785	1.10904	H	-2.46717	-3.97011	-3.21337
C	-4.55671	-0.94564	1.12794	C	1.52295	-2.06092	2.38160
C	-2.63829	-2.30439	1.67945	H	0.63901	-1.88736	3.00089
C	-5.39654	-1.89108	1.71314	H	1.97971	-3.01123	2.67340
H	-4.98536	-0.05777	0.67581	H	2.23664	-1.24991	2.55455
C	-3.48119	-3.24895	2.26934	C	2.57960	-2.65380	-0.20034
H	-1.57737	-2.51032	1.61774	C	3.83923	-2.18507	0.19386
C	-4.86029	-3.04515	2.29035	C	2.49385	-3.51742	-1.30405
H	-6.47096	-1.72742	1.71726	C	4.98835	-2.57331	-0.49665
H	-3.05316	-4.15212	2.69539	H	3.93674	-1.50543	1.03344
H	-5.51660	-3.78393	2.74240	C	3.64125	-3.89831	-1.99746
C	-3.12972	0.91656	-0.82817	H	1.52215	-3.89385	-1.60697
C	-3.48621	2.27239	-0.79844	C	4.89412	-3.42723	-1.59540
C	-3.57551	0.13306	-1.90910	H	5.95596	-2.19800	-0.17559
C	-4.26504	2.83014	-1.81618	H	3.55935	-4.57017	-2.84800
H	-3.16080	2.90897	0.01648	H	5.78927	-3.72703	-2.13370
C	-4.35766	0.68764	-2.91890				



TS-1a-S

P	-1.76068	-0.81738	-0.45433	C	-4.91351	-3.10364	1.00411
P	1.61548	-0.97393	-0.60687	H	-5.28566	-4.11960	0.90244
C	-2.29500	0.72918	-1.30530	C	2.50866	2.94586	-1.36151
C	3.23799	-1.65857	-0.05814	H	2.58060	3.83941	-0.74891
C	-0.20696	-1.75624	-2.63783	C	-5.04384	-0.91171	2.00089
H	-0.15553	-0.70017	-2.93048	H	-5.52010	-0.21081	2.68126
H	-0.26164	-2.32097	-3.57977	C	2.54903	1.85827	-3.51689
C	-3.30732	-1.39184	0.36273	H	2.66644	1.90631	-4.59617
C	2.11227	0.54839	-1.51591	C	2.65914	3.01818	-2.74891
C	-1.54618	-2.00563	-1.90295	H	2.85851	3.97240	-3.22881
H	-1.50502	-2.99994	-1.44379	C	-5.53766	-2.21433	1.87674
C	1.11577	-2.18209	-1.94985	H	-6.39770	-2.53129	2.45968
H	1.89625	-2.19191	-2.72266	C	-2.95519	3.11765	-2.63473
C	-1.30385	1.66873	-1.62775	H	-3.21411	4.04122	-3.14539
H	-0.27782	1.48403	-1.33746	C	1.04062	-3.59355	-1.35192
C	5.61003	-2.09021	-0.33080	H	0.39993	-3.61615	-0.46298
H	6.51964	-1.99618	-0.91807	H	0.63269	-4.30147	-2.08417
C	4.41493	-1.55397	-0.81134	Ni	-2.70100	-1.97609	-2.91263
H	4.39913	-1.03621	-1.76637	H	-2.71953	-1.02419	-3.45268
C	-3.93577	-0.51092	1.26090	C	-2.58520	-2.78052	-3.64996
H	-3.54765	0.49760	1.37672	H	-3.67288	-2.10000	-2.42642
C	-3.62548	1.00664	-1.65499	C	2.03146	-2.42253	2.90446
H	-4.40779	0.29719	-1.40580	C	-0.61724	2.28189	-1.05270
C	-3.80941	-2.69534	0.25068	H	-1.46236	2.67896	1.53423
H	-3.34250	-3.40652	-0.42262	C	-1.46007	2.81885	2.75755
C	3.28021	-2.31074	1.18309	H	-0.48089	2.21796	1.14139
H	2.36398	-2.38692	1.76558	C	0.63118	4.00895	0.73766
C	2.28134	0.63143	-2.90504	H	-1.23194	4.45733	2.68662
H	2.19264	-0.25591	-3.52308	C	2.46541	4.72394	0.49709
C	2.23495	1.72289	-0.75302	H	0.74431	5.78338	2.11838
H	2.08072	1.68211	0.31961	C	-0.90785	0.20313	4.11838
C	-3.95241	2.19406	-2.31011	H	-1.88370	0.58739	3.80479
H	-4.98789	2.39777	-2.56969	H	-0.52717	0.79982	4.95386
C	4.47321	-2.85489	1.66133	P	0.23481	1.65299	3.53753
H	4.49218	-3.35894	2.62376	O	-0.03696	-0.83623	4.43744
C	5.64120	-2.74220	0.90456	H	1.27772	-1.03147	6.57400
H	6.57400	-3.15567					
C	-1.62851	2.85042	-2.29392				
H	-0.84070	3.55973	-2.53137				

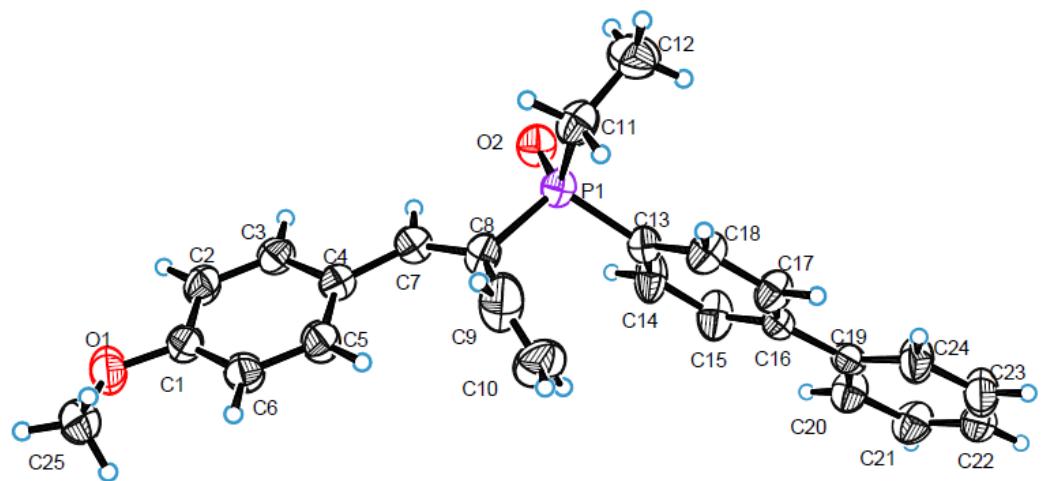


TS-1-P

P	1.16141	-1.22550	0.63629	C	3.43614	-4.35893	-0.75504	
P	-2.11343	-0.50637	0.32238	H	3.28415	-5.42026	-0.93118	
C	1.91173	0.22471	1.47330	C	-1.98806	3.56847	0.62599	
C	-3.79102	-0.77919	-0.37261	H	-1.81014	4.38567	-0.06722	
C	-0.80993	-1.58655	2.62135	C	4.82785	-2.39351	-0.86896	
H	-0.58149	-0.54360	2.87238	H	5.76735	-1.91508	-1.13225	
H	-1.02063	-2.08457	3.57843	C	-2.40400	2.76942	2.86577	
C	2.58367	-2.22805	0.05520	H	-2.17863	3.82781	1.98579	
C	-2.22047	1.18542	1.03412	C	-2.15158	4.84854	2.35693	
C	0.45951	-2.25294	2.04379	C	2.90597	2.53582	2.72054	
H	0.16963	-3.19594	1.56773	H	3.29561	3.42911	3.20117	
C	-2.11558	-1.66504	1.79253	C	-2.41469	-3.08943	1.30220	
H	-2.93679	-1.36531	2.45681	H	-1.74171	-3.38456	0.48905	
C	1.27243	1.46104	1.30572	H	-2.29469	-3.80973	2.12077	
H	0.40223	1.53041	0.66729	C	-3.43748	-3.16723	0.92500	
C	-6.20554	-0.82030	-0.15313	C	1.45445	-2.57291	3.16394	
H	-7.09785	-0.66275	0.44658	H	1.72296	-1.67024	3.72142	
C	-4.94727	-0.58575	0.39745	H	1.01139	-3.28473	3.87169	
H	-4.86394	-0.23497	1.42282	Ni	-0.34984	-0.57587	-0.85669	
C	3.80536	-1.63439	-0.29948	H	-1.37367	0.22685	-1.93519	
H	3.95856	-0.57581	-0.12317	C	1.46968	1.87249B	-2.12100	
C	3.06849	0.16362	2.26829	C	1.4671	2.81129	1.65626	-1.77391
H	3.59334	-0.77766	2.39103	C	0.91724	3.14621	-1.94195	
C	2.41159	-3.60011	-0.19082	C	3.58455	2.69099	-1.25295	
H	1.46929	-4.08344	0.05120	H	3.24671	2.69099	-1.89585	
C	-3.91237	-1.19883	-1.70180	C	1.69186	4.18402	-1.41984	
H	-3.01316	-1.31430	-2.30039	H	-0.11984	3.30485	-2.22168	
C	-2.42928	1.45573	2.39256	C	3.02383	3.95798	-1.06868	
H	-2.60037	0.64798	3.09608	H	4.62047	2.50992	-0.97823	
C	-2.00682	2.25887	0.15081	H	1.25509	5.17068	-1.28537	
H	-1.82468	2.05972	-0.90118	C	3.62295	4.76252	-0.65106	
C	3.56289	1.31287	2.88360	H	1.23106	-0.10636	-4.16005	
H	4.46159	1.25392	3.49168	C	2.26098	-0.40426	-3.93546	
C	-5.17342	-1.43533	-2.25256	H	1.23714	0.69041	-4.91246	
H	-5.25879	-1.75623	-3.28685	P	0.38271	0.48389	-2.63184	
C	-6.31930	-1.24920	-1.47902	O	-1.04399	1.10924	-3.02344	
H	-7.30109	-1.42872	-1.90833	H	0.69118	-0.97165	-4.55554	
C	1.75930	2.60785	1.93079					
H	1.24750	3.55237	1.77872					

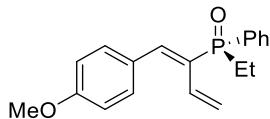
INT-2-P				H	-3.21299	-4.16592	-1.94036
P	-0.88602	0.05252	-1.02963	C	2.44703	2.98006	2.08972
P	2.37117	-0.30336	-0.34725	H	2.07528	3.20644	3.08471
C	-1.35109	1.80077	-0.76020	C	-4.78590	-1.15568	-1.77508
C	3.88470	-1.25546	0.05443	H	-5.77482	-0.71287	-1.85013
C	1.29978	0.63252	-2.77869	C	3.54562	3.65816	0.04893
H	1.24536	1.61911	-2.30163	H	4.04439	4.41725	-0.54743
H	1.53433	0.82319	-3.83512	C	3.09360	3.95987	1.33452
C	-2.41580	-0.90108	-1.35328	H	3.23842	4.95703	1.74110
C	2.70377	1.39089	0.27446	C	-4.61783	-2.52691	-1.96105
C	-0.08913	-0.04060	-2.73418	H	-5.47243	-3.15448	-2.19764
H	0.03500	-1.12249	-2.85895	C	-1.89306	4.50620	-0.23189
C	2.48303	-0.17197	-2.20232	H	-2.10000	5.55389	-0.03114
H	3.40311	0.37299	-2.44801	C	2.60572	-1.57518	-2.81492
C	-0.89615	2.40121	0.42410	H	1.82064	-2.24964	-2.45557
H	-0.38050	1.81187	1.17423	H	2.52973	-1.52024	-3.90764
C	6.29771	-1.48469	0.11249	H	3.56646	-2.02950	-2.56012
H	7.28563	-1.05604	-0.03153	C	-0.95173	0.45516	-3.90148
C	5.16360	-0.71406	-0.13881	H	-0.97095	1.54797	-3.94189
H	5.27251	0.31526	-0.46831	H	-0.52414	0.10017	-4.84707
C	-3.69166	-0.34377	-1.47239	H	-1.98022	0.08782	-3.83835
H	-3.84127	0.71456	-1.29691	Ni	0.43018	-0.83929	0.54025
C	-2.10250	2.57016	-1.66710	H	1.21337	-1.55895	1.60852
H	-2.49370	2.12456	-2.57257	C	-2.67334	-0.69848	2.01694
C	-2.25740	-2.28778	-1.50967	C	-3.42331	-1.83509	1.68437
H	-1.27519	-2.73350	-1.36851	C	-3.32033	0.53927	2.11559
C	3.75734	-2.57327	0.50959	C	-4.79746	-1.73987	1.47716
H	2.76402	-2.97537	0.68497	H	-2.93314	-2.79887	1.57863
C	3.35380	2.38041	-0.47798	C	-4.69534	0.63777	1.89377
H	3.70688	2.16890	-1.48236	H	-2.73452	1.41108	2.38673
C	2.24858	1.70277	1.56687	C	-5.43729	-0.50186	1.58125
H	1.69138	0.97310	2.14961	H	-5.36794	-2.62740	1.21857
C	-2.37099	3.91201	-1.40273	H	-5.18828	1.60329	1.97615
H	-2.95448	4.49322	-2.11146	H	-6.50866	-0.42765	1.41362
C	4.89368	-3.34569	0.75455	C	-0.76252	-2.19538	3.48243
H	4.78617	-4.36693	1.10924	H	-1.02469	-3.12788	2.97087
C	6.16392	-2.80311	0.55565	H	-1.43385	-2.04466	4.33447
H	7.04873	-3.40187	0.75292	P	-0.85910	-0.76256	2.32512
C	-1.16247	3.74676	0.68065	O	-0.42270	0.54710	2.99797
H	-0.79842	4.19104	1.60220	H	0.27024	-2.26975	3.83315
C	-3.34915	-3.09477	-1.81927				

8. ORTEP drawing of 3ka at 50% probability.



These data can be obtained free of charge from the Cambridge crystallographic data centre (CCDC
2056434).

9. Spectroscopic data of products.



3aa: 89% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.86 – 7.68 (m, 2H), 7.55 – 7.44 (m, 5H), 7.40 (d, *J* = 19.5 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.60 (dd, *J* = 18.1, 16.7, 11.6, 1.5 Hz, 1H), 5.33 – 5.29 (m, 1H), 5.28 (td, *J* = 2.8, 1.2 Hz, 1H), 3.83 (s, 3H), 2.37 – 2.14 (m, 2H), 1.22 (dt, *J* = 17.3, 7.7 Hz, 3H).

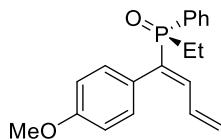
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.1, 142.2 (d, *J* = 8.0 Hz), 133.2 (d, *J* = 97.0 Hz), 131.9 (d, *J* = 9.2 Hz), 131.8, 131.5 (d, *J* = 2.6 Hz), 130.8 (d, *J* = 9.2 Hz), 129.0 (d, *J* = 90.7 Hz), 128.6 (d, *J* = 11.5 Hz), 128.2 (d, *J* = 17.0 Hz), 120.3 (d, *J* = 5.9 Hz), 113.8, 55.3, 20.2 (d, *J* = 73.7 Hz), 5.4 (d, *J* = 4.7 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 36.0.

HRMS (ESI) [M+H]⁺: calcd. 313.1357, found. 313.1360.

Optical Rotation: $[\alpha]_D^{20} = +99.0$ (*c* = 0.847, acetone).

HPLC: Daicel Chiralcel OD-H (91 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, λ = 297 nm, *t* (major) = 13.4 min, *t* (minor) = 14.5 min.

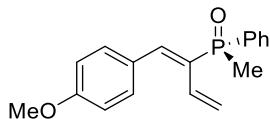


3aa': colorless oil.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.46 (m, 3H), 7.41 (td, *J* = 7.5, 2.5 Hz, 2H), 7.22 (dd, *J* = 17.6, 11.0 Hz, 1H), 6.81 (s, 4H), 6.34 – 6.14 (m, 1H), 5.56 (d, *J* = 16.9 Hz, 1H), 5.32 (dd, *J* = 10.0, 2.0 Hz, 1H), 3.80 (s, 3H), 1.98 (dq, *J* = 11.0, 7.5 Hz, 2H), 1.16 (dt, *J* = 17.0, 7.6 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 159.1, 142.7 (d, *J* = 8.0 Hz), 136.2 (d, *J* = 91.0 Hz), 132.7 (d, *J* = 15.4 Hz), 131.6 (d, *J* = 97.2 Hz), 131.5 (d, *J* = 2.7 Hz), 131.1 (d, *J* = 8.7 Hz), 130.7 (d, *J* = 4.1 Hz), 128.3 (d, *J* = 11.4 Hz), 127.2 (d, *J* = 10.3 Hz), 124.1, 113.8, 55.2, 20.1 (d, *J* = 74.2 Hz), 5.2 (d, *J* = 5.0 Hz).

³¹P NMR (162 MHz, Chloroform-*d*) δ 33.7.



3ba: 74% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.76 (ddt, *J* = 11.9, 6.7, 1.5 Hz, 2H), 7.57 – 7.47 (m, 3H), 7.45 (d, *J* = 8.7 Hz, 2H), 7.37 (d, *J* = 20.4 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.61 (tdd, *J* = 17.9, 11.6, 1.4 Hz, 1H), 5.37 – 5.27 (m, 1H), 5.31 (dd, *J* = 2.7, 1.4 Hz, 1H), 3.83 (s, 3H), 1.94 (d, *J* = 13.1 Hz, 3H).

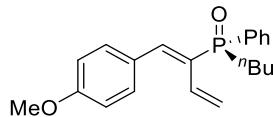
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.2, 141.6 (d, *J* = 8.7 Hz), 134.1 (d, *J* = 100.6 Hz), 131.8, 131.7 (d, *J* = 9.3 Hz), 131.6 (d, *J* = 2.7 Hz), 130.5 (d, *J* = 9.8 Hz), 129.9, 128.6 (d, *J* = 11.8 Hz), 128.0 (d, *J* = 17.3 Hz), 120.5 (d, *J* = 6.0 Hz), 113.8, 55.3, 14.8 (d, *J* = 74.6 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 31.8.

HRMS (ESI) [M+H]⁺: calcd. 299.1201, found. 299.1196.

Optical Rotation: $[\alpha]_D^{20} = +97.3$ (*c* = 0.987, acetone).

HPLC: Daicel Chiralcel AD-H (80 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 297 nm, *t* (major) = 7.3 min, *t* (minor) = 11.7 min.



3ca: 89% yield, yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.89 – 7.69 (m, 2H), 7.55 – 7.45 (m, 5H), 7.41 (d, *J* = 19.6 Hz, 1H), 6.90 (d, *J* = 8.9 Hz, 2H), 6.60 (dd, *J* = 18.4, 17.0, 11.7, 1.5 Hz, 1H), 5.30 (dd, *J* = 2.6, 0.8 Hz, 1H), 5.29 – 5.26 (m, 1H), 3.83 (s, 3H), 2.40 – 2.12 (m, 2H), 1.80 – 1.57 (m, 2H), 1.58 – 1.35 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H).

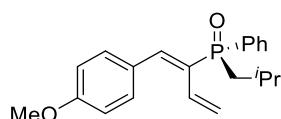
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.0, 142.0 (d, *J* = 7.8 Hz), 133.5 (d, *J* = 97.0 Hz), 131.9 (d, *J* = 9.2 Hz), 131.8, 131.5 (d, *J* = 2.7 Hz), 130.7 (d, *J* = 9.2 Hz), 129.2 (d, *J* = 90.8 Hz), 128.5 (d, *J* = 11.5 Hz), 128.1 (d, *J* = 16.6 Hz), 120.3 (d, *J* = 5.8 Hz), 113.7, 55.2, 26.8 (d, *J* = 73.0 Hz), 24.1 (d, *J* = 15.3 Hz), 23.3 (d, *J* = 3.8 Hz), 13.6.

³¹P NMR (202 MHz, Chloroform-*d*) δ 34.3.

HRMS (ESI) [M+H]⁺: calcd. 341.1670, found. 341.1677.

Optical Rotation: [α]_D²⁰ = +79.1 (*c* = 1.45, acetone).

HPLC: Daicel Chiralcel AD-H (93 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 299 nm, *t* (major) = 7.4 min, *t* (minor) = 14.0 min.



3da: 85% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 9.7, 6.8, 1.5 Hz, 2H), 7.55 – 7.39 (m, 6H), 6.99 – 6.80 (m, 2H), 6.58 (dd, *J* = 18.0, 16.4, 11.6, 1.4 Hz, 1H), 5.29 (dq, *J* = 2.5, 1.3 Hz, 1H), 5.28 (dd, *J* = 31.1, 2.6, 1.4 Hz, 1H), 3.83 (s, 3H), 2.30 – 2.11 (m, 3H), 1.07 (dd, *J* = 9.4, 6.0 Hz, 6H).

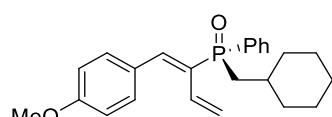
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.0, 141.8 (d, *J* = 7.7 Hz), 134.0 (d, *J* = 96.5 Hz), 132.1 (d, *J* = 9.2 Hz), 131.8, 131.4 (d, *J* = 2.8 Hz), 130.8 (d, *J* = 9.2 Hz), 130.1 (d, *J* = 90.2 Hz), 128.5 (d, *J* = 11.4 Hz), 128.2 (d, *J* = 16.6 Hz), 120.4 (d, *J* = 5.8 Hz), 113.7, 55.3, 35.4 (d, *J* = 71.9 Hz), 24.7 (dd, *J* = 19.5, 8.9 Hz), 23.6 (d, *J* = 3.7 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 32.6.

HRMS (ESI) [M+H]⁺: calcd. 341.1670, found. 341.1674.

Optical Rotation: [α]_D²⁰ = +50.6 (*c* = 0.887, acetone).

HPLC: Daicel Chiralcel AD-H (93 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 297 nm, *t* (major) = 6.1 min, *t* (minor) = 15.0 min.



3ea: 53% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.85 – 7.67 (m, 2H), 7.53 – 7.44 (m, 5H), 7.42 (d, *J* = 19.9 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.58 (dd, *J* = 18.0, 16.5, 11.6, 1.4 Hz, 1H), 5.28 (dt, *J* = 2.6, 1.5 Hz, 1H), 5.27 (ddd, *J* = 31.2, 2.6, 1.4 Hz, 1H), 3.83 (s, 3H), 2.17 (qdd, *J* = 15.1, 11.2, 6.1 Hz, 2H), 1.96 – 1.77 (m, 3H), 1.62 (ddtd, *J* = 19.6, 12.4, 3.6, 1.6 Hz, 3H), 1.25 (ddt, *J* = 12.9, 9.4, 3.3 Hz, 2H), 1.17 – 1.02 (m, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 160.2, 142.5 (d, *J* = 7.8 Hz), 141.4 (d, *J* = 15.3 Hz), 133.2 (d, *J* = 97.5 Hz), 131.9, 131.8, 131.7 (d, *J* = 2.7 Hz), 130.8 (d, *J* = 9.3 Hz), 129.2, 128.7 (d, *J* = 11.6 Hz), 128.4,

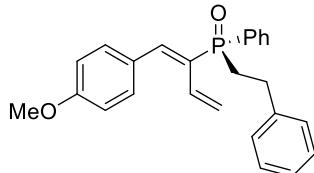
128.4 (d, $J = 56.4$ Hz), 128.0, 126.3, 120.5 (d, $J = 5.9$ Hz), 113.8, 55.3, 29.3 (d, $J = 70.7$ Hz), 27.5 (d, $J = 2.9$ Hz).

^{31}P NMR (202 MHz, Chloroform-d) δ 33.1.

HRMS(ESI) [M+Na] $^+$: calcd. 403.1803, found. 403.1804

Optical Rotation: $[\alpha]_D^{20} = +36.0$ ($c = 0.807$, acetone).

HPLC: Daicel Chiralcel OD-H (93 % ee), *n*-Hexanes/*i*-PrOH = 95/5, 1 mL/min, $\lambda = 296$ nm, t (major) = 13.1 min, t (minor) = 15.1 min.



3fa: 93% yield, colorless oil.

^1H NMR (500 MHz, Chloroform-d) δ 7.83 – 7.74 (m, 2H), 7.57 – 7.43 (m, 6H), 7.31 – 7.15 (m, 5H), 6.90 (d, $J = 8.8$ Hz, 2H), 6.61 (dddd, $J = 18.0, 16.8, 12.0, 1.5$ Hz, 1H), 5.32 (d, $J = 2.5$ Hz, 1H), 5.29 (dt, $J = 8.0, 1.4$ Hz, 1H), 3.83 (s, 3H), 3.03 – 2.91 (m, 2H), 2.62 – 2.49 (m, 2H).

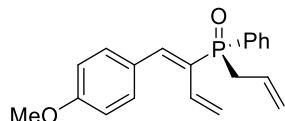
^{13}C NMR (126 MHz, Chloroform-d) δ 160.2, 142.5 (d, $J = 7.8$ Hz), 141.4 (d, $J = 15.3$ Hz), 133.2 (d, $J = 97.5$ Hz), 131.9, 131.8, 131.7 (d, $J = 2.7$ Hz), 130.8 (d, $J = 9.3$ Hz), 128.8 (d, $J = 91.1$ Hz), 128.8 – 128.5 (m), 128.1, 128.0, 120.5 (d, $J = 5.9$ Hz), 113.8, 55.3, 29.3 (d, $J = 70.7$ Hz), 27.5 (d, $J = 2.9$ Hz).

^{31}P NMR (202 MHz, Chloroform-d) δ 33.1.

HRMS (ESI) [M+H] $^+$: calcd. 389.1670, found. 389.1663.

Optical Rotation: $[\alpha]_D^{20} = +80.9$ ($c = 1.45$, acetone).

HPLC: Daicel Chiralcel AD-H (90 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, $\lambda = 299$ nm, t (major) = 12.3 min, t (minor) = 20.3 min.



3ga: 90% yield, yellow oil.

^1H NMR (500 MHz, Chloroform-d) δ 7.80 – 7.74 (m, 2H), 7.55 – 7.47 (m, 3H), 7.46 (d, $J = 8.8$ Hz, 2H), 7.38 (d, $J = 19.9$ Hz, 1H), 6.89 (d, $J = 8.8$ Hz, 2H), 6.61 (dddd, $J = 18.5, 17.5, 11.6, 1.4$ Hz, 1H), 5.93 – 5.82 (m, 1H), 5.36 – 5.33 (m, 1H), 5.33 – 5.31 (m, 1H), 5.24 – 5.22 (m, 1H), 5.21 – 5.19 (m, 1H), 3.83 (s, 3H), 3.12 (ddt, $J = 14.2, 7.4, 1.3$ Hz, 2H).

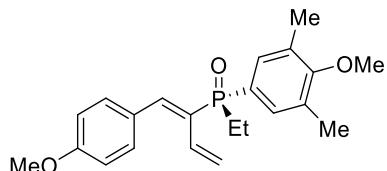
^{13}C NMR (126 MHz, Chloroform-d) δ 160.2, 142.7 (d, $J = 8.0$ Hz), 132.9 (d, $J = 97.6$ Hz), 131.9, 131.9 (d, $J = 9.2$ Hz), 131.7 (d, $J = 2.7$ Hz), 131.0 (d, $J = 9.3$ Hz), 128.8 (d, $J = 92.3$ Hz), 128.5 (d, $J = 11.6$ Hz), 128.0 (d, $J = 17.1$ Hz), 127.3 (d, $J = 9.0$ Hz), 120.6 (d, $J = 18.6$ Hz), 120.6, 113.8, 55.3, 33.6 (d, $J = 69.8$ Hz).

^{31}P NMR (202 MHz, Chloroform-d) δ 31.7.

HRMS (ESI) [M+H] $^+$: calcd. 325.1357, found. 325.1353.

Optical Rotation: $[\alpha]_D^{20} = +79.6$ ($c = 0.920$, acetone).

HPLC: Daicel Chiralcel AD-H (85 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, $\lambda = 254$ nm, t (major) = 7.8 min, t (minor) = 17.9 min.



3ha: 68% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.31 (m, 3H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.61 (td, *J* = 17.6, 11.9 Hz, 1H), 5.36 – 5.28 (m, 1H), 5.34 – 5.27 (m, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 2.31 (s, 6H), 2.24 – 2.16 (m, 2H), 1.21 (dt, *J* = 17.1, 7.6 Hz, 3H).

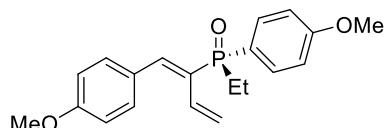
¹³C NMR (126 MHz, Chloroform-*d*) δ 159.9, 159.7 (d, *J* = 3.2 Hz), 141.9 (d, *J* = 7.8 Hz), 131.9 (d, *J* = 9.2 Hz), 131.8, 131.4 (d, *J* = 9.9 Hz), 131.4 (d, *J* = 12.7 Hz), 129.1 (d, *J* = 90.7 Hz), 128.2 (d, *J* = 3.4 Hz), 127.8 (d, *J* = 78.9 Hz), 120.2 (d, *J* = 5.7 Hz), 113.6, 59.6, 55.2, 20.0 (d, *J* = 73.8 Hz), 16.2, 5.4 (d, *J* = 4.9 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.6.

HRMS (ESI) [M+H]⁺: calcd. 371.1776, found. 371.1781.

Optical Rotation: $[\alpha]_D^{20} = +61.6$ (*c* = 1.63, acetone).

HPLC: Daicel Chiralcel OD-H (92 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, λ = 296 nm, *t* (major) = 10.4 min, *t* (minor) = 12.1 min.



3ia: 53% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 10.9, 8.7 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.37 (d, *J* = 19.5 Hz, 1H), 6.99 (dd, *J* = 8.8, 2.1 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.60 (dd, *J* = 18.2, 16.8, 11.7, 1.5 Hz, 1H), 5.34 – 5.30 (m, 1H), 5.29 – 5.27 (m, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 2.29 – 2.15 (m, 2H), 1.20 (dt, *J* = 17.3, 7.6 Hz, 3H).

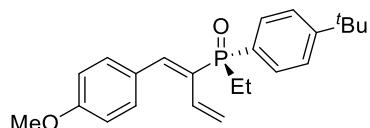
¹³C NMR (126 MHz, Chloroform-*d*) δ 162.2 (d, *J* = 2.8 Hz), 160.0, 142.0 (d, *J* = 7.9 Hz), 132.7 (d, *J* = 10.5 Hz), 132.0 (d, *J* = 9.1 Hz), 131.8, 129.3 (d, *J* = 91.4 Hz), 128.2 (d, *J* = 16.8 Hz), 124.2 (d, *J* = 102.9 Hz), 120.2 (d, *J* = 5.7 Hz), 114.1 (d, *J* = 12.4 Hz), 113.7, 55.3, 55.3, 20.3 (d, *J* = 74.1 Hz), 5.5 (d, *J* = 4.9 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.8.

HRMS (ESI) [M+Na]⁺: calcd. 365.1283, found. 365.1291.

Optical Rotation: $[\alpha]_D^{20} = +69.9$ (*c* = 0.800, acetone).

HPLC: Daicel Chiralcel OD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, λ = 296 nm, *t* (major) = 15.0 min, *t* (minor) = 20.1 min.



3ja: 76% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.71 – 7.62 (m, 2H), 7.54 – 7.45 (m, 4H), 7.41 (d, *J* = 19.5 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 6.61 (dd, *J* = 18.2, 16.8, 11.6, 1.4 Hz, 1H), 5.31 (dd, *J* = 25.3, 2.6, 1.4 Hz, 1H), 5.33 – 5.30 (m, 1H), 3.83 (s, 3H), 2.37 – 2.16 (m, 2H), 1.33 (s, 9H), 1.28 – 1.13 (m, 3H).

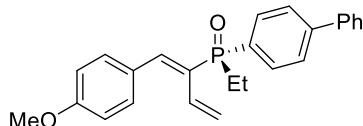
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.0, 154.96 (d, *J* = 2.7 Hz), 142.1 (d, *J* = 7.7 Hz), 132.0 (d, *J* = 9.1 Hz), 131.8, 130.6 (d, *J* = 9.4 Hz), 129.8 (d, *J* = 91.9 Hz), 129.0 (d, *J* = 83.2 Hz), 128.2 (d, *J* = 16.7 Hz), 125.5 (d, *J* = 11.5 Hz), 120.2 (d, *J* = 5.7 Hz), 113.7, 55.2, 34.9, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 4.9 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 36.0.

HRMS (ESI) [M+Na]⁺: calcd. 391.1803, found. 391.1799.

Optical Rotation: [α]_D²⁰ = +73.5 (*c* = 1.55, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 299 nm, *t* (major) = 5.4 min, *t* (minor) = 15.2 min.



3ka: 90% yield, white powder.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.86 – 7.79 (m, 2H), 7.73 – 7.68 (m, 2H), 7.64 – 7.60 (m, 2H), 7.52 – 7.36 (m, 6H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.63 (dddd, *J* = 18.2, 16.8, 11.6, 1.4 Hz, 1H), 5.36 (ddd, *J* = 18.4, 2.5, 1.4 Hz, 1H), 5.34 – 5.31 (m, 1H), 3.83 (s, 3H), 2.32 – 2.24 (m, 2H), 1.35 – 1.15 (m, 3H).

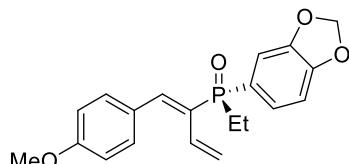
¹³C NMR (126 MHz, Chloroform-d) δ 160.1, 144.3 (d, *J* = 2.8 Hz), 142.3 (d, *J* = 7.9 Hz), 140.0, 131.9 (d, *J* = 9.1 Hz), 131.8, 131.7 (d, *J* = 98.2 Hz), 131.4 (d, *J* = 9.5 Hz), 128.9 (d, *J* = 91.0 Hz), 128.9, 128.1 (d, *J* = 16.9 Hz), 128.0, 127.2 (d, *J* = 11.8 Hz), 127.2, 120.4 (d, *J* = 5.8 Hz), 113.8, 55.3, 20.2 (d, *J* = 74.0 Hz), 5.5 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 36.0.

HRMS (ESI) [M+Na]⁺: calcd. 411.1490, found. 411.1491.

Optical Rotation: [α]_D²⁰ = +61.6 (*c* = 0.947, acetone).

HPLC: Daicel Chiralcel AS-H (88 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 306 nm, *t* (major) = 13.4 min, *t* (minor) = 15.8 min.



3la: 80% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.7 Hz, 2H), 7.37 (d, *J* = 19.6 Hz, 1H), 7.28 (ddd, *J* = 11.8, 7.9, 1.5 Hz, 1H), 7.17 (dd, *J* = 10.7, 1.5 Hz, 1H), 6.94 – 6.87 (m, 3H), 6.60 (dddd, *J* = 18.2, 16.9, 11.6, 1.4 Hz, 1H), 6.02 (s, 2H), 5.35 (dt, *J* = 18.6, 1.8 Hz, 1H), 5.33 – 5.29 (m, 1H), 3.83 (s, 3H), 2.27 – 2.12 (m, 2H), 1.21 (dt, *J* = 17.4, 7.6 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-d) δ 160.0, 150.4 (d, *J* = 2.8 Hz), 148.0 (d, *J* = 17.1 Hz), 142.0 (d, *J* = 8.0 Hz), 131.9 (d, *J* = 9.1 Hz), 131.8, 129.1 (d, *J* = 91.5 Hz), 128.1 (d, *J* = 16.8 Hz), 126.2 (d, *J* = 100.5 Hz), 126.0 (d, *J* = 10.1 Hz), 120.3 (d, *J* = 5.7 Hz), 113.7, 110.4 (d, *J* = 11.8 Hz), 108.7 (d, *J* = 14.3 Hz), 101.5, 55.3, 20.3 (d, *J* = 74.5 Hz), 5.5 (d, *J* = 4.9 Hz).

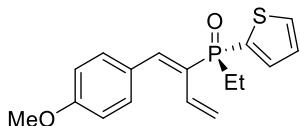
³¹P NMR (202 MHz, Chloroform-*d*) δ 36.0.

HRMS (ESI) [M+Na]⁺: calcd. 379.1075, found. 379.1076.

Optical Rotation: [α]_D²⁰ = +75.8 (*c* = 0.827, acetone).

HPLC: Daicel Chiralcel OJ-H (90 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 296 nm, *t* (major)

= 8.9 min, *t* (minor) = 7.8 min.



3ma: 89% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.70 (ddd, *J* = 4.7, 3.7, 1.1 Hz, 1H), 7.58 (ddd, *J* = 6.7, 3.6, 1.1 Hz, 1H), 7.51 – 7.44 (m, 3H), 7.19 (ddd, *J* = 5.1, 3.5, 1.7 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.61 (tdd, *J* = 17.6, 12.0, 1.4 Hz, 1H), 5.38 – 5.36 (m, 1H), 5.33 (ddd, *J* = 6.5, 2.8, 1.3 Hz, 1H), 3.83 (s, 3H), 2.37 – 2.17 (m, 2H), 1.25 (dt, *J* = 18.4, 7.6 Hz, 3H).

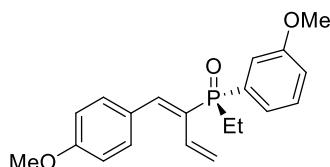
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.1, 142.6 (d, *J* = 8.1 Hz), 135.0 (d, *J* = 9.1 Hz), 134.0 (d, *J* = 102.1 Hz), 132.6 (d, *J* = 4.5 Hz), 131.9, 131.6 (d, *J* = 9.7 Hz), 128.7 (d, *J* = 96.2 Hz), 128.1 (d, *J* = 12.8 Hz), 127.9, 120.4 (d, *J* = 6.0 Hz), 113.7, 55.2, 22.3 (d, *J* = 77.4 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 29.6.

HRMS (ESI) [M+Na]⁺: calcd. 341.0741, found. 341.0804

Optical Rotation: $[\alpha]_D^{20} = +76.7$ (*c* = 1.63, acetone).

HPLC: Daicel Chiralcel AD-H (88 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 298 nm, *t* (major) = 10.6 min, *t* (minor) = 21.4 min.



3na: 90% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.8 Hz, 2H), 7.41 – 7.27 (m, 4H), 7.05 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.60 (dddd, *J* = 18.2, 16.8, 11.6, 1.4 Hz, 1H), 5.36 (dt, *J* = 18.2, 1.7 Hz, 1H), 5.31 (ddt, *J* = 11.6, 2.6, 1.2 Hz, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 2.29 – 2.18 (m, 2H), 1.27 – 1.13 (m, 3H).

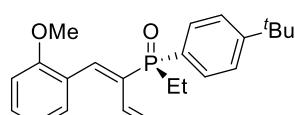
¹³C NMR (126 MHz, Chloroform-*d*) δ 160.0, 159.6 (d, *J* = 14.2 Hz), 142.1 (d, *J* = 8.1 Hz), 134.4 (d, *J* = 96.1 Hz), 131.8 (d, *J* = 9.1 Hz), 131.8, 129.7 (d, *J* = 13.5 Hz), 128.9 (d, *J* = 90.9 Hz), 128.1 (d, *J* = 16.7 Hz), 122.8 (d, *J* = 9.4 Hz), 120.4 (d, *J* = 5.8 Hz), 117.5 (d, *J* = 2.6 Hz), 115.9 (d, *J* = 10.0 Hz), 113.7, 55.3 (d, *J* = 14.3 Hz), 20.2 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 4.9 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 36.3.

HRMS (ESI) [M+Na]⁺: calcd. 365.1283, found. 365.1289.

Optical Rotation: $[\alpha]_D^{20} = +84.0$ (*c* = +1.45, acetone).

HPLC: Daicel Chiralcel AD-H (92 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 293 nm, *t* (major) = 7.4 min, *t* (minor) = 11.3 min.



3jb: 87% yield, yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.71 (dd, *J* = 11.1, 8.2 Hz, 2H), 7.55 – 7.46 (m, 3H), 7.39 (d, *J* = 7.4 Hz, 1H), 7.31 (td, *J* = 7.9, 1.7 Hz, 1H), 6.95 – 6.88 (m, 2H), 6.64 – 6.52 (m, 1H), 5.57 (dt, *J* = 18.1,

1.4 Hz, 1H), 5.28 – 5.22 (m, 1H), 3.83 (s, 3H), 2.33 – 2.15 (m, 2H), 1.33 (s, 9H), 1.23 (dt, J = 17.3, 7.4 Hz, 3H).

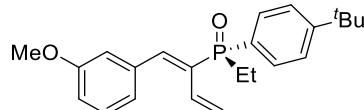
^{13}C NMR (126 MHz, Chloroform-*d*) δ 157.7, 154.9 (d, J = 2.7 Hz), 138.3 (d, J = 10.1 Hz), 131.7, 131.6, 131.0 (d, J = 1.7 Hz), 130.8 (d, J = 9.6 Hz), 130.2, 129.6 (d, J = 99.1 Hz), 125.5 (d, J = 11.8 Hz), 124.5 (d, J = 16.3 Hz), 120.5 (d, J = 5.2 Hz), 120.0, 110.6, 55.5, 35.0, 31.2, 21.2 (d, J = 73.5 Hz), 5.7 (d, J = 5.0 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 37.2.

HRMS (ESI) [M+H]⁺: calcd. 369.1983, found. 369.1984.

Optical Rotation: $[\alpha]_D^{20} = +29.7$ (c = 3.13, acetone).

HPLC: Daicel Chiralcel AD-H (89 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 315 nm, t (major) = 5.9 min, t (minor) = 6.6 min.



3jc: 96% yield, colorless oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.68 (dd, J = 11.1, 8.1 Hz, 2H), 7.49 (dd, J = 8.3, 2.5 Hz, 2H), 7.45 (d, J = 19.4 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.07 (d, J = 7.7 Hz, 1H), 7.03 (t, J = 1.9 Hz, 1H), 6.88 (dd, J = 8.3, 2.5 Hz, 1H), 6.67 – 6.56 (m, 1H), 5.35 (dd, J = 18.1, 2.0 Hz, 1H), 5.33 – 5.28 (m, 1H), 3.80 (s, 3H), 2.24 (dq, J = 11.3, 7.6 Hz, 2H), 1.33 (s, 9H), 1.23 (dt, J = 17.4, 7.4 Hz, 3H).

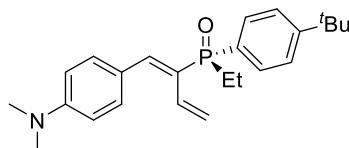
^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.4, 155.2 (d, J = 2.8 Hz), 142.5 (d, J = 7.7 Hz), 136.8 (d, J = 16.3 Hz), 132.0 (d, J = 88.7 Hz), 131.7 (d, J = 8.9 Hz), 130.7 (d, J = 9.5 Hz), 129.6 (d, J = 99.6 Hz), 129.3, 125.7 (d, J = 11.8 Hz), 122.6, 120.8 (d, J = 5.5 Hz), 115.3, 114.6, 55.3, 35.0, 31.1, 20.3 (d, J = 73.9 Hz), 5.5 (d, J = 4.8 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 35.6.

HRMS (ESI) [M+H]⁺: calcd. 369.1983, found. 369.1989.

Optical Rotation: $[\alpha]_D^{20} = +43.9$ (c = 0.673, acetone).

HPLC: Daicel Chiralcel AD-H (97 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 274 nm, t (major) = 7.4 min, t (minor) = 8.8 min.



3jd: 42% yield, yellow oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.68 (dd, J = 11.0, 8.1 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.36 (d, J = 19.5 Hz, 1H), 6.75 – 6.60 (m, 3H), 5.27 (dt, J = 25.2, 1.5 Hz, 1H), 5.28 – 5.25 (m, 1H), 3.00 (s, 6H), 2.28 – 2.17 (m, 2H), 1.32 (s, 9H), 1.20 (dt, J = 16.8, 7.6 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 154.7 (d, J = 2.6 Hz), 150.5, 142.8 (d, J = 7.8 Hz), 132.6 (d, J = 9.4 Hz), 131.8, 130.7 (d, J = 9.6 Hz), 130.3 (d, J = 99.2 Hz), 125.6 (d, J = 93.0 Hz), 125.4 (d, J = 11.6 Hz), 123.6 (d, J = 16.8 Hz), 119.2 (d, J = 5.7 Hz), 111.4, 40.1, 34.9, 31.1, 20.1 (d, J = 74.0 Hz), 5.5 (d, J = 4.8 Hz).

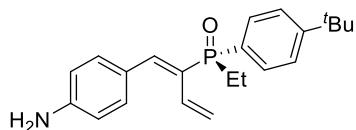
^{31}P NMR (202 MHz, Chloroform-*d*) δ 36.3.

HRMS (ESI) [M+H]⁺: calcd. 382.2300, found. 382.2296.

Optical Rotation: $[\alpha]_D^{20} = +186$ (c = 1.19, acetone).

HPLC: Daicel Chiralcel OD-H (91 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, λ = 343 nm, t (major)

= 9.7 min, *t* (minor) = 11.3 min.



3je: 95% yield, brown oil.

$^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.67 (dd, *J* = 11.0, 8.0 Hz, 2H), 7.50 – 7.43 (m, 2H), 7.38 – 7.31 (m, 3H), δ 6.72 – 6.55 (m, 1H), 6.64 (d, *J* = 8.6 Hz, 2H), 5.32 – 5.24 (m, 1H), 5.27 (s, 1H), 4.01 (s, 2H), 2.32 – 2.13 (m, 2H), 1.32 (s, 9H), 1.20 (dt, *J* = 15.9, 7.6 Hz, 3H).

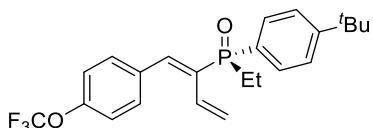
$^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 155.2 (d, *J* = 2.7 Hz), 141.0 (d, *J* = 7.7 Hz), 134.6, 133.9 (d, *J* = 16.4 Hz), 132.6 (d, *J* = 88.5 Hz), 131.3 (d, *J* = 9.0 Hz), 131.2, 130.6 (d, *J* = 9.5 Hz), 129.2 (d, *J* = 99.6 Hz), 128.5, 125.6 (d, *J* = 11.8 Hz), 121.3 (d, *J* = 5.9 Hz), 34.9, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 5.1 Hz).

$^{31}\text{P NMR}$ (202 MHz, Chloroform-*d*) δ 36.1.

HRMS (ESI) [M+H] $^+$: calcd. 354.1987, found. 354.1984.

Optical Rotation: $[\alpha]_D^{20} = +102$ (*c* = 1.69, acetone).

HPLC: Daicel Chiralcel AD-H (94 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 284 nm, *t* (major) = 5.6 min, *t* (minor) = 13.1 min.



3jf: 91% yield, yellow oil.

$^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 11.0, 8.0 Hz, 2H), 7.55 – 7.47 (m, 4H), 7.45 (d, *J* = 19.2 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 2H), 6.54 (td, *J* = 17.0, 11.6 Hz, 1H), 5.36 (d, *J* = 7.5 Hz, 1H), 5.34 (d, *J* = 2.2 Hz, 1H), 2.24 (dq, *J* = 15.2, 7.8 Hz, 2H), 1.34 (s, 9H), 1.23 (dt, *J* = 16.3, 7.4 Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 155.4 (d, *J* = 2.7 Hz), 140.7 (d, *J* = 7.7 Hz), 138.9 (d, *J* = 17.0 Hz), 134.6 (d, *J* = 87.1 Hz), 131.0 (d, *J* = 8.8 Hz), 130.7 (d, *J* = 9.6 Hz), 130.3 (d, *J* = 32.8 Hz), 130.1, 129.0 (d, *J* = 99.9 Hz), 125.7 (d, *J* = 11.8 Hz), 125.2 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 272.3 Hz), 121.8 (d, *J* = 5.9 Hz), 35.0, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 5.1 Hz).

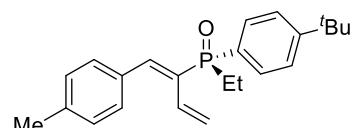
$^{31}\text{P NMR}$ (202 MHz, Chloroform-*d*) δ 35.2.

$^{19}\text{F NMR}$ (471 MHz, Chloroform-*d*) δ -57.8.

HRMS (ESI) [M+H] $^+$: calcd. 423.1701, found. 423.1703.

Optical Rotation: $[\alpha]_D^{20} = +46.1$ (*c* = 1.10, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 272 nm, *t* (major) = 4.8 min, *t* (minor) = 7.8 min.



3jg: 78% yield, yellow oil.

$^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 7.73 – 7.64 (m, 2H), 7.49 (dd, *J* = 8.3, 2.5 Hz, 2H), 7.44 (d, *J* = 19.5 Hz, 1H), 7.39 (d, *J* = 7.9 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 6.68 – 6.55 (m, 1H), 5.37 – 5.32 (m, 1H), 5.31 – 5.27 (m, 1H), 2.36 (s, 3H), 2.29 – 2.19 (m, 2H), 1.33 (s, 9H), 1.28 – 1.17 (m, 3H).

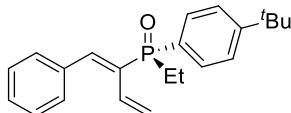
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.0 (d, *J* = 2.7 Hz), 142.6 (d, *J* = 7.8 Hz), 138.9, 132.7 (d, *J* = 16.5 Hz), 131.8 (d, *J* = 9.0 Hz), 130.6 (d, *J* = 9.5 Hz), 130.5 (d, *J* = 89.9 Hz), 130.0, 129.2, 129.0, 125.5 (d, *J* = 11.7 Hz), 120.4 (d, *J* = 5.7 Hz), 34.9, 31.0, 21.3, 20.2 (d, *J* = 73.8 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.9.

HRMS (ESI) [M+H]⁺: calcd. 353.2034, found. 353.2030.

Optical Rotation: [α]_D²⁰ = +36.6 (*c* = 1.35, acetone).

HPLC: Daicel Chiralcel OD-H (87 % ee), *n*-Hexanes/*i*-PrOH = 93/7, 1 mL/min, λ = 281 nm, *t* (major) = 7.2 min, *t* (minor) = 8.7 min.



3jh: 95% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.65 (m, 2H), 7.53 – 7.43 (m, 5H), 7.35 (dt, *J* = 16.6, 7.1 Hz, 3H), 6.61 (td, *J* = 17.6, 11.7 Hz, 1H), 5.40 – 5.34 (m, 1H), 5.33 – 5.28 (m, 1H), 2.31 – 2.19 (m, 2H), 1.33 (s, 9H), 1.23 (dt, *J* = 17.0, 7.4 Hz, 3H).

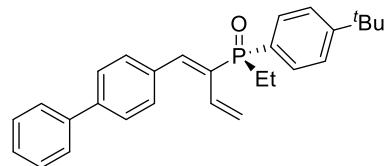
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.0 (d, *J* = 2.8 Hz), 142.5 (d, *J* = 7.6 Hz), 135.4 (d, *J* = 16.3 Hz), 131.7 (d, *J* = 89.1 Hz), 131.6 (d, *J* = 9.1 Hz), 130.6 (d, *J* = 9.5 Hz), 130.0, 129.5 (d, *J* = 99.5 Hz), 128.6, 128.2, 125.6 (d, *J* = 11.8 Hz), 120.7 (d, *J* = 5.6 Hz), 34.9, 31.0, 20.2 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 36.1.

HRMS (ESI) [M+H]⁺: calcd. 339.1878, found. 339.1875.

Optical Rotation: [α]_D²⁰ = +61.2 (*c* = 1.52, acetone).

HPLC: Daicel Chiralcel AD-H (94 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 273 nm, *t* (major) = 7.5 min, *t* (minor) = 11.4 min.



3ji: 70% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.74 – 7.67 (m, 2H), 7.63 – 7.55 (m, 6H), 7.54 – 7.48 (m, 3H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.33 (m, 1H), 6.66 (dd, *J* = 18.1, 16.8, 11.6, 1.5 Hz, 1H), 5.38 (dt, *J* = 18.3, 1.8 Hz, 1H), 5.36 – 5.32 (m, 1H), 2.30 – 2.22 (m, 2H), 1.34 (s, 9H), 1.24 (dt, *J* = 17.3, 7.5 Hz, 3H).

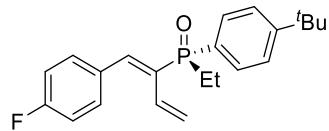
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.1 (d, *J* = 2.8 Hz), 142.0 (d, *J* = 7.6 Hz), 141.4, 140.2, 134.5 (d, *J* = 16.5 Hz), 131.7 (d, *J* = 8.9 Hz), 131.7 (d, *J* = 89.0 Hz), 130.7, 130.6, 130.6, 129.6 (d, *J* = 99.4 Hz), 128.8, 127.6, 126.9 (d, *J* = 10.6 Hz), 125.6 (d, *J* = 11.7 Hz), 120.8 (d, *J* = 5.8 Hz), 34.9, 31.1, 20.2 (d, *J* = 73.9 Hz), 5.5 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.6.

HRMS (ESI) [M+H]⁺: calcd. 415.2191, found. 415.2190.

Optical Rotation: [α]_D²⁰ = +27.9 (*c* = 2.76, acetone).

HPLC: Daicel Chiralcel AD-H (94 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 303 nm, *t* (major) = 5.8 min, *t* (minor) = 12.4 min.



3jj: 83% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.72 – 7.64 (m, 2H), 7.54 – 7.38 (m, 5H), 7.08 – 7.01 (m, 2H), 6.55 (dd, *J* = 17.9, 16.2, 11.7, 1.4 Hz, 1H), 5.37 – 5.33 (m, 1H), 5.33 – 5.31 (m, 1H), 2.23 (dq, *J* = 11.2, 7.6 Hz, 2H), 1.33 (s, 9H), 1.22 (dt, *J* = 17.4, 7.6 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 162.7 (d, *J* = 249.9 Hz), 155.2 (d, *J* = 2.7 Hz), 141.3 (d, *J* = 7.6 Hz), 131.9 (d, *J* = 8.0 Hz), 131.6 (dd, *J* = 16.6, 3.3 Hz), 131.5 (d, *J* = 9.0 Hz), 131.2, 130.7 (d, *J* = 9.6 Hz), 129.4 (d, *J* = 99.5 Hz), 125.6 (d, *J* = 11.6 Hz), 121.1 (d, *J* = 5.9 Hz), 115.3 (d, *J* = 21.6 Hz), 35.0, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 5.0 Hz).

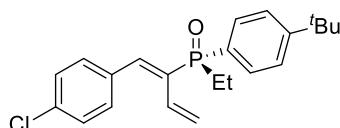
³¹P NMR (202 MHz, Chloroform-*d*) δ 35.5.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -111.6.

HRMS (ESI) [M+H]⁺: calcd. 357.1784, found. 357.1783.

Optical Rotation: [α]_D²⁰ = +53.4 (*c* = 1.02, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 273 nm, *t* (major) = 4.6 min, *t* (minor) = 8.6 min.



3jk: 76% yield, yellow powder.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.68 (dd, *J* = 11.1, 8.0 Hz, 2H), 7.50 (dd, *J* = 8.3, 2.5 Hz, 2H), 7.46 – 7.38 (m, 3H), 7.33 (d, *J* = 8.2 Hz, 2H), 6.54 (td, *J* = 17.1, 11.5 Hz, 1H), 5.38 – 5.32 (m, 1H), 5.32 (d, *J* = 3.2 Hz, 1H), 2.23 (dq, *J* = 11.2, 7.6 Hz, 2H), 1.33 (s, 9H), 1.22 (dt, *J* = 17.4, 7.5 Hz, 3H).

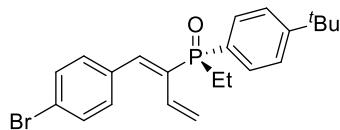
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.2 (d, *J* = 2.7 Hz), 141.1 (d, *J* = 7.7 Hz), 134.6, 133.9 (d, *J* = 16.4 Hz), 132.6 (d, *J* = 88.3 Hz), 131.4 (d, *J* = 9.1 Hz), 131.2, 130.6 (d, *J* = 9.6 Hz), 129.3 (d, *J* = 99.6 Hz), 128.5, 125.6 (d, *J* = 11.7 Hz), 121.3 (d, *J* = 5.8 Hz), 35.0, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 4.9 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.4.

HRMS (ESI) [M+H]⁺: calcd. 373.1488 (³⁷Cl), found. 373.1483.

Optical Rotation: [α]_D²⁰ = +46.4 (*c* = 1.88, acetone).

HPLC: Daicel Chiralcel AD-H (96 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 279 nm, *t* (major) = 4.9 min, *t* (minor) = 10.9 min.



3jl: 90% yield, white powder.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.70 – 7.64 (m, 2H), 7.52 – 7.47 (m, 4H), 7.40 (d, *J* = 19.3 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 6.52 (dd, *J* = 17.7, 16.1, 11.6, 1.4 Hz, 1H), 5.37 – 5.32 (m, 1H), 5.35 – 5.31 (m, 1H), 2.23 (dq, *J* = 11.2, 7.6 Hz, 2H), 1.33 (s, 9H), 1.22 (dt, *J* = 17.4, 7.7 Hz, 3H).

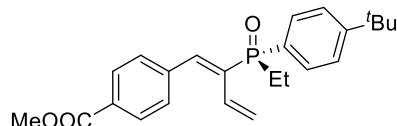
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.1, 138.9 (d, *J* = 18.7 Hz), 134.7 (d, *J* = 8.7 Hz), 132.2, 131.4 (d, *J* = 8.9 Hz), 130.6 (d, *J* = 9.6 Hz), 129.5 (d, *J* = 100.1 Hz), 129.3, 128.3 (d, *J* = 91.3 Hz), 127.1, 125.6 (d, *J* = 11.6 Hz), 122.1 (d, *J* = 6.2 Hz), 35.0, 31.1, 20.1 (d, *J* = 74.5 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.2.

HRMS (ESI) [M+H]⁺: calcd. 417.0983 (⁷⁹Br), found. 417.0975.

Optical Rotation: [α]_D²⁰ = +64.2 (*c* = 1.19, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 60/40, 1 mL/min, λ = 280 nm, *t* (major) = 5.1 min, *t* (minor) = 11.8 min.



3jm: 88% yield, yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 7.9 Hz, 2H), 7.69 (t, *J* = 9.5 Hz, 2H), 7.56 – 7.44 (m, 5H), 6.55 (td, *J* = 17.1, 11.7 Hz, 1H), 5.37 (d, *J* = 30.3 Hz, 1H), 5.36 (s, 1H), 3.92 (s, 3H), 2.25 (dq, *J* = 15.5, 8.0 Hz, 2H), 1.34 (s, 9H), 1.24 (dt, *J* = 16.2, 7.3 Hz, 3H).

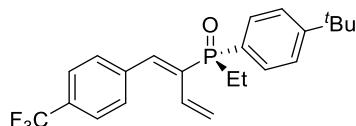
¹³C NMR (126 MHz, Chloroform-*d*) δ 166.5, 155.3 (d, *J* = 2.7 Hz), 141.2 (d, *J* = 7.6 Hz), 139.9 (d, *J* = 16.2 Hz), 134.4 (d, *J* = 87.2 Hz), 131.2 (d, *J* = 8.8 Hz), 130.7 (d, *J* = 9.5 Hz), 129.8, 129.8, 129.4, 129.1 (d, *J* = 99.6 Hz), 125.7 (d, *J* = 11.7 Hz), 121.6 (d, *J* = 5.9 Hz), 52.2, 35.0, 31.1, 20.2 (d, *J* = 73.8 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.2.

HRMS (ESI) [M+Na]⁺: calcd. 419.1752, found. 419.1749.

Optical Rotation: [α]_D²⁰ = +41.8 (*c* = 1.18, acetone).

HPLC: Daicel Chiralcel AD-H (93 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 304 nm, *t* (major) = 9.1 min, *t* (minor) = 16.6 min.



3jn: 75% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.73 – 7.65 (m, 2H), 7.64 – 7.55 (m, 4H), 7.55 – 7.46 (m, 3H), 6.53 (dd, *J* = 17.5, 15.8, 11.6, 1.4 Hz, 1H), 5.40 – 5.36 (m, 1H), 5.34 (dd, *J* = 4.2, 2.0 Hz, 1H), 2.25 (dq, *J* = 11.1, 7.6 Hz, 2H), 1.34 (s, 9H), 1.24 (dt, *J* = 17.5, 7.6 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 155.4 (d, *J* = 2.7 Hz), 140.7 (d, *J* = 7.7 Hz), 138.9 (d, *J* = 17.0 Hz), 134.6 (d, *J* = 87.1 Hz), 131.0 (d, *J* = 8.8 Hz), 130.7 (d, *J* = 9.6 Hz), 130.3 (d, *J* = 32.8 Hz), 130.1, 129.0 (d, *J* = 99.9 Hz), 125.7 (d, *J* = 11.8 Hz), 125.2 (q, *J* = 3.8 Hz), 123.9 (d, *J* = 272.2 Hz), 121.8 (d, *J* = 5.9 Hz), 35.0, 31.1, 20.1 (d, *J* = 73.9 Hz), 5.4 (d, *J* = 5.1 Hz).

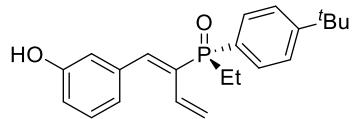
³¹P NMR (202 MHz, Chloroform-*d*) δ 35.0.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -62.8.

HRMS (ESI) [M+H]⁺: calcd. 407.1752, found. 407.1749.

Optical Rotation: [α]_D²⁰ = +38.2 (*c* = 1.07, acetone).

HPLC: Daicel Chiralcel AD-H (94 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 288 nm, *t* (major) = 6.6 min, *t* (minor) = 13.4 min.



3jo: 45% yield, white powder.

¹H NMR (500 MHz, Chloroform-*d*) δ 10.19 (s, 1H), δ 7.67 (dd, *J* = 11.2, 8.0 Hz, 2H), 7.56 (d, *J* = 19.7 Hz, 1H), 7.49 (d, *J* = 6.9 Hz, 2H), 7.31 (s, 1H), 7.19 (t, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 1H), 6.70 (td, *J* = 18.1, 11.6 Hz, 1H), 5.32 – 5.28 (m, 1H), 5.26 (d, *J* = 3.5 Hz, 1H), 2.27 (dq, *J* = 11.0, 7.7 Hz, 2H), 1.32 (s, 9H), 1.28 – 1.15 (m, 3H).

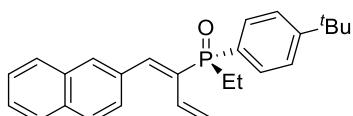
¹³C NMR (126 MHz, Chloroform-*d*) δ 158.0, 155.4 (d, *J* = 2.7 Hz), 144.2 (d, *J* = 7.1 Hz), 136.1 (d, *J* = 16.4 Hz), 131.8 (d, *J* = 9.7 Hz), 130.7 (d, *J* = 9.8 Hz), 129.6 (d, *J* = 91.3 Hz), 129.2, 128.7 (d, *J* = 100.6 Hz), 125.8 (d, *J* = 11.9 Hz), 120.4 (d, *J* = 5.5 Hz), 120.4, 117.7, 116.9, 35.0, 31.1, 19.9 (d, *J* = 73.7 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 38.1.

HRMS (ESI) [M+Na]⁺: calcd. 377.1646, found. 377.1635.

Optical Rotation: [α]_D²⁰ = +61.6 (*c* = 0.680, acetone).

HPLC: Daicel Chiralcel OD-H (96 % ee), *n*-Hexanes/*i*-PrOH = 93/7, 1 mL/min, λ = 280 nm, *t* (major) = 9.4 min, *t* (minor) = 11.8 min.



3jp: 73% yield, white powder.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.94 (s, 1H), 7.86 – 7.79 (m, 3H), 7.73 (dd, *J* = 11.1, 8.1 Hz, 2H), 7.67 – 7.58 (m, 2H), 7.50 (ddd, *J* = 10.1, 6.5, 2.1 Hz, 4H), 6.75 – 6.62 (m, 1H), 5.41 (dt, *J* = 18.0, 1.6 Hz, 1H), 5.38 – 5.32 (m, 1H), 2.32 – 2.21 (m, 2H), 1.34 (s, 9H), 1.31 – 1.19 (m, 3H).

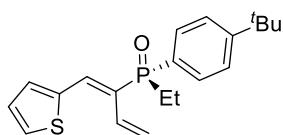
¹³C NMR (126 MHz, Chloroform-*d*) δ 155.1 (d, *J* = 2.7 Hz), 142.6 (d, *J* = 7.8 Hz), 133.1, 132.9, 132.6 (d, *J* = 83.6 Hz), 131.7 (d, *J* = 9.0 Hz), 131.6, 130.7 (d, *J* = 9.6 Hz), 130.0, 129.5 (d, *J* = 99.6 Hz), 129.5 (d, *J* = 136.8 Hz), 128.3, 127.7 (d, *J* = 23.7 Hz), 127.1, 126.8, 126.4, 125.6 (d, *J* = 11.7 Hz), 121.0 (d, *J* = 5.7 Hz), 34.9, 31.1, 20.3 (d, *J* = 73.7 Hz), 5.5 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 35.7.

HRMS (ESI) [M+H]⁺: calcd. 389.2034, found. 389.2031.

Optical Rotation: [α]_D²⁰ = +48.6 (*c* = 2.40, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 265 nm, *t* (major) = 8.2 min, *t* (minor) = 12.0 min.



3jq: 24% yield, light yellow oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.76 – 7.59 (m, 3H), 7.48 (dd, *J* = 8.4, 2.6 Hz, 2H), 7.42 (d, *J* = 5.1 Hz, 1H), 7.30 (d, *J* = 3.6 Hz, 1H), 7.07 (dd, *J* = 5.1, 3.7 Hz, 1H), 6.68 (dd, *J* = 17.8, 14.4, 11.5, 1.5 Hz, 1H), 5.46 – 5.40 (m, 1H), 5.32 (ddd, *J* = 17.7, 2.6, 1.3 Hz, 1H), 2.22 (dq, *J* = 10.4, 7.5, 3.6 Hz, 2H), 1.33 (s, 9H), 1.22 (dt, *J* = 17.3, 7.6 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 155.1 (d, *J* = 2.8 Hz), 138.9 (d, *J* = 18.7 Hz), 134.7 (d, *J* = 8.7 Hz), 132.2, 131.4 (d, *J* = 8.9 Hz), 130.6 (d, *J* = 9.6 Hz), 129.5 (d, *J* = 100.2 Hz), 129.3, 128.3 (d, *J* = 91.2

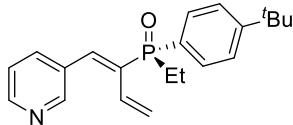
Hz), 127.1, 125.6 (d, J = 11.6 Hz), 122.1 (d, J = 6.2 Hz), 35.0, 31.1, 20.1 (d, J = 74.5 Hz), 5.4 (d, J = 5.1 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 34.9.

HRMS (ESI) [M+H] $^+$: calcd. 345.1442, found. 345.1440.

Optical Rotation: $[\alpha]_D^{20} = +8.00$ (c = 2.95, acetone).

HPLC: Daicel Chiralcel AD-H (95 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, λ = 305 nm, t (major) = 7.7 min, t (minor) = 14.7 min.



3jr: 76% yield, yellow oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.64 (d, J = 2.3 Hz, 1H), 8.50 – 8.43 (m, 1H), 7.78 – 7.70 (m, 1H), 7.61 (dd, J = 11.1, 8.1 Hz, 2H), 7.44 (dd, J = 8.3, 2.6 Hz, 2H), 7.38 (d, J = 19.1 Hz, 1H), 7.26 – 7.20 (m, 1H), 6.46 (ddd, J = 17.9, 15.1, 11.2 Hz, 1H), 5.34 – 5.30 (m, 1H), 5.30 – 5.26 (m, 1H), 2.17 (dq, J = 11.0, 7.6 Hz, 2H), 1.26 (s, 9H), 1.16 (dt, J = 17.2, 7.6 Hz, 3H).

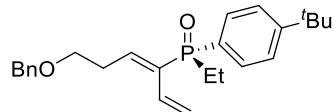
^{31}P NMR (202 MHz, Chloroform-*d*) δ 34.9.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 155.3 (d, J = 2.7 Hz), 150.7, 149.3, 138.6 (d, J = 7.7 Hz), 136.8, 134.7 (d, J = 87.1 Hz), 131.3 (d, J = 16.1 Hz), 130.9 (d, J = 8.9 Hz), 130.6 (d, J = 9.6 Hz), 128.8 (d, J = 99.9 Hz), 125.7 (d, J = 11.8 Hz), 123.1, 121.9 (d, J = 5.9 Hz), 34.9, 31.0, 20.0 (d, J = 74.0 Hz), 5.4 (d, J = 5.1 Hz).

HRMS (ESI) [M+Na] $^+$: calcd. 362.1650, found. 362.1646.

Optical Rotation: $[\alpha]_D^{20} = +30.8$ (c = 0.860, acetone).

HPLC: Daicel Chiralcel AD-H (92 % ee), *n*-Hexanes/*i*-PrOH = 70/30, 1 mL/min, λ = 261 nm, t (major) = 6.8 min, t (minor) = 11.4 min.



3js: 59% yield, colorless oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.60 (dd, J = 10.9, 8.0 Hz, 2H), 7.43 (dd, J = 8.3, 2.5 Hz, 2H), 7.31 (m, 5H), 6.60 (dt, J = 19.4, 7.2 Hz, 1H), 6.32 (dt, J = 17.7, 12.3 Hz, 1H), 5.33 (d, J = 10.5 Hz, 1H), 5.31 – 5.28 (m, 1H), 4.51 (s, 2H), 3.60 (t, J = 6.6 Hz, 2H), 2.66 (dd, J = 6.8, 2.8 Hz, 2H), 2.08 (dt, J = 15.1, 7.7 Hz, 2H), 1.31 (s, 9H), 1.22 – 1.11 (m, 3H).

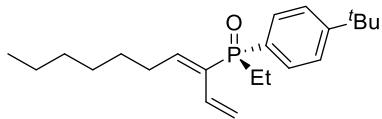
^{13}C NMR (126 MHz, Chloroform-*d*) δ 154.8 (d, J = 2.8 Hz), 142.8 (d, J = 7.0 Hz), 138.1, 133.4 (d, J = 91.3 Hz), 130.5 (d, J = 9.5 Hz), 130.0 (d, J = 10.7 Hz), 129.1 (d, J = 99.2 Hz), 128.3, 127.5 (d, J = 1.8 Hz), 125.4 (d, J = 11.5 Hz), 125.1, 120.9 (d, J = 7.2 Hz), 73.0, 68.8, 34.9, 31.0, 29.9 (d, J = 13.0 Hz), 20.7 (d, J = 73.4 Hz), 5.3 (d, J = 5.0 Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 34.3.

HRMS (ESI) [M+H] $^+$: calcd. 397.2296, found. 397.2298.

Optical Rotation: $[\alpha]_D^{20} = +22.2$ (c = 1.56, acetone).

HPLC: Daicel Chiralcel AD-H (>99 % ee), *n*-Hexanes/*i*-PrOH = 93/7, 0.5 mL/min, λ = 228 nm, t (major) = 40.9 min, t (minor) = 34.6 min.



3jt: 90% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.66 – 7.56 (m, 2H), 7.47 (dd, *J* = 8.4, 2.5 Hz, 2H), 6.58 (dt, *J* = 19.5, 7.4 Hz, 1H), 6.34 (ddd, *J* = 17.8, 14.0, 11.5 Hz, 1H), 5.28 – 5.26 (m, 1H), 5.30 – 5.22 (m, 1H), 2.33 (qd, *J* = 7.5, 2.8 Hz, 2H), 2.10 (dddd, *J* = 15.0, 9.2, 7.5, 2.3 Hz, 2H), 1.47 (p, *J* = 7.2 Hz, 2H), 1.36 – 1.24 (m, 6H), 1.32 (s, 9H), 1.16 (dt, *J* = 17.2, 7.6 Hz, 3H), 0.88 (t, *J* = 6.7 Hz, 3H).

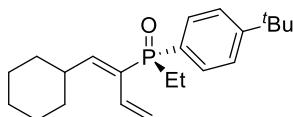
¹³C NMR (126 MHz, Chloroform-*d*) δ 154.8 (d, *J* = 2.7 Hz), 147.3 (d, *J* = 6.0 Hz), 131.3 (d, *J* = 91.8 Hz), 130.5 (d, *J* = 9.6 Hz), 130.2 (d, *J* = 11.1 Hz), 129.5 (d, *J* = 98.8 Hz), 125.4 (d, *J* = 11.5 Hz), 120.3 (d, *J* = 7.2 Hz), 34.9, 31.5, 31.1, 29.2 (d, *J* = 12.8 Hz), 29.0, 28.8 (d, *J* = 1.6 Hz), 22.5, 20.7 (d, *J* = 73.4 Hz), 14.0, 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 34.3.

HRMS (ESI) [M+H]⁺: calcd. 347.2504, found. 347.2504.

Optical Rotation: [α]_D²⁰ = -5.39 (*c* = 1.32, acetone).

HPLC: Daicel Chiralcel IA-H (99 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 0.5 mL/min, λ = 256 nm, *t* (major) = 14.9 min, *t* (minor) = 16.6 min.



3ju: 61% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 10.9, 8.0 Hz, 2H), 7.46 (dd, *J* = 8.3, 2.3 Hz, 2H), 6.55 – 6.24 (m, 2H), 5.26 (s, 1H), 5.24 – 5.21 (m, 1H), 2.58 (q, *J* = 10.8 Hz, 1H), 2.16 – 2.05 (m, 2H), 1.82 – 1.60 (m, 6H), 1.32 (s, 9H), 1.30 – 1.20 (m, 4H), 1.22 – 1.10 (m, 3H).

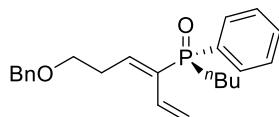
¹³C NMR (126 MHz, Chloroform-*d*) δ 154.8 (d, *J* = 2.5 Hz), 152.1 (d, *J* = 5.4 Hz), 130.5 (d, *J* = 9.6 Hz), 130.3 (d, *J* = 11.0 Hz), 129.7 (d, *J* = 52.3 Hz), 129.0 (d, *J* = 45.1 Hz), 125.4 (d, *J* = 11.6 Hz), 120.0 (d, *J* = 7.0 Hz), 38.1 (d, *J* = 12.2 Hz), 34.9, 32.3 (d, *J* = 21.1 Hz), 31.0, 25.7, 25.4, 20.6 (d, *J* = 73.4 Hz), 5.4 (d, *J* = 5.0 Hz).

³¹P NMR (202 MHz, Chloroform-*d*) δ 34.3.

HRMS (ESI) [M+Na]⁺: calcd. 367.2167, found. 367.2162.

Optical Rotation: [α]_D²⁰ = +7.41 (*c* = 0.870, acetone).

HPLC: Daicel Chiralcel AD-H (97 % ee), *n*-Hexanes/*i*-PrOH = 95/5, 1 mL/min, λ = 235 nm, *t* (major) = 16.4 min, *t* (minor) = 19.0 min.



3jv: 92% yield, colorless oil.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.75 – 7.61 (m, 2H), 7.55 – 7.46 (m, 1H), 7.44 (td, *J* = 7.6, 2.6 Hz, 2H), 7.37 – 7.24 (m, 5H), 6.62 (dt, *J* = 19.6, 7.2 Hz, 1H), 6.32 (ddd, *J* = 17.6, 13.5, 11.6 Hz, 1H), 5.32 (d, *J* = 2.5 Hz, 1H), 5.30 – 5.27 (m, 1H), 4.51 (s, 2H), 3.60 (t, *J* = 6.6 Hz, 2H), 2.66 (qd, *J* = 6.7, 2.8 Hz, 2H), 2.12 (td, *J* = 10.9, 6.6 Hz, 2H), 1.56 (dt, *J* = 14.3, 7.4 Hz, 2H), 1.41 (h, *J* = 7.3 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 143.3 (d, *J* = 7.0 Hz), 138.0, 133.1 (d, *J* = 91.5 Hz), 132.2 (d, *J* = 97.1 Hz), 131.6 (d, *J* = 2.7 Hz), 130.6 (d, *J* = 9.4 Hz), 129.7 (d, *J* = 10.7 Hz), 128.5 (d, *J* = 11.5 Hz),

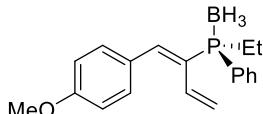
128.3, 127.5, 127.5, 121.1 (d, $J = 7.3$ Hz), 72.9, 68.6 (d, $J = 1.6$ Hz), 29.9 (d, $J = 13.1$ Hz), 27.2 (d, $J = 72.1$ Hz), 24.0 (d, $J = 15.2$ Hz), 23.2 (d, $J = 3.9$ Hz), 13.5.

^{31}P NMR (202 MHz, Chloroform-*d*) δ 34.4.

HRMS (ESI) [M+Na] $^+$: calcd. 391.1803, found. 391.1806.

Optical Rotation: $[\alpha]_D^{20} = +12.7$ ($c = 1.79$, acetone).

HPLC: Daicel Chiralcel AD-H (92 % ee), *n*-Hexanes/*i*-PrOH = 80/20, 1 mL/min, $\lambda = 208$ nm, t (major) = 8.0 min, t (minor) = 12.4 min.



4: 60% yield, colorless oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.65 (ddd, $J = 10.0, 7.6, 1.9$ Hz, 2H), 7.48 – 7.42 (m, 5H), 7.39 (d, $J = 20.1$ Hz, 1H), 6.90 (d, $J = 8.7$ Hz, 2H), 6.55 (dt, $J = 18.0, 11.8$ Hz, 1H), 5.23 (d, $J = 11.5$ Hz, 1H), 5.10 (d, $J = 18.0$ Hz, 1H), 3.84 (s, 3H), 2.32 – 2.20 (m, 1H), 2.13 (dq, $J = 14.3, 7.9$ Hz, 1H), 1.16 (dt, $J = 17.8, 7.6$ Hz, 3H), 1.06 – 0.75 (m, 3H).

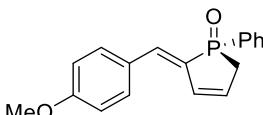
^{13}C NMR (126 MHz, Chloroform-*d*) δ 160.0, 144.7 (d, $J = 16.8$ Hz), 131.8, 131.4 (d, $J = 8.6$ Hz), 130.6 (d, $J = 2.3$ Hz), 130.3 (d, $J = 54.7$ Hz), 129.4 (d, $J = 89.7$ Hz), 128.7 (d, $J = 9.7$ Hz), 128.4 (d, $J = 17.1$ Hz), 125.2 (d, $J = 48.2$ Hz), 119.9 (d, $J = 4.9$ Hz), 113.7, 55.3, 16.1 (d, $J = 38.7$ Hz), 6.9.

^{31}P NMR (202 MHz, Chloroform-*d*) δ 24.36 (q, $J = 58.2$ Hz).

HRMS(ESI) [M+H] $^+$: calcd. 311.1736, found. 311.1729.

Optical Rotation: $[\alpha]_D^{20} = +34.9$ ($c = 1.51$, acetone).

HPLC: Daicel Chiralcel AD-H (88 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, $\lambda = 297$ nm, t (major) = 6.7 min, t (minor) = 8.5 min.



5: 92% yield, yellow oil.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.83 – 7.72 (m, 2H), 7.54 (td, $J = 7.2, 1.5$ Hz, 1H), 7.47 (td, $J = 7.5, 2.3$ Hz, 2H), 7.38 (d, $J = 8.6$ Hz, 2H), 7.34 – 7.23 (m, 1H), 6.90 (d, $J = 8.8$ Hz, 2H), 6.79 (d, $J = 18.7$ Hz, 1H), 6.31 (dddd, $J = 24.9, 6.3, 3.4, 1.6$ Hz, 1H), 3.82 (s, 3H), 2.95 (ddt, $J = 18.4, 15.4, 2.8$ Hz, 1H), 2.77 (dddd, $J = 19.3, 6.2, 3.4, 2.2$ Hz, 1H).

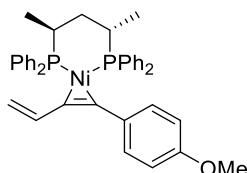
^{13}C NMR (126 MHz, Chloroform-*d*) δ 159.9, 134.6 (d, $J = 9.6$ Hz), 133.9 (d, $J = 75.7$ Hz), 133.1 (d, $J = 75.3$ Hz), 131.9 (d, $J = 3.0$ Hz), 131.7 (d, $J = 31.3$ Hz), 131.2 (d, $J = 8.1$ Hz), 130.6, 130.2 (d, $J = 10.2$ Hz), 129.2 (d, $J = 17.5$ Hz), 128.6 (d, $J = 12.0$ Hz), 114.0, 55.3, 33.0 (d, $J = 70.5$ Hz).

^{31}P NMR (202 MHz, Chloroform-*d*) δ 45.4.

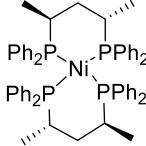
HRMS (ESI) [M+H] $^+$: calcd. 297.1044, found. 297.1045.

Optical Rotation: $[\alpha]_D^{20} = +39.8$ ($c = 1.40$, acetone).

HPLC: Daicel Chiralcel OJ-H (88 % ee), *n*-Hexanes/*i*-PrOH = 90/10, 1 mL/min, $\lambda = 315$ nm, t (major) = 19.4 min, t (minor) = 25.0 min.

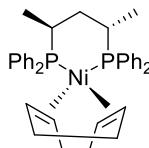


A: **¹H NMR** (500 MHz, Benzene-*d*₆) δ 7.87 – 7.68 (m, 4H), 7.51 (t, *J* = 8.6 Hz, 2H), 7.49 – 7.41 (m, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.96 (t, *J* = 7.4 Hz, 2H), 6.85 – 6.75 (m, 7H), 6.70 (d, *J* = 8.1 Hz, 3H), 6.63 (dt, *J* = 10.5, 6.0 Hz, 1H), 6.27 (d, *J* = 8.2 Hz, 2H), 5.09 (d, *J* = 17.1 Hz, 1H), 4.73 (d, *J* = 9.5 Hz, 1H), 2.94 (s, 3H), 2.42 – 2.18 (m, 2H), 1.62 – 1.38 (m, 2H), 0.69 – 0.55 (m, 6H).
³¹P NMR (202 MHz, Benzene-*d*₆) δ 35.6 (d, *J* = 20.2 Hz), 34.6 (d, *J* = 20.1 Hz).



B: **¹H NMR** (400 MHz, Benzene-*d*₆) δ 7.66 (s, 7H), 7.22 (s, 8H), 7.10 (dd, *J* = 12.3, 7.0 Hz, 12H), 6.94 (t, *J* = 7.3 Hz, 5H), 6.77 (t, *J* = 7.5 Hz, 8H), 2.38 (q, *J* = 6.5 Hz, 4H), 1.75 (d, *J* = 13.5 Hz, 4H), 0.92 (dt, *J* = 11.3, 5.3 Hz, 12H).

³¹P NMR (162 MHz, Benzene-*d*₆) δ 28.0.

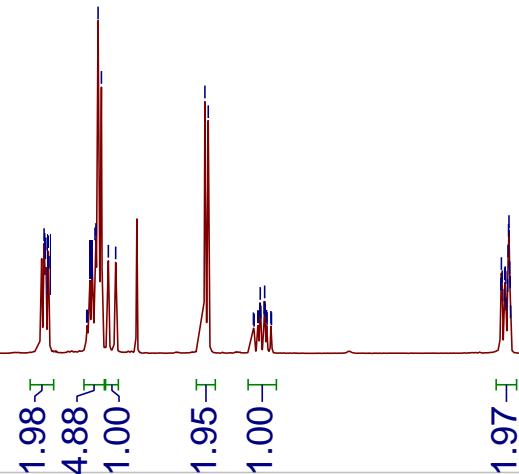
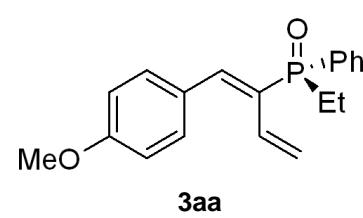


C: **¹H NMR** (400 MHz, Benzene-*d*₆) δ 7.71 – 7.55 (m, 4H), 7.41 (t, *J* = 7.4 Hz, 4H), 7.13 (d, *J* = 11.5 Hz, 4H), 7.10 – 7.03 (m, 8H), 4.61 – 4.35 (m, 4H), 2.75 – 2.64 (m, 2H), 2.34 – 2.26 (m, 2H), 2.07 (s, 2H), 1.93 – 1.82 (m, 2H), 1.79 – 1.71 (m, 2H), 1.61 – 1.46 (m, 2H), 0.95 (dd, *J* = 10.5, 6.8 Hz, 6H).

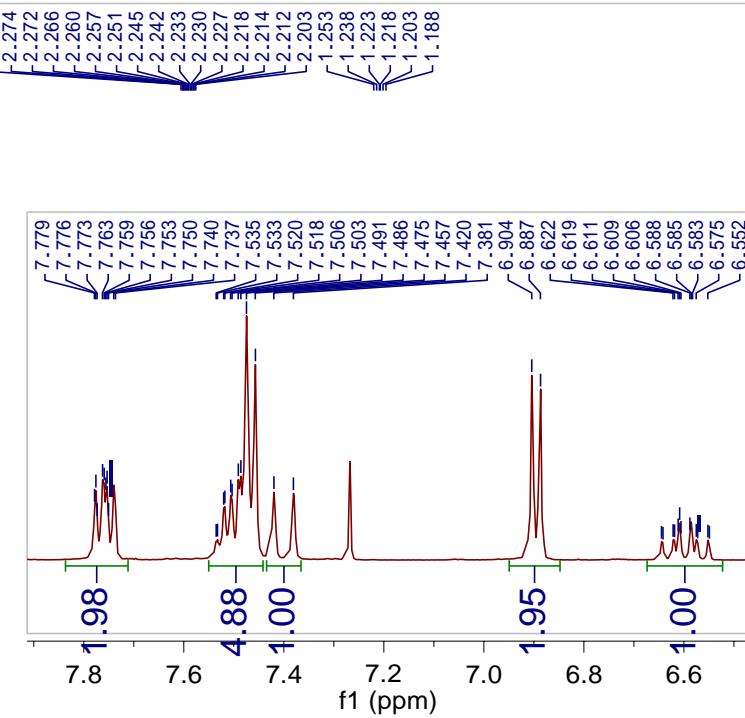
³¹P NMR (162 MHz, Benzene-*d*₆) δ 34.4.

10. Supplementary References:

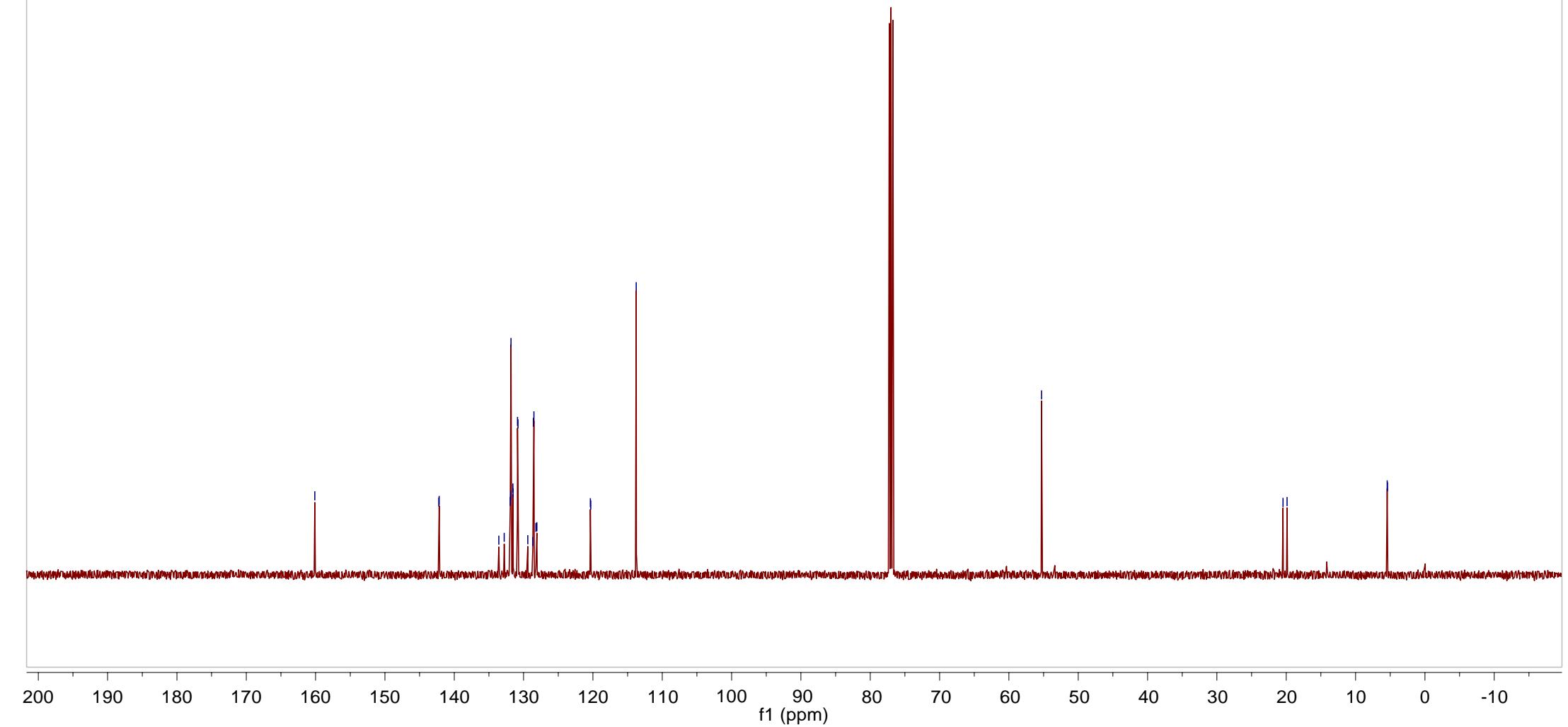
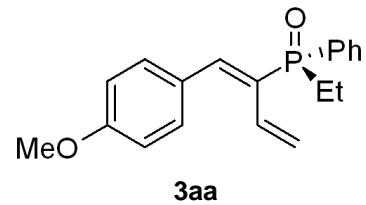
1. Y. Zhang, B. Yu, B. Gao, T. Zhang and H. Huang, *Org. Lett.*, 2019, **21**, 535.
2. R. Beaud, R. J. Phipps and M. J. Gaunt, *J. Am. Chem. Soc.*, 2016, **138**, 13183.
3. L. Duan, K. Zhao, Z. Wang, F.-L. Zhang and Z. Gu, *ACS Catal.*, 2019, **9**, 9852.
4. K. V. Rajendran and D. G. Gilheany, *Chem. Commun.*, 2012, **48**, 817.
5. Gaussian 16, Revision C.01, 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. V. 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., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. 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, Inc., Wallingford CT, **2016**.
6. S. Grimme, *J. Chem. Theory Comput.*, 2019, **15**, 2847.
7. P. Pracht, F. Bohle and S. Grimme, *Phys. Chem. Chem. Phys.*, 2020, **22**, 7169.
8. P. Pracht and S. Grimme, *Chem. Sci.*, 2021, **12**, 6551.
9. G. Luchini, J. V. Alegre-Quena, Y. Guan, I. Funes-Ardoiz, R. S. Paton, 2019, GoodVibes: GoodVibes 3.0.1 <http://doi.org/10.5281/zenodo.595246>.
10. S. Grimme, *Chem. Eur. J.*, 2012, **18**, 9955.

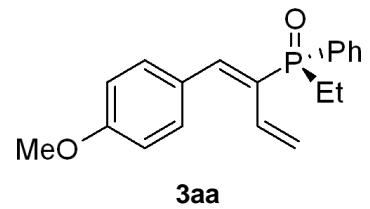


f1 (ppm)

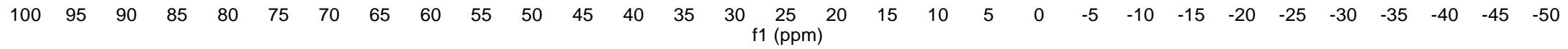


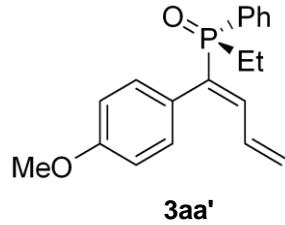
f1 (ppm)





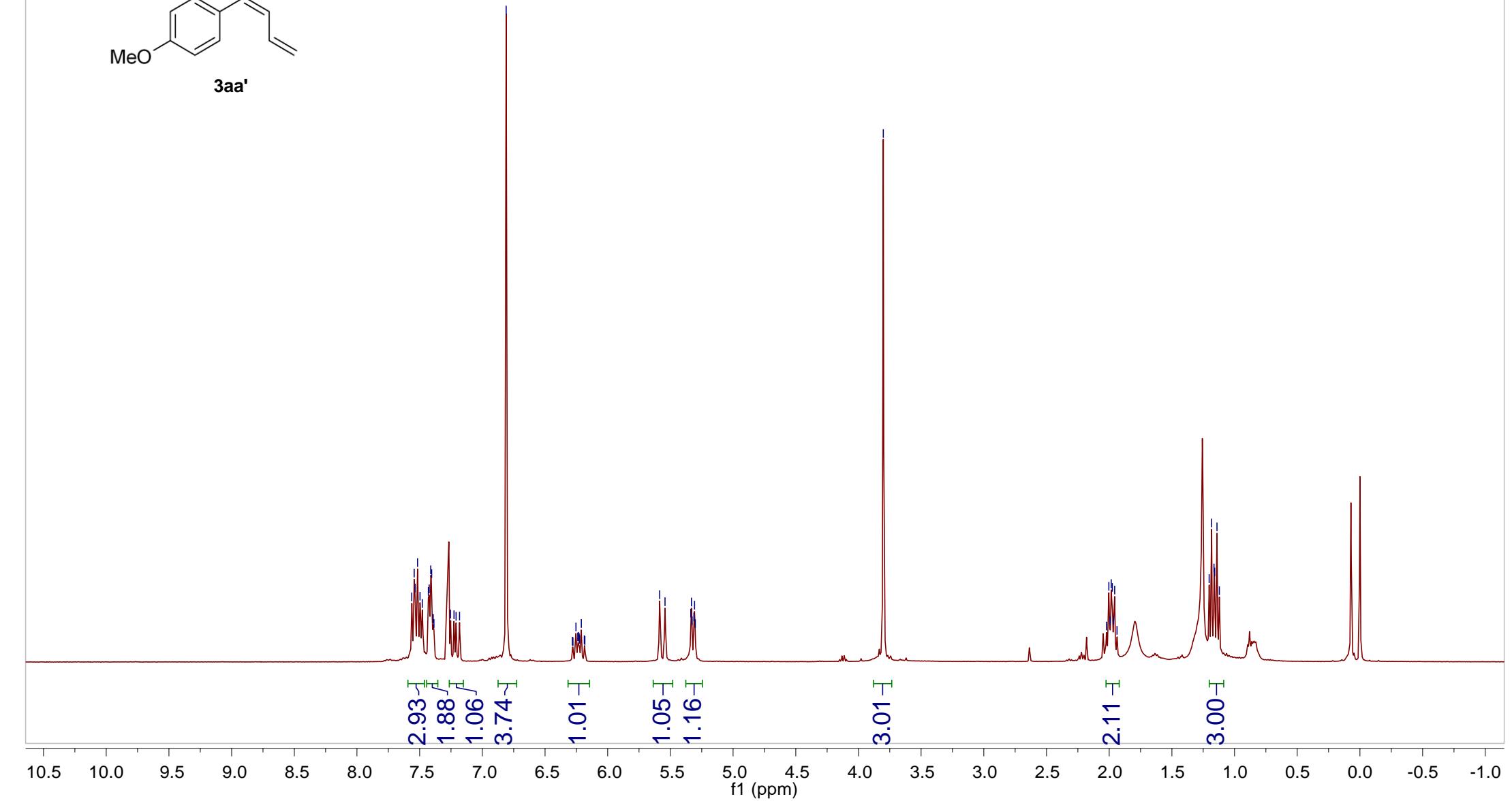
-35.954

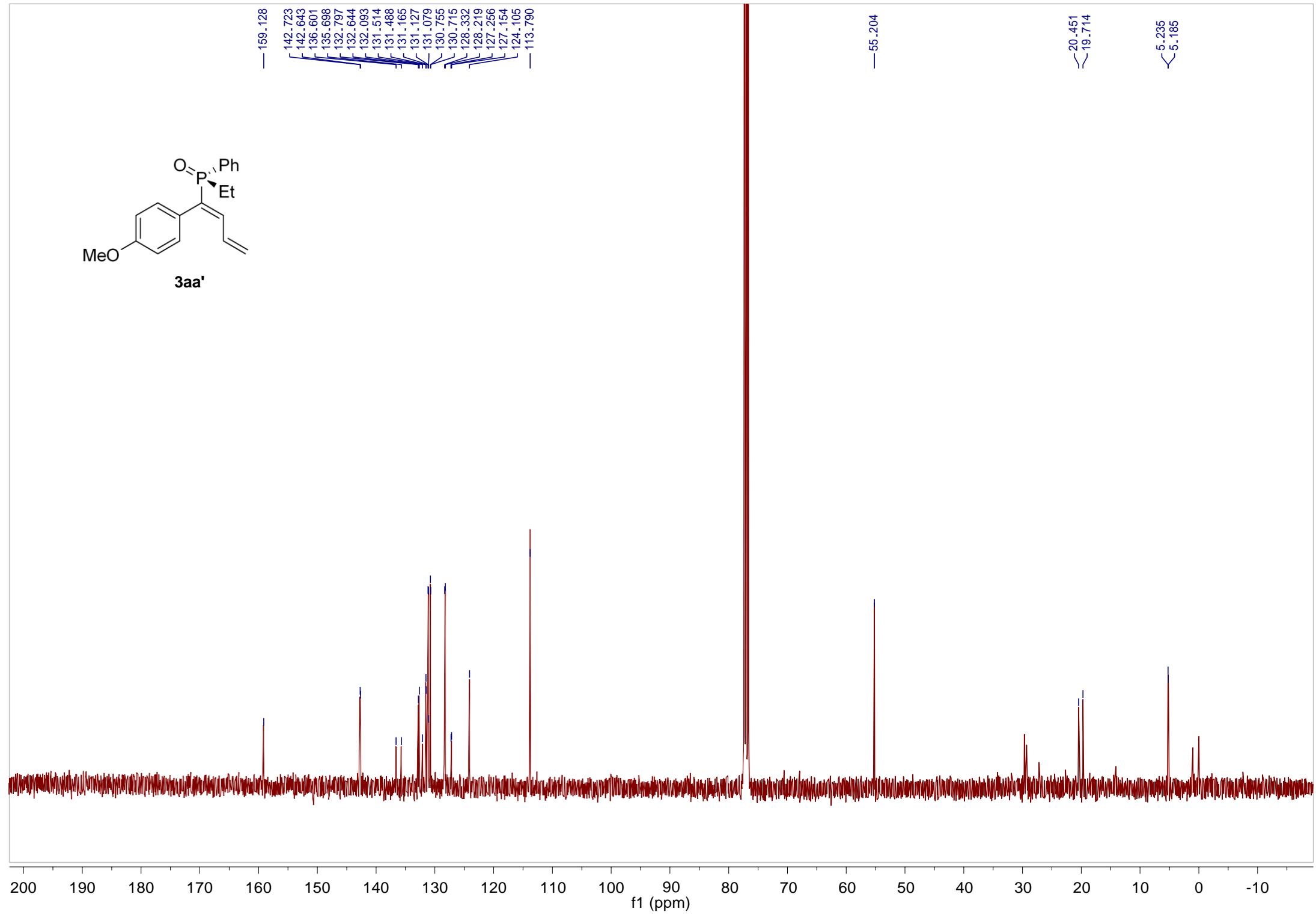
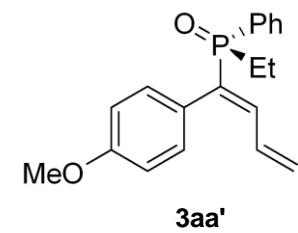


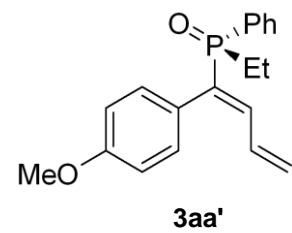


7.563
7.544
7.535
7.517
7.497
7.479
7.430
7.424
7.411
7.405
7.392
7.386
7.254
7.226
7.209
7.182
6.810
6.281
6.277
6.263
6.239
6.234
6.228
6.225
6.211
6.186
6.182
5.385
5.543
5.537
5.332
5.327
5.312
5.307
5.302

—3.802
2.022
2.003
1.994
1.984
1.975
1.965
1.956
1.937
1.202
1.183
1.164
1.159
1.140
1.121



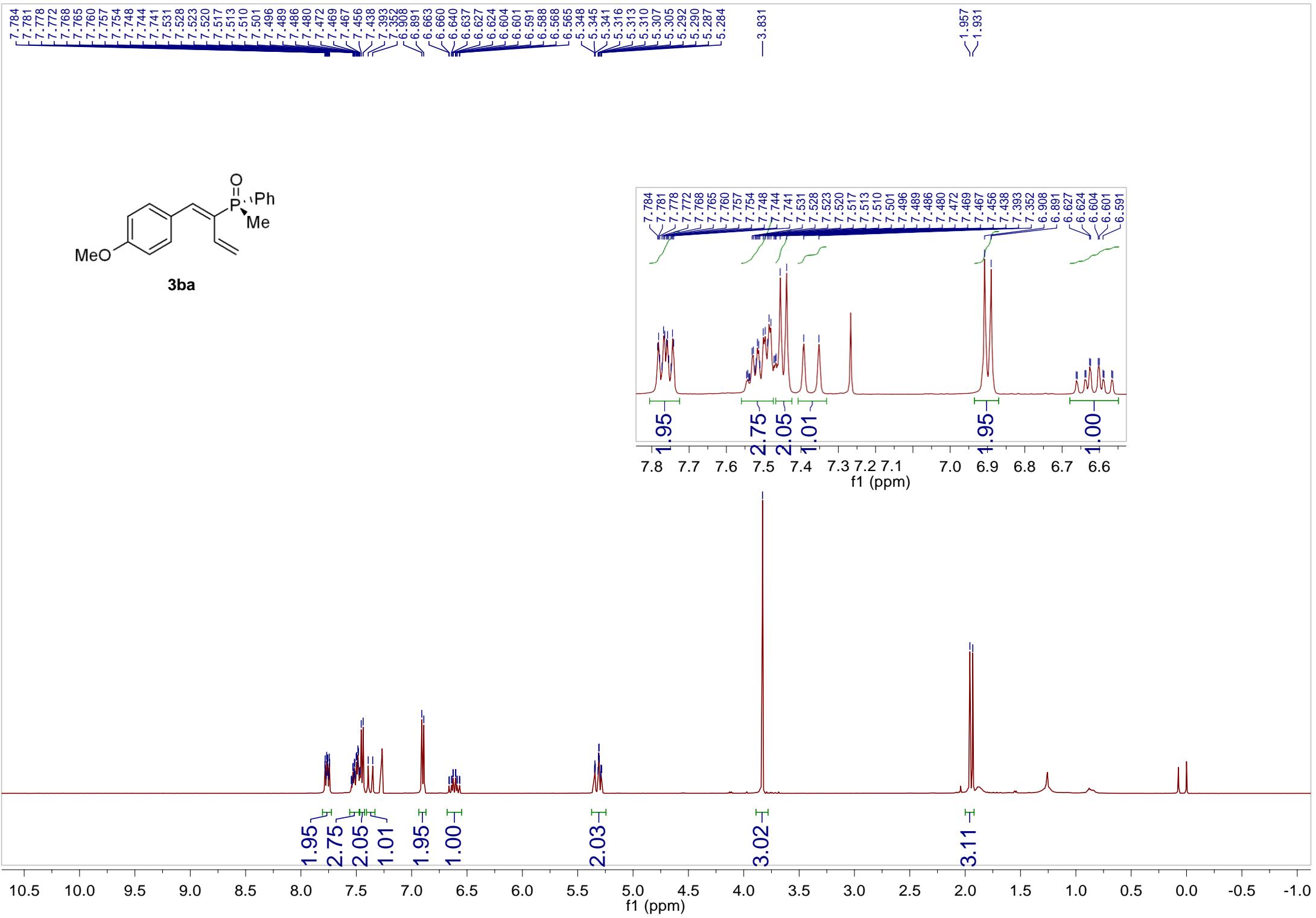


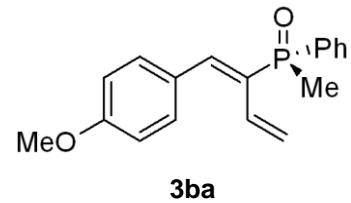


-33.731

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

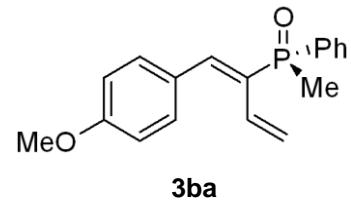
f1 (ppm)





200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

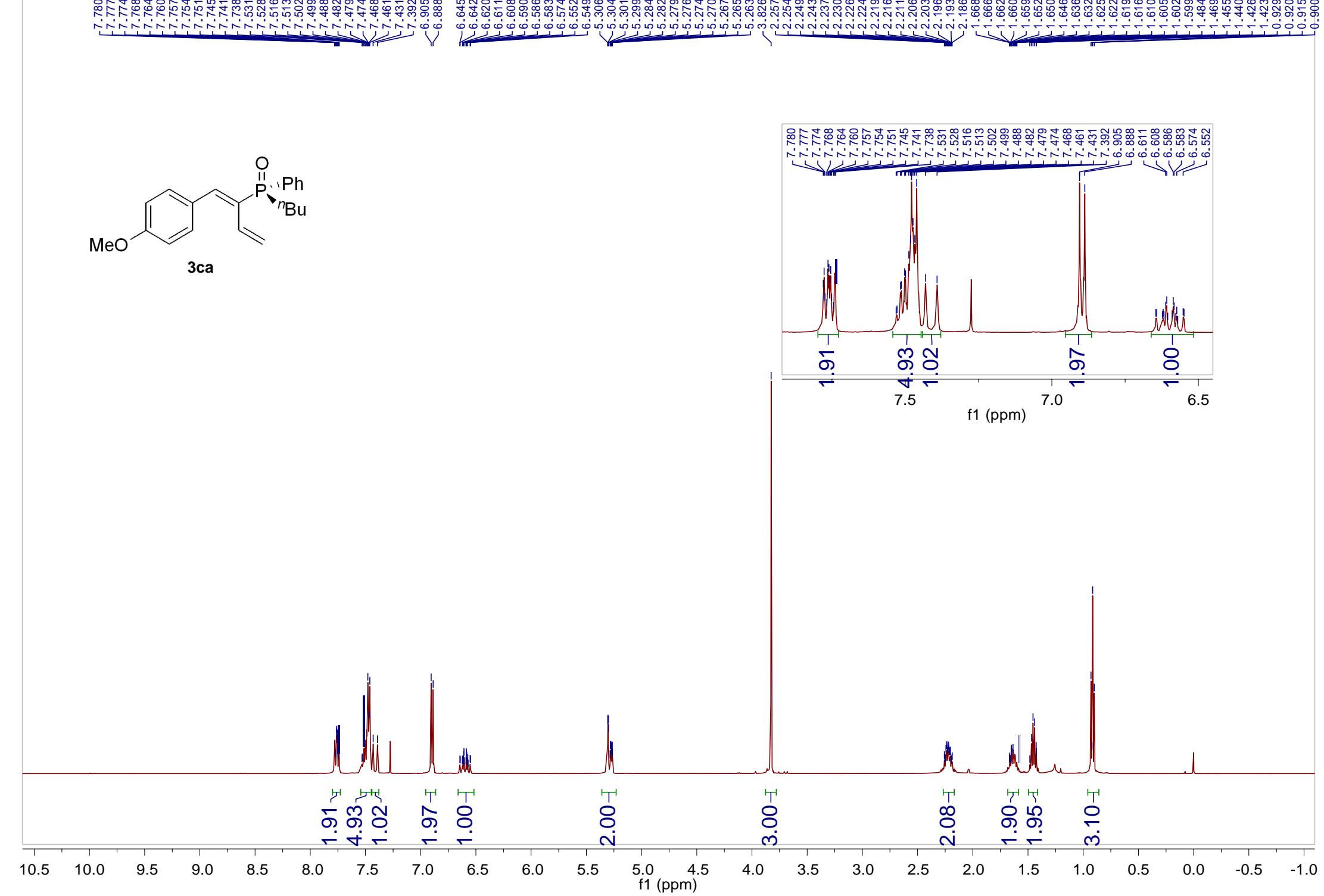
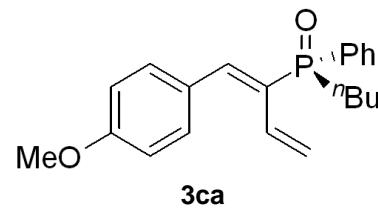


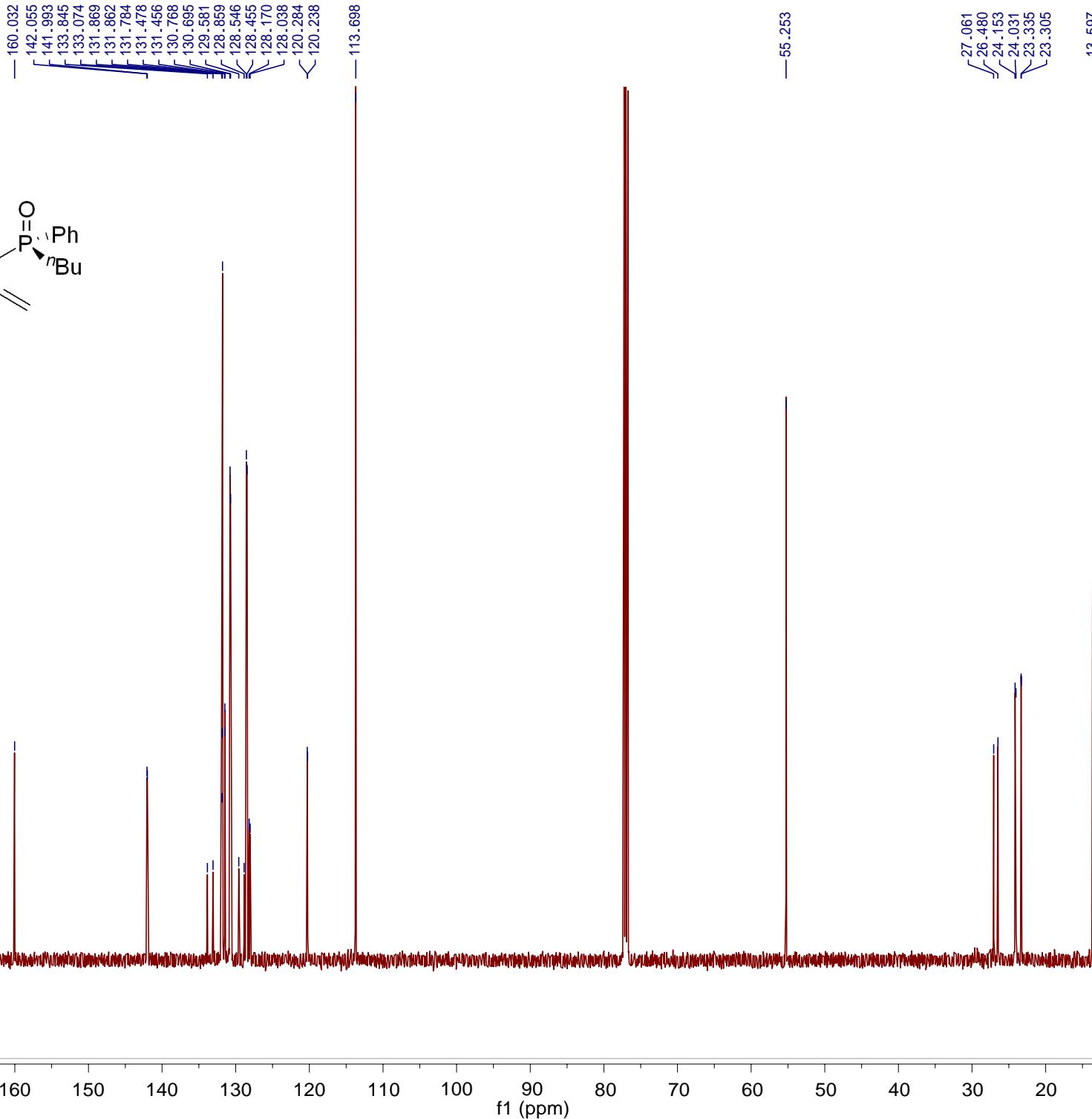
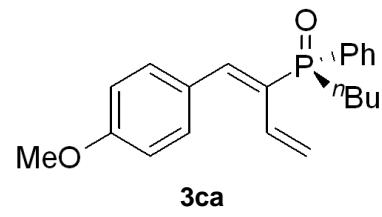
-31.729

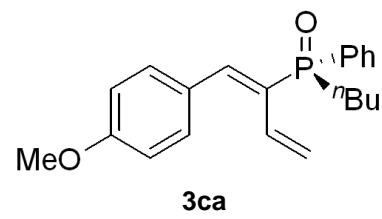
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

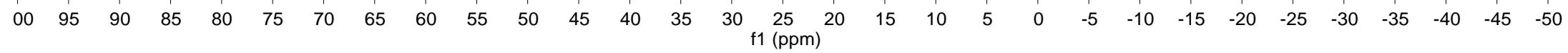
7.780
7.777
7.774
7.768
7.764
7.760
7.757
7.754
7.751
7.745
7.741
7.738
7.531
7.528
7.516
7.513
7.502
7.499
7.488
7.482
7.479
7.474
7.468
7.461
7.431
7.416
7.304
5.301
6.611
6.620
6.608
6.590
6.586
6.583
6.574
6.552
6.549
5.306
5.304
5.301
5.299
5.284
5.282
5.279
5.276
5.274
5.270
5.267
5.265
5.263
3.826
2.257
2.254
2.249
2.243
2.237
2.230
2.226
2.224
2.219
2.216
2.211
2.206
2.203
2.196
2.193
2.186
1.668
1.666
1.662
1.636
1.610
1.608
1.605
1.602
1.599
1.574
6.552

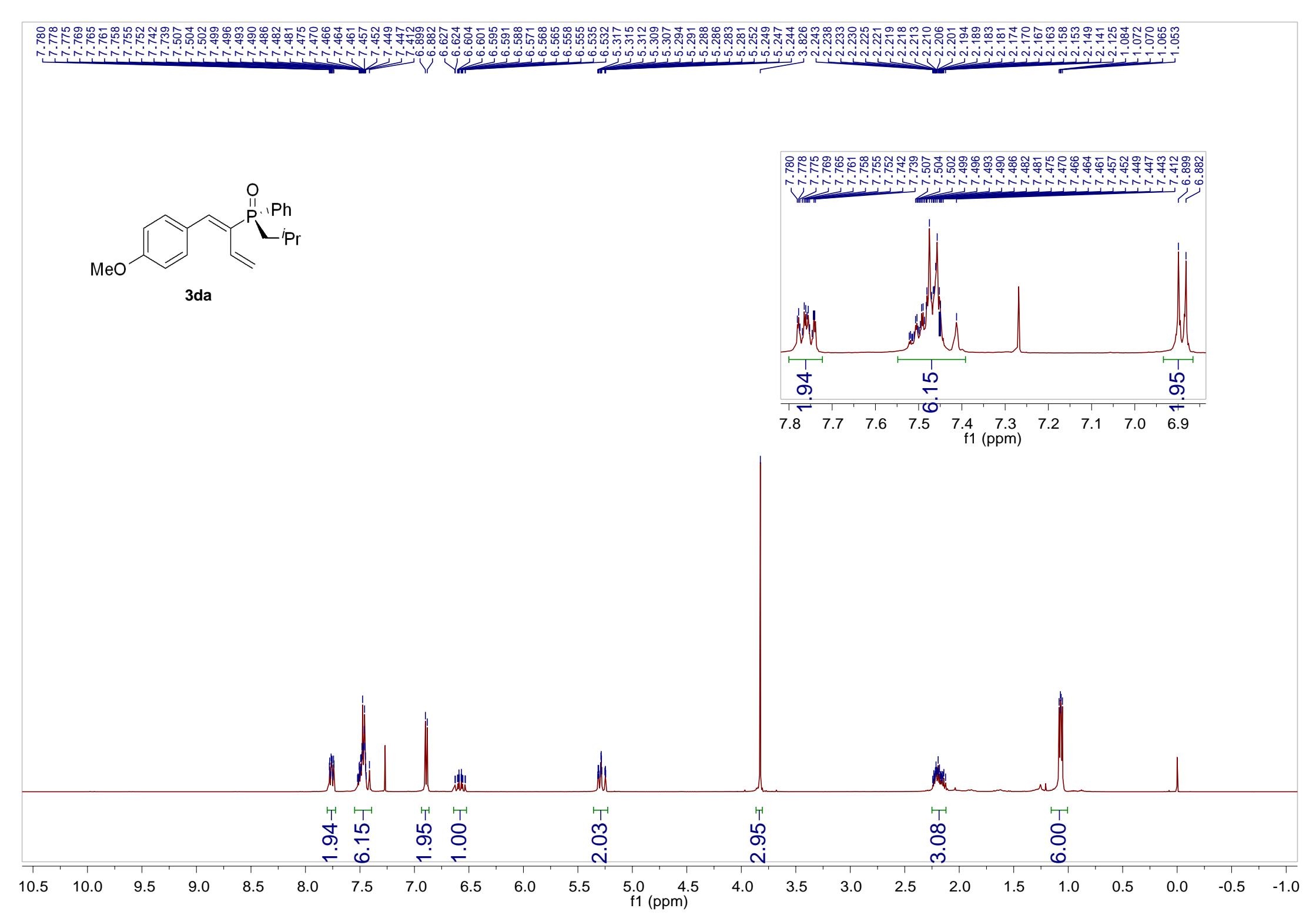






-34.301

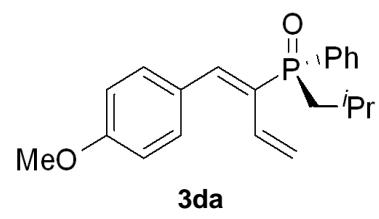






190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

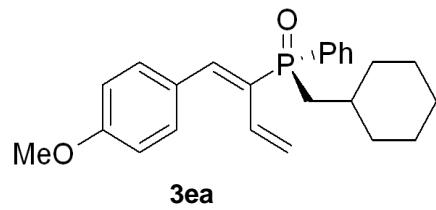
f1 (ppm)



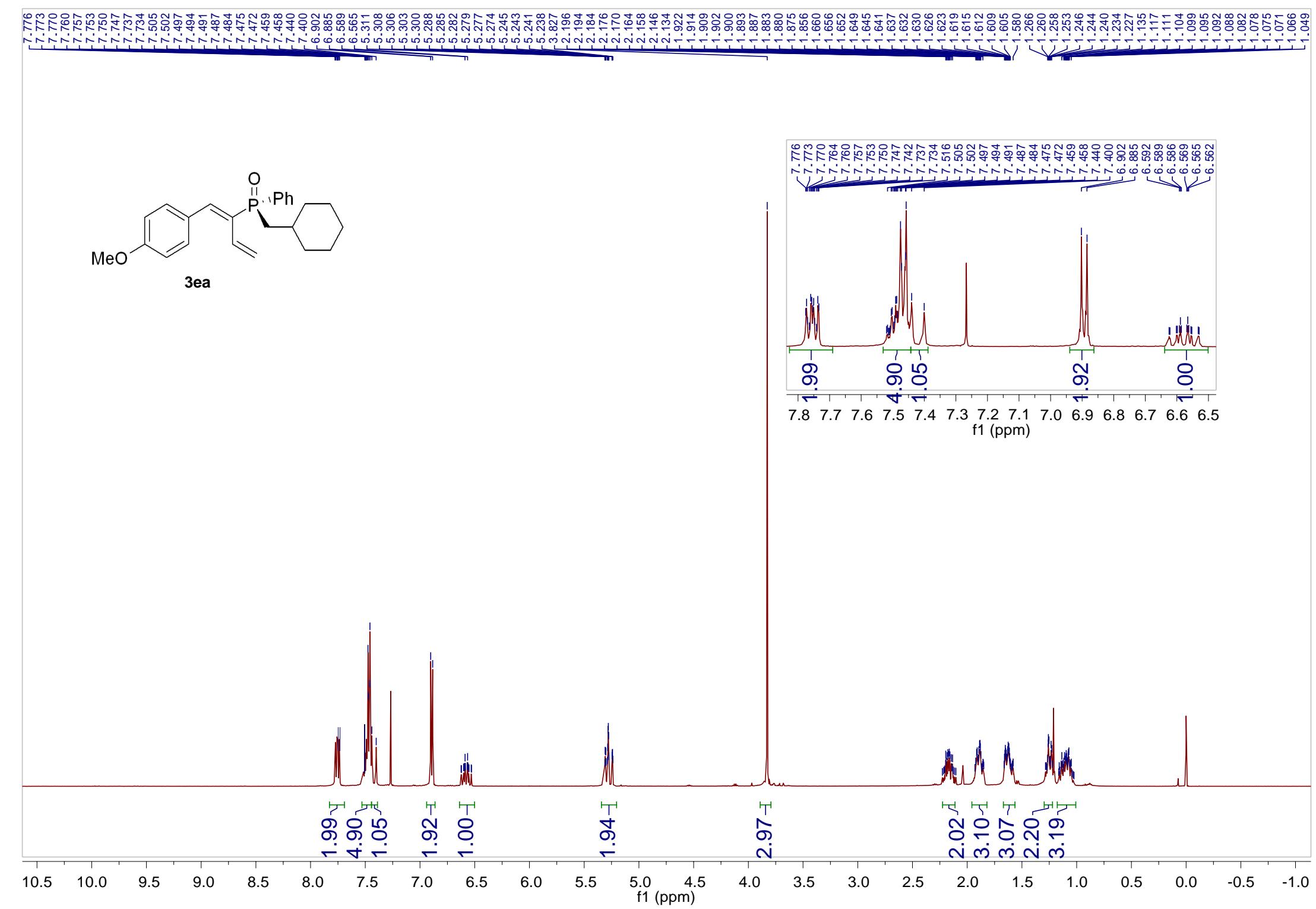
-32.599

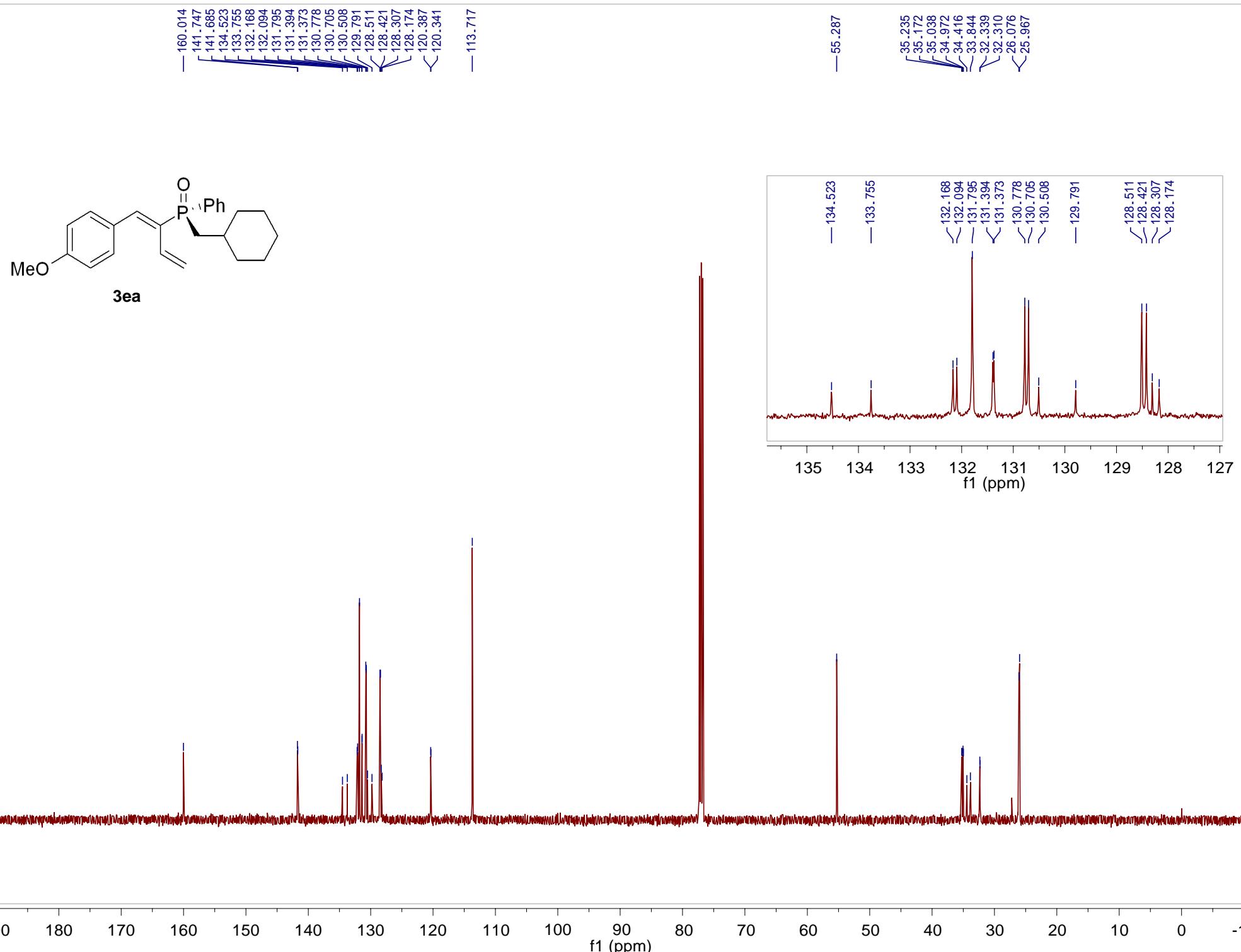
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

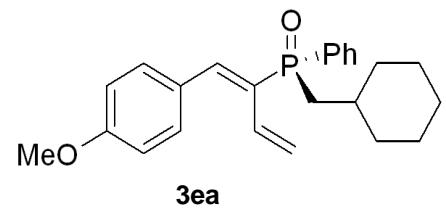
f1 (ppm)



3ea



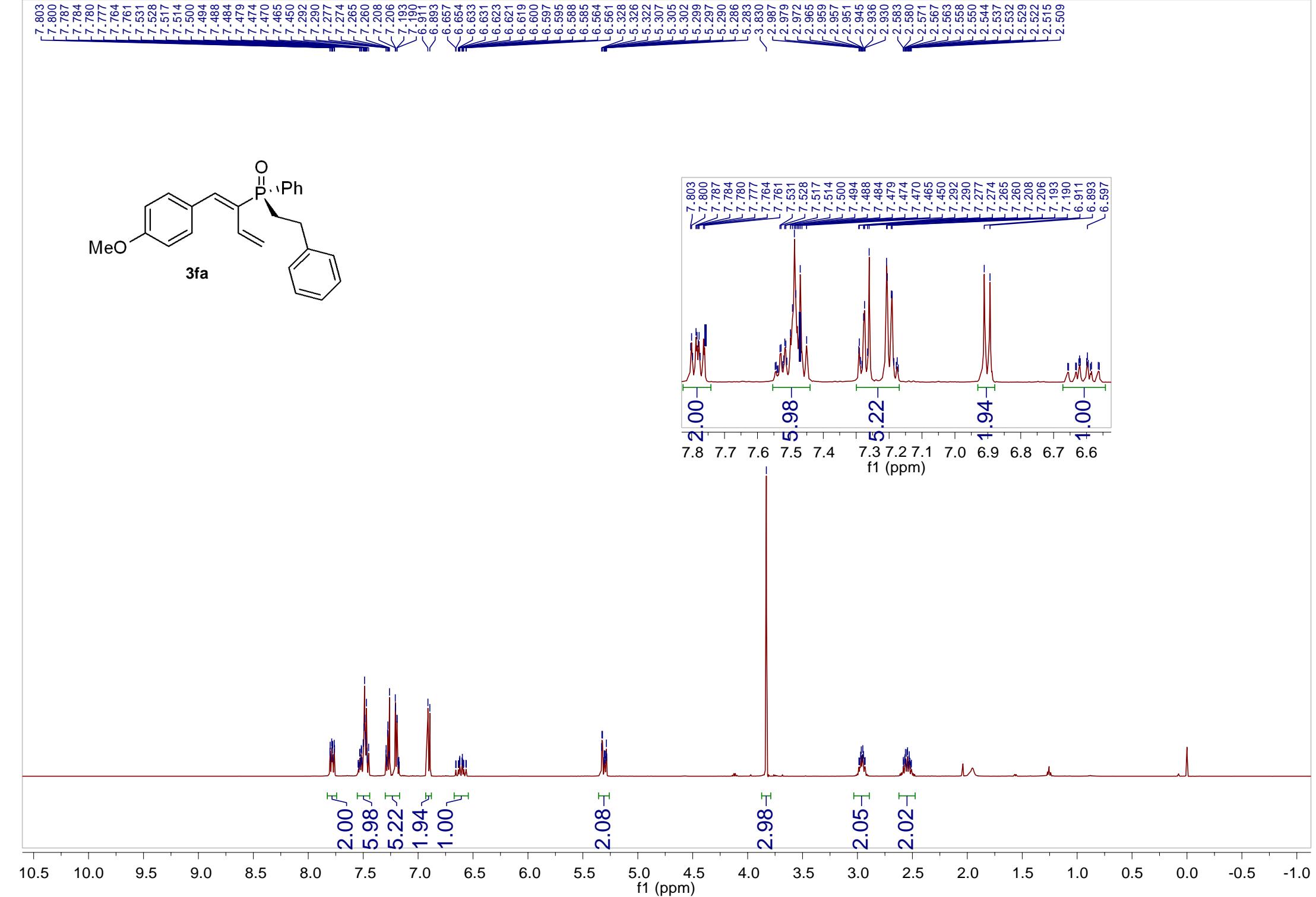


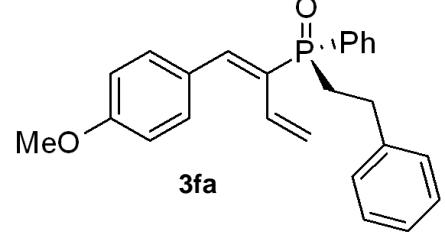


-32.798

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)



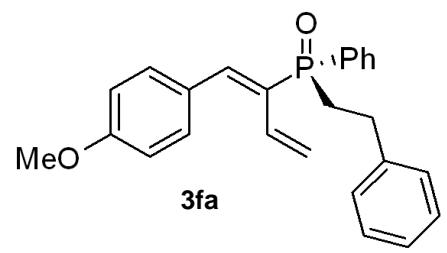


— 160.184

142.570
142.508
141.482
141.361
133.554
132.778
131.899
131.835
131.711
131.690
130.813
130.739
129.165
128.704
128.613
128.580
128.440
128.131
127.984
126.270
120.489
120.443
113.784

— 55.312

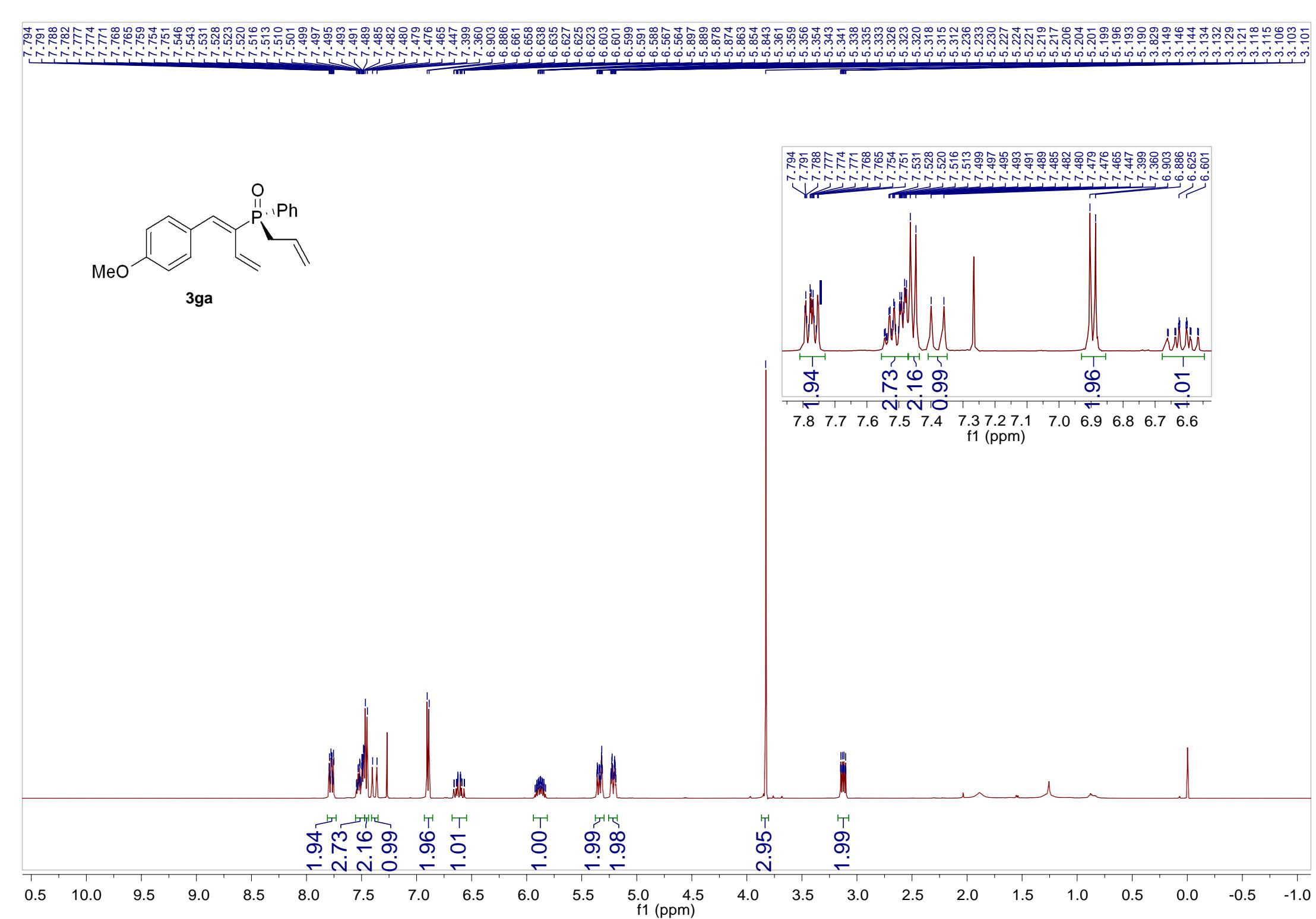
29.593
29.031
27.523
27.500

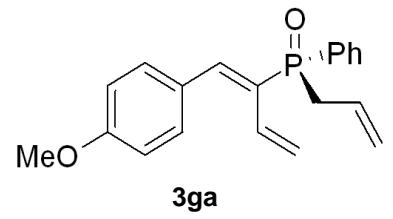


—33.125

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)





— 160.168

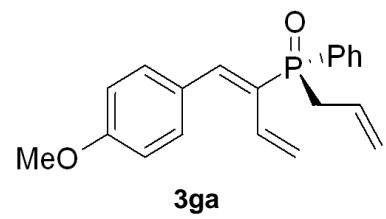
< 142.700
142.636
133.279
132.503
< 131.897
131.871
131.824
< 131.720
131.699
< 131.010
130.936
129.109
128.586
128.494
128.376
128.066
127.930
127.300
127.228
120.696
120.599
120.549
113.758

— 55.302

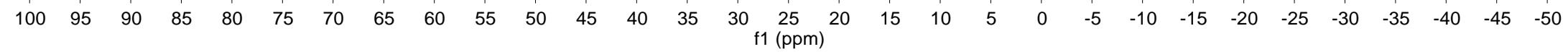
< 33.858
< 33.303

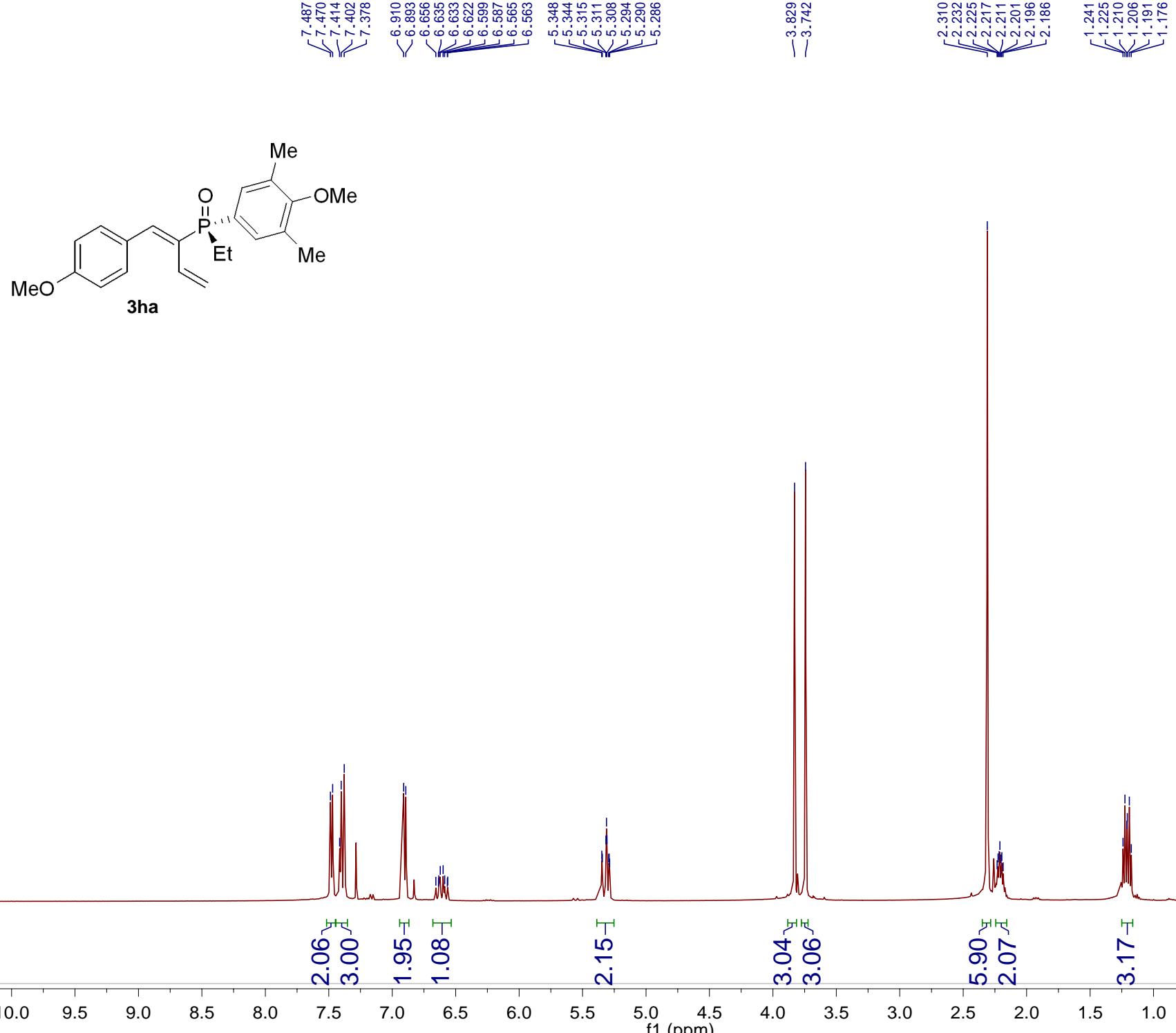
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

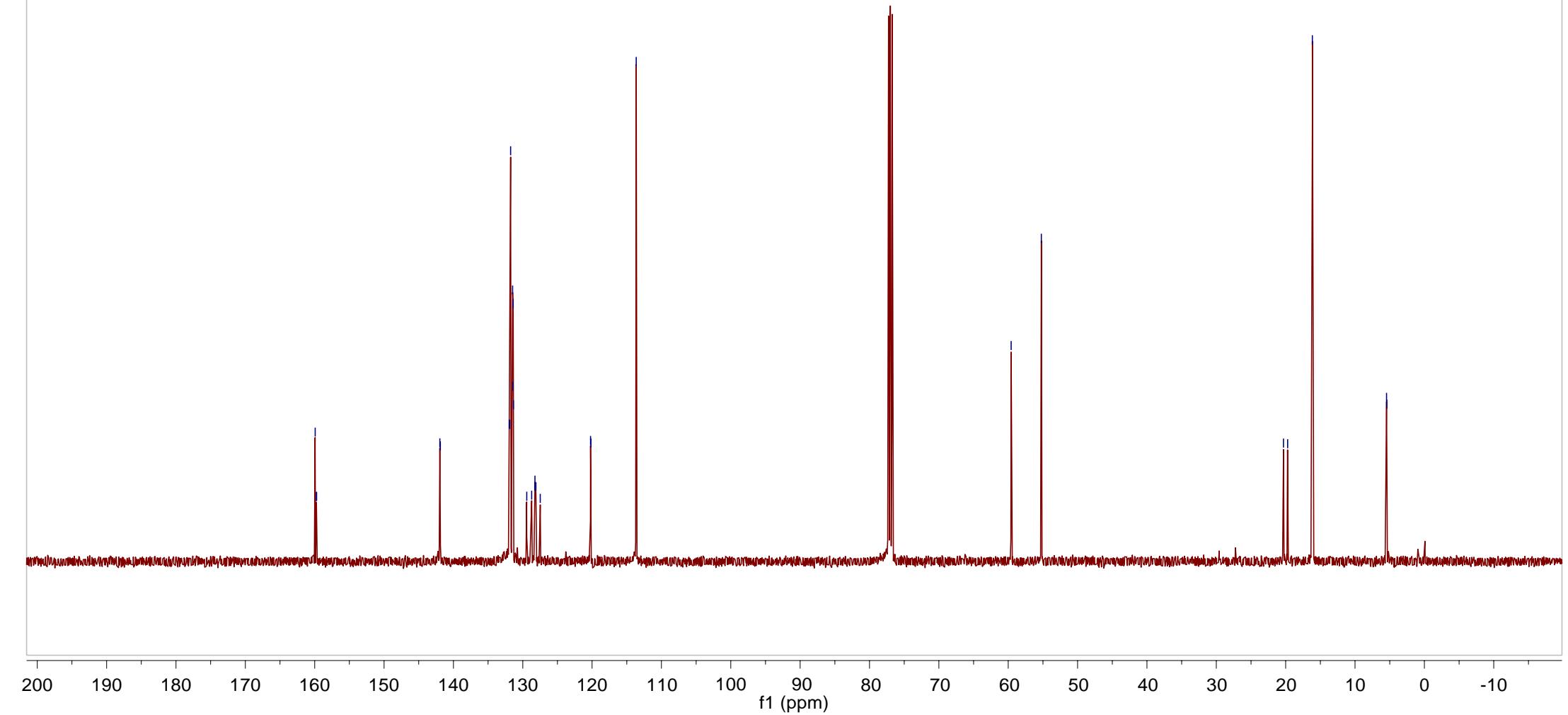
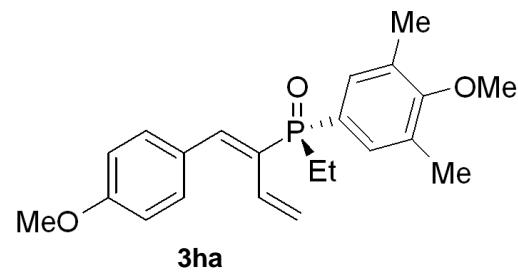
f1 (ppm)

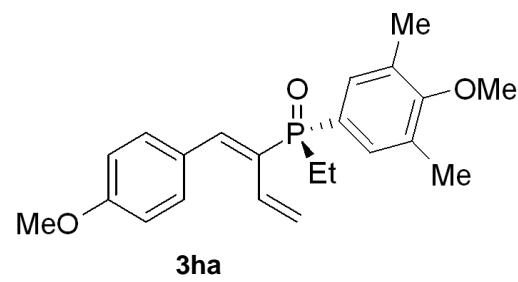


31.690





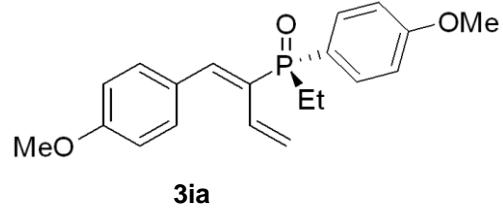




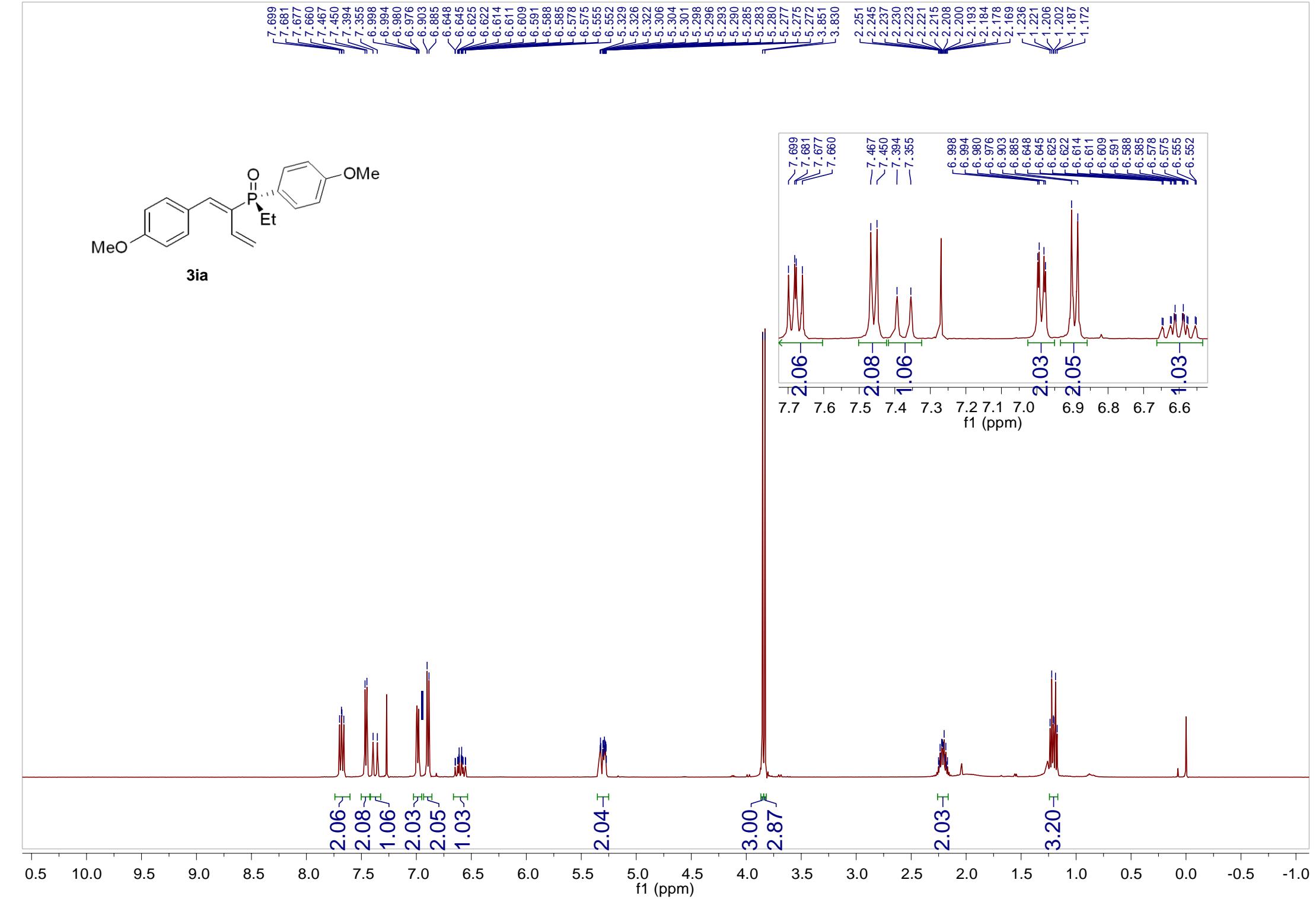
-35.620

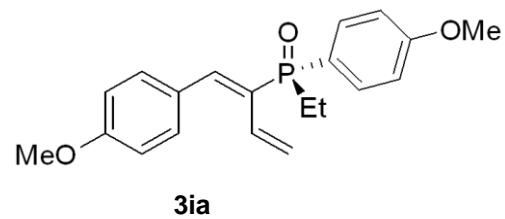
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

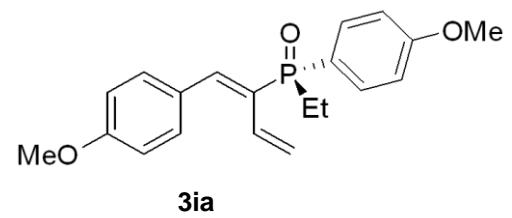
f1 (ppm)



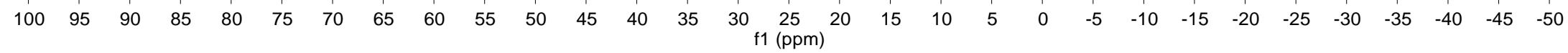
3ia

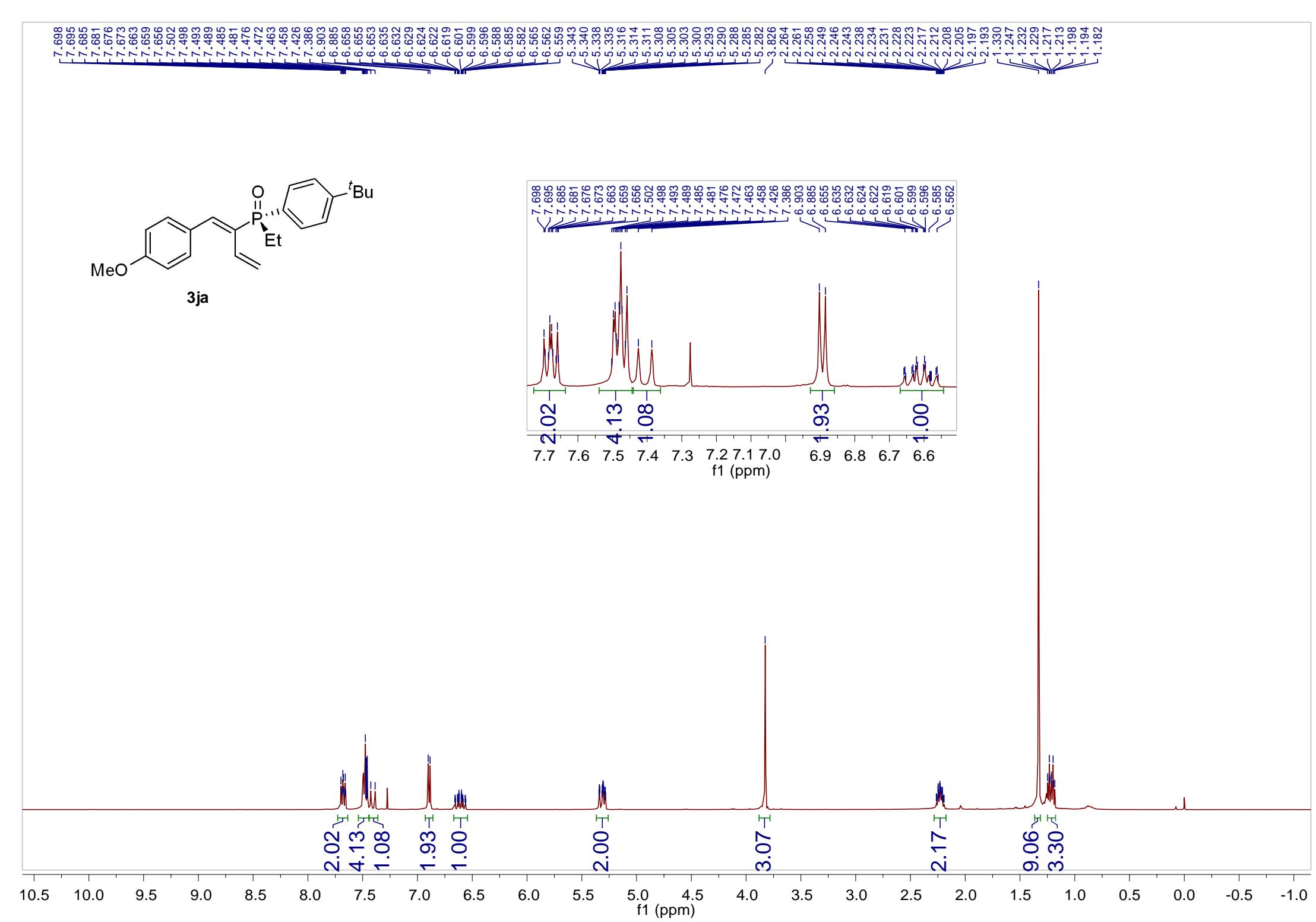


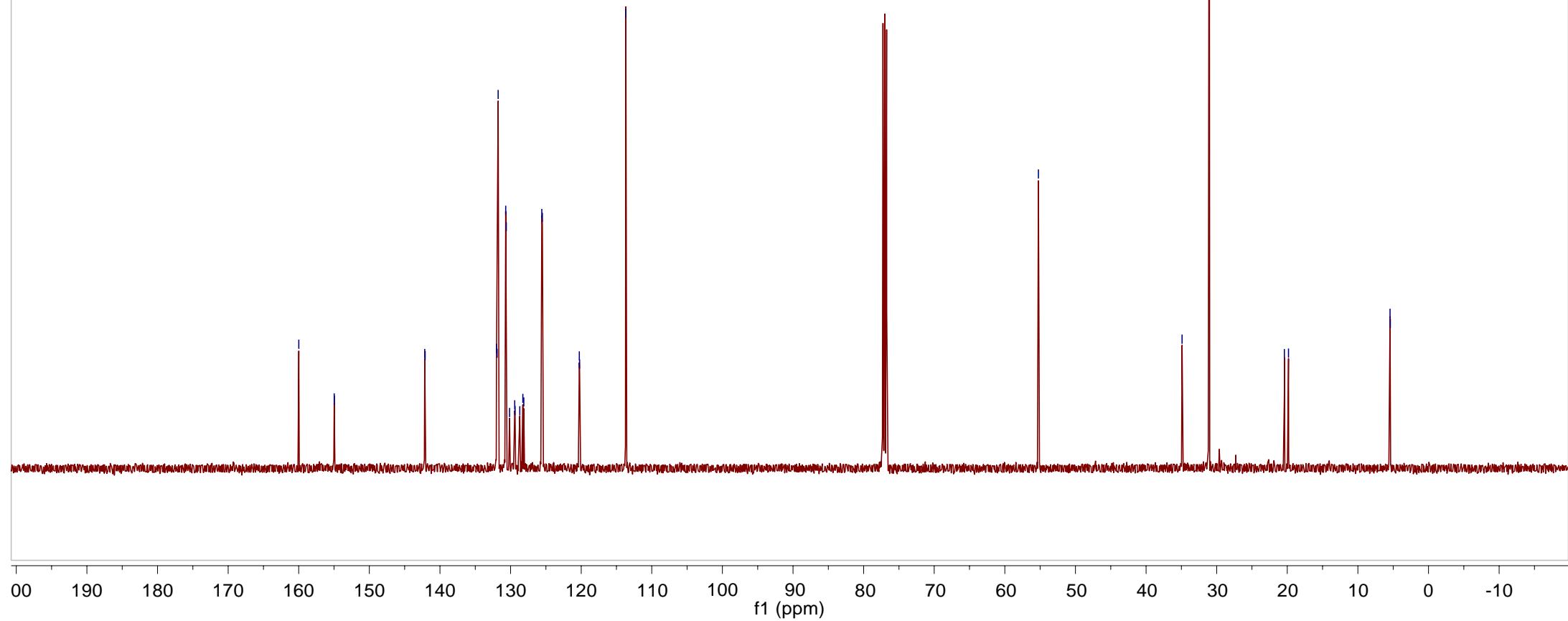
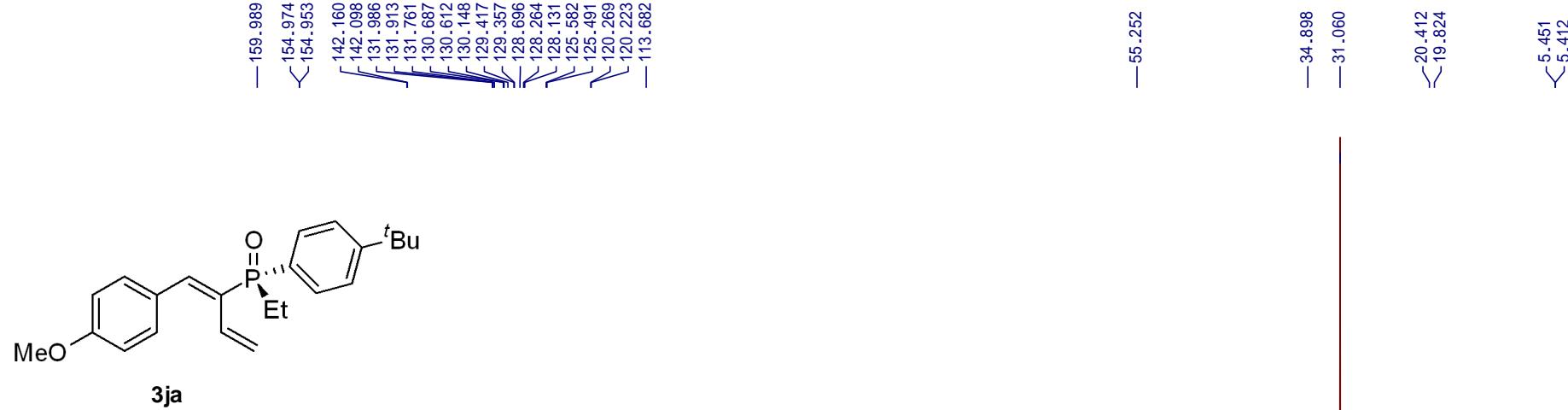


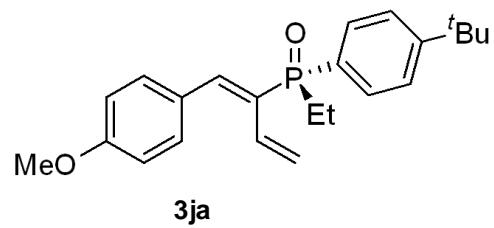


-35.806





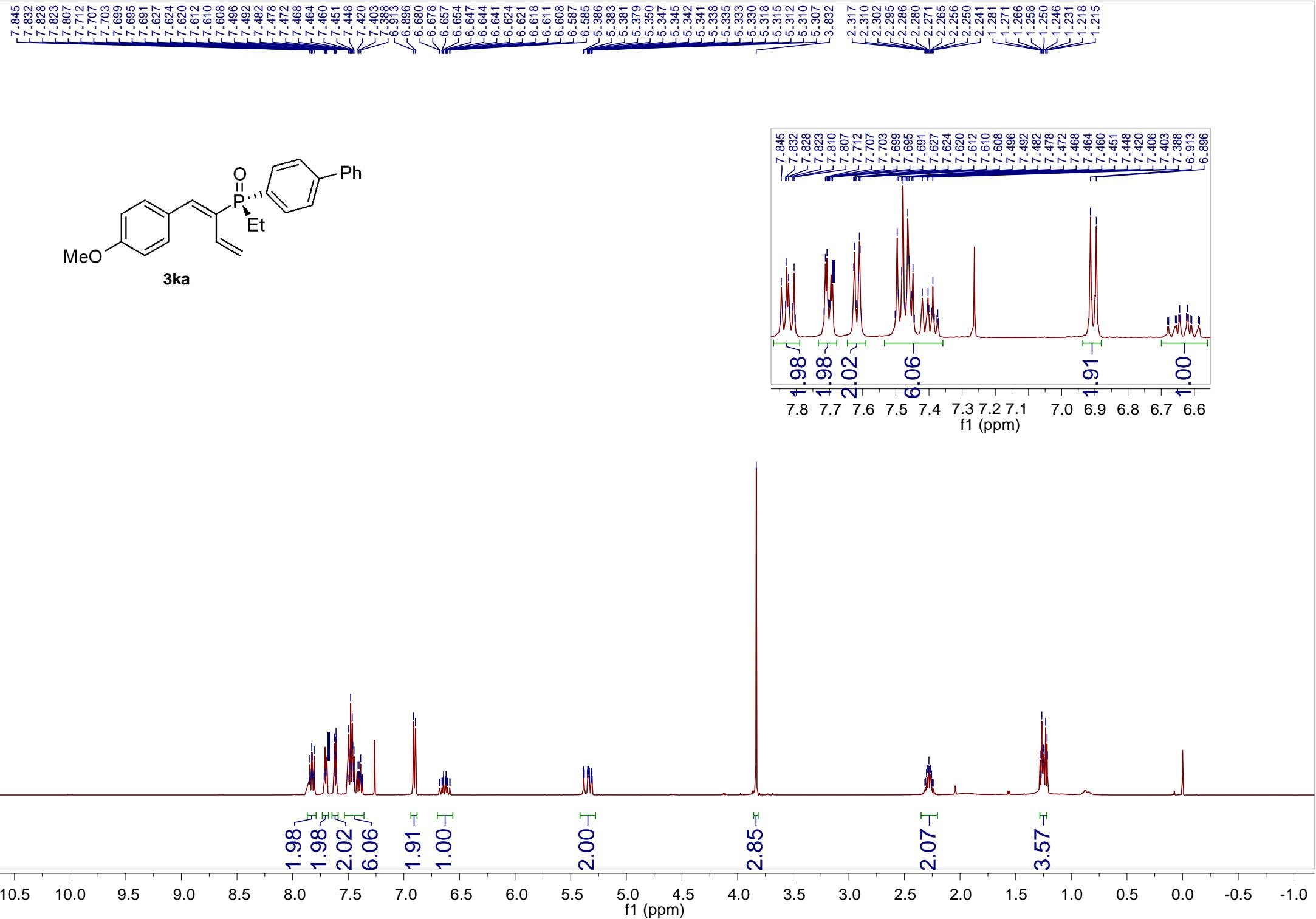


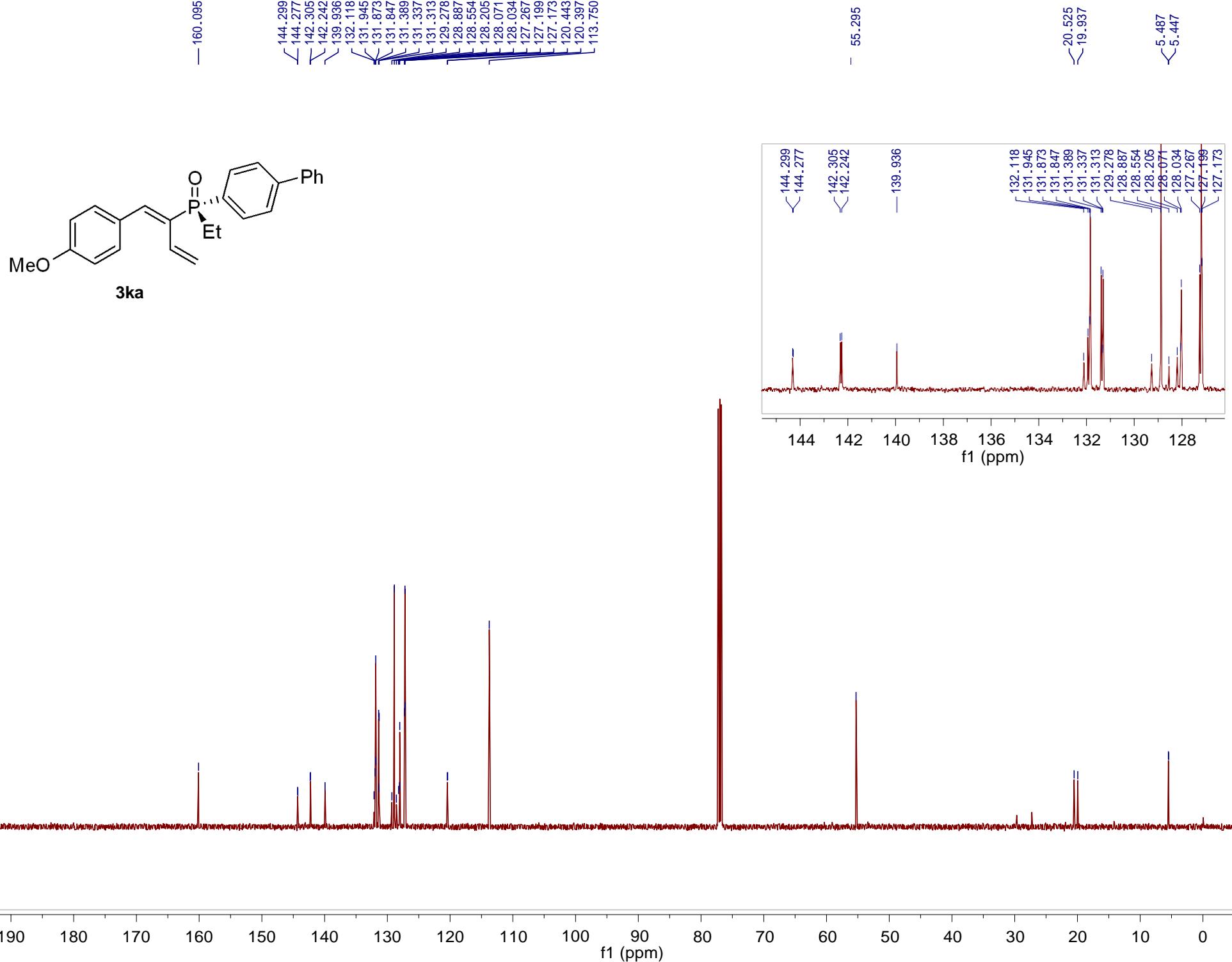


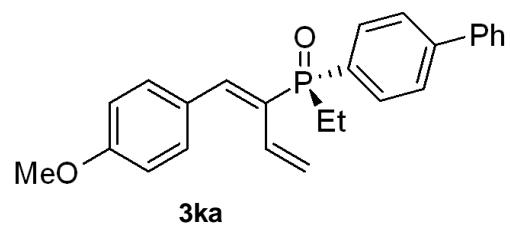
-35.973

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

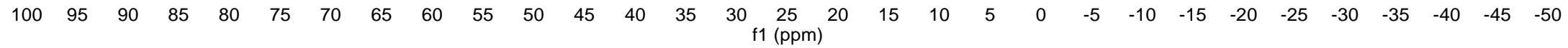
f1 (ppm)

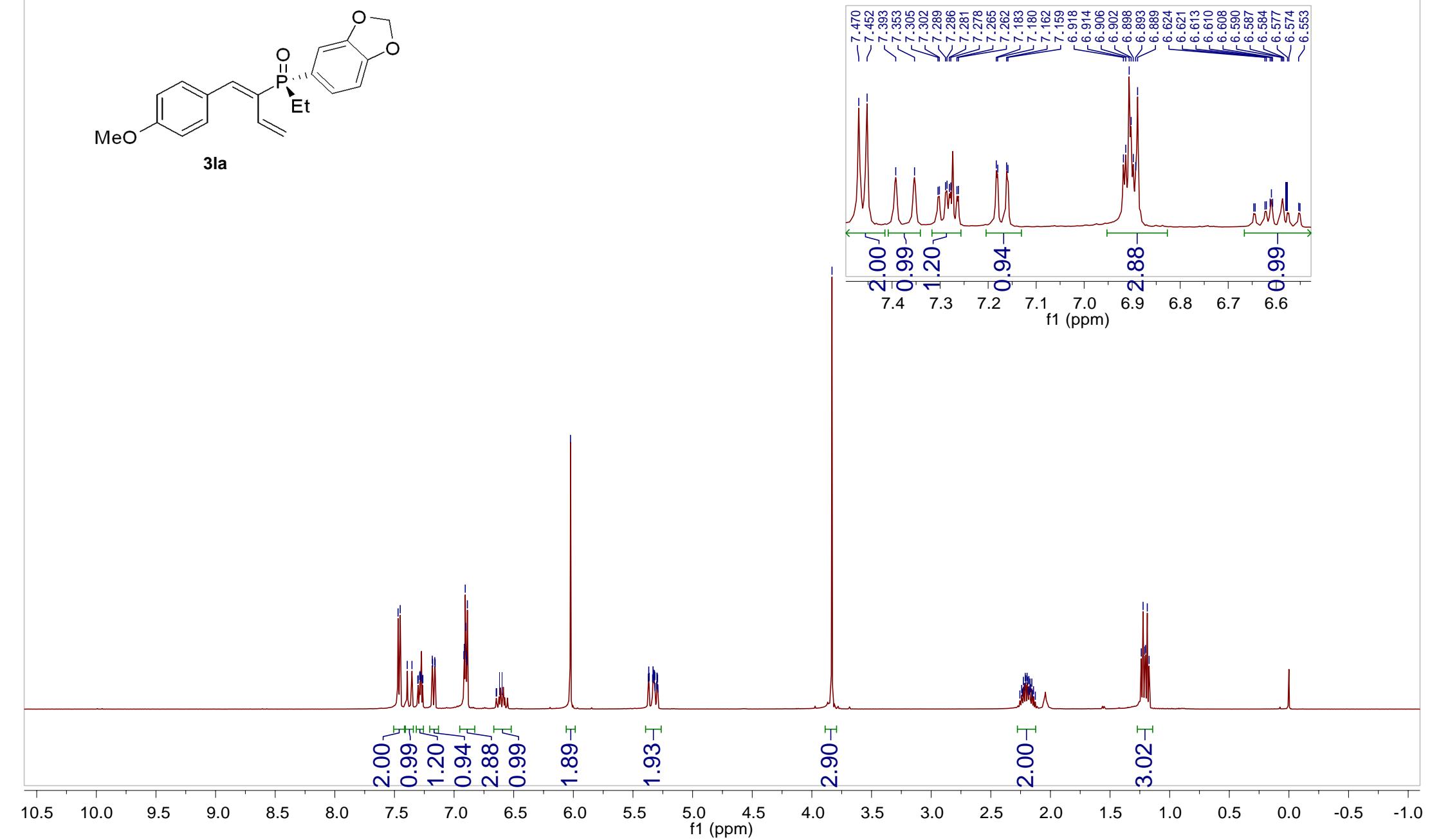
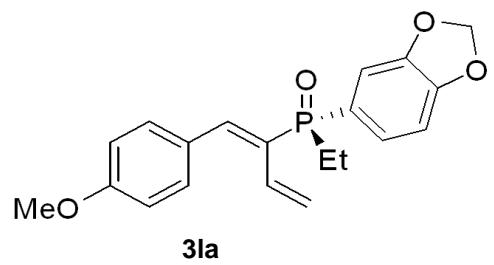


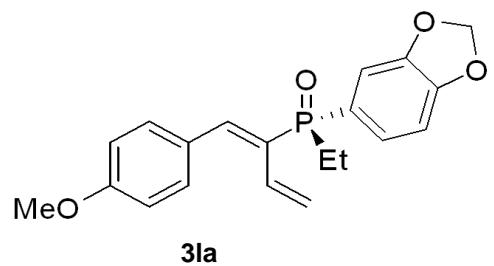




-35.928



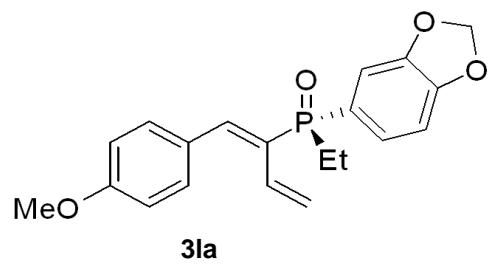




— 160.106
 ↘ 150.490
 ↘ 150.468
 ↘ 148.100
 ↘ 147.364
 ↘ 142.102
 ↘ 142.038
 ↘ 131.362
 ↘ 131.890
 ↘ 131.848
 ↘ 129.519
 ↘ 128.791
 ↘ 128.219
 ↘ 128.085
 ↘ 126.711
 ↘ 126.073
 ↘ 125.992
 ↘ 125.912
 ↘ 120.375
 ↘ 120.330
 ↘ 113.775
 ↘ 110.509
 ↘ 110.415
 ↘ 108.836
 ↘ 108.723
 ↘ 101.532
 — 55.335
 ↘ 20.663
 ↘ 20.071
 ↘ 5.536
 ↘ 5.497

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

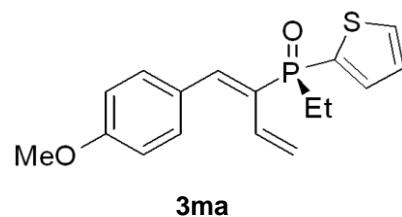


-35.917

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

7.714
7.708
7.705
7.700
7.698
7.696
7.691
7.688
7.596
7.594
7.589
7.587
7.583
7.580
7.575
7.573
7.510
7.499
7.494
7.480
7.476
7.469
7.466
7.463
7.456
7.205
7.201
7.198
7.195
7.192
7.188
7.185
6.914
6.908
6.904
6.895
6.890
6.638
6.636
6.628
6.625
6.621
6.611
6.607
6.604
6.601
6.593
6.590
6.569
6.566
5.378
5.368
5.366
5.361
5.347
5.344
5.342



0.91
0.97
2.99
0.96
1.92
1.00

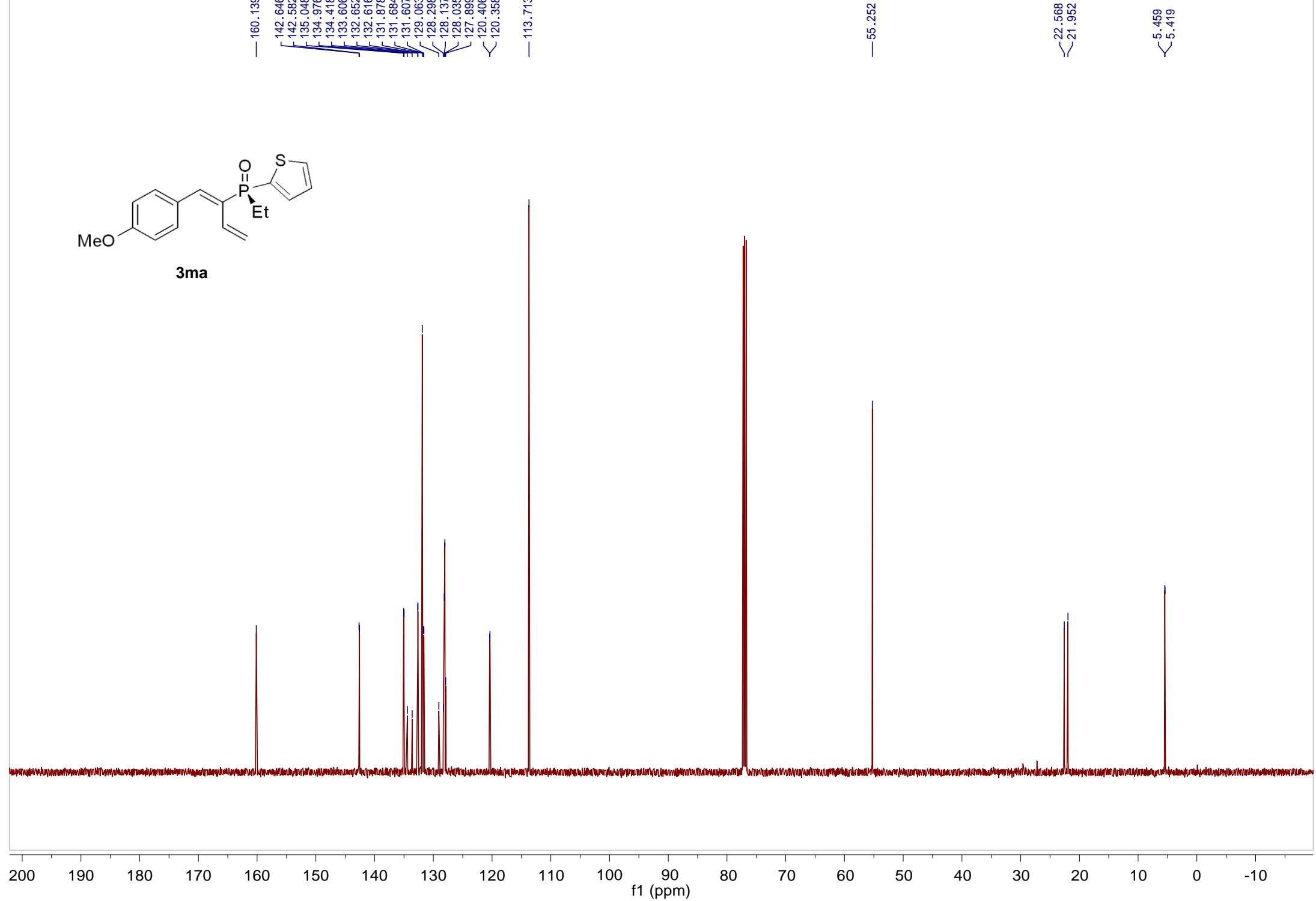
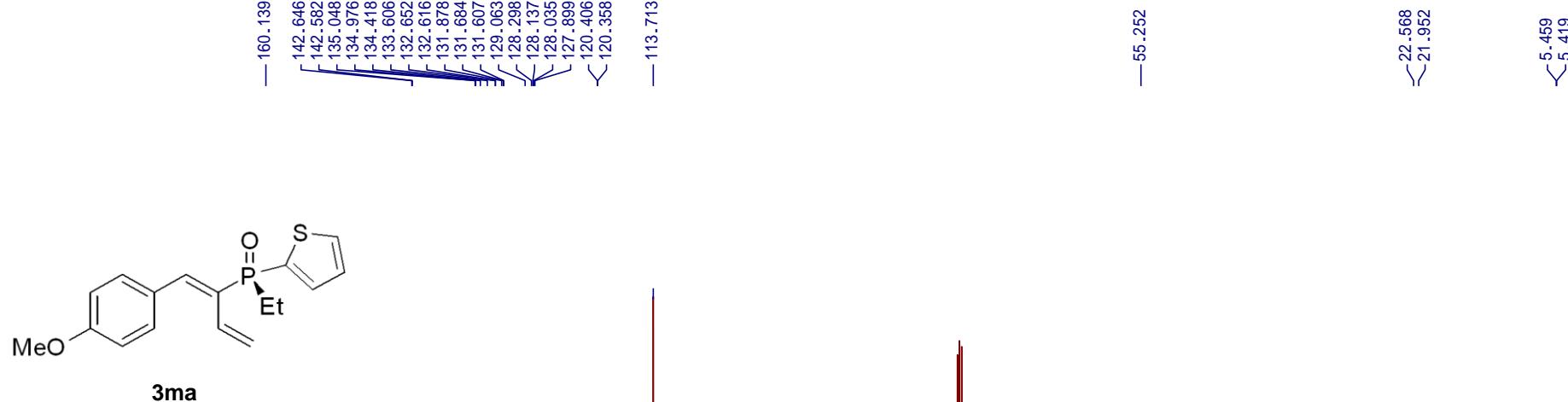
2.01

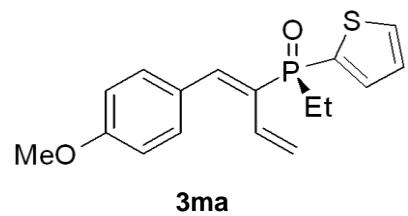
3.00

2.18

3.30

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 -0.5 -1.0

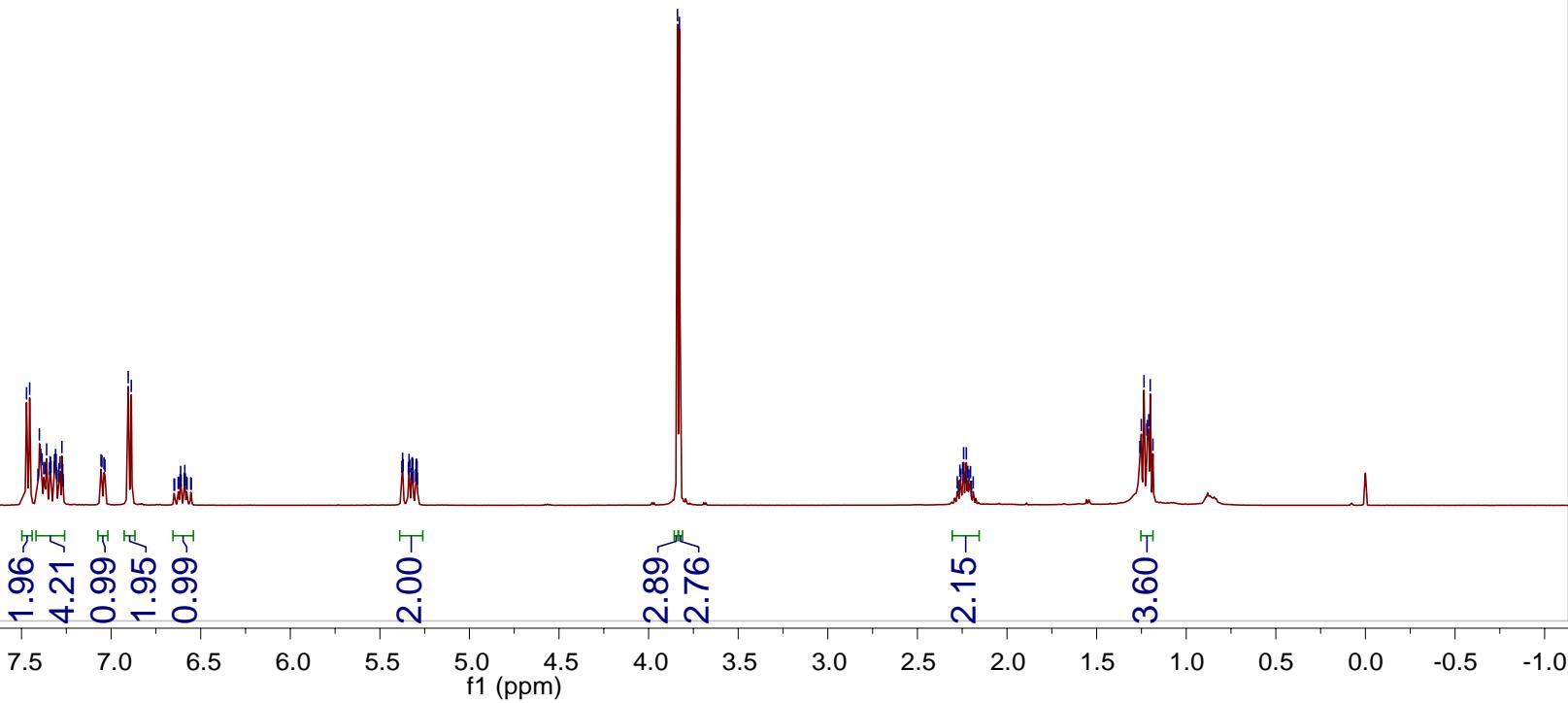
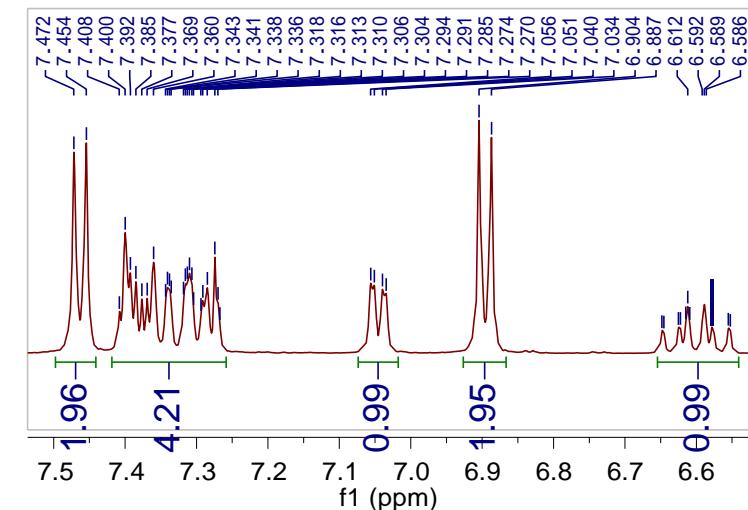
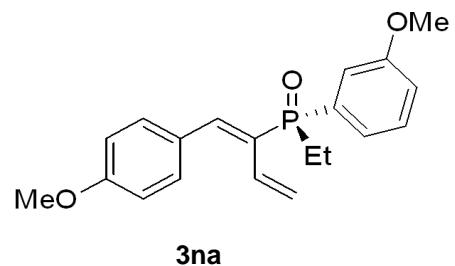


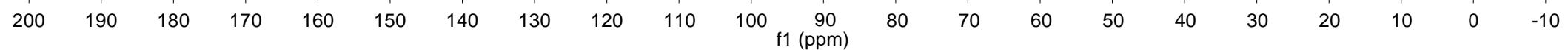
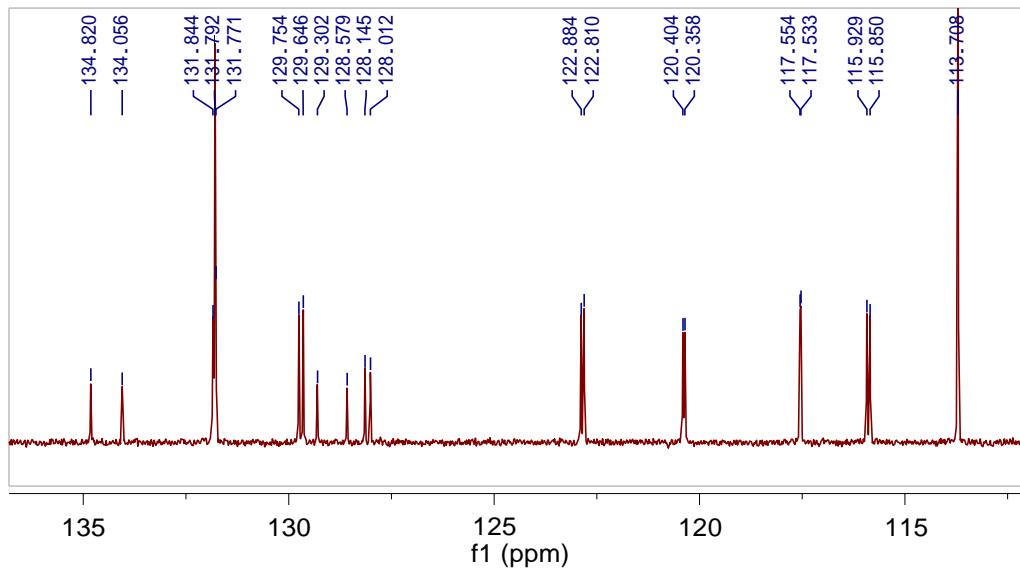
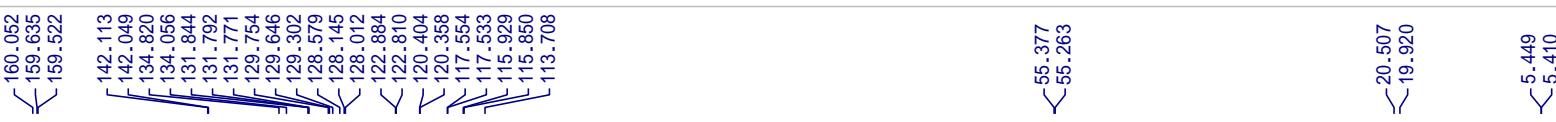
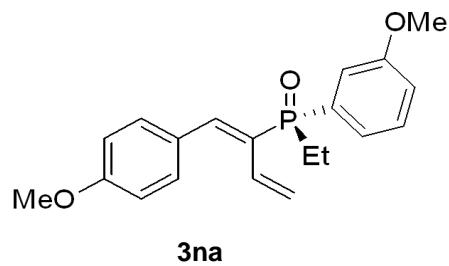


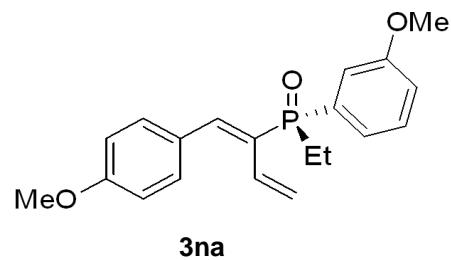
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

7.472
7.454
7.408
7.400
7.392
7.385
7.377
7.369
7.360
7.356
7.343
7.341
7.338
7.336
7.318
7.316
7.313
7.310
7.306
7.304
7.294
7.291
7.285
7.274
7.270
7.267
7.056
7.051
6.625
6.622
6.615
6.612
6.609
6.592
6.589
6.586
6.579
6.576
6.555
6.553
5.377
5.374
5.370
5.341
5.337
5.334
5.324
5.321
5.319
5.316
5.313
5.301
5.298
5.295
5.293
5.290
3.839
3.828
2.278
2.272
7.385
7.377
7.369
7.360
7.343
7.341
7.338
7.336
7.318
7.316
7.313
7.310
7.306
7.304
7.294
7.291
7.285
7.274
7.270
7.056
7.051
7.040
6.612
6.592
6.589
6.586
6.579
6.576
6.555
6.553
5.377
5.374
5.370
5.341
5.337
5.334
5.324
5.321
5.319
5.316
5.313
5.301
5.298
5.295
5.293
5.290
3.839
3.828
2.278
2.272
7.385
7.377
7.369
7.360
7.343
7.341
7.338
7.336
7.318
7.316
7.313
7.310
7.306
7.304
7.294
7.291
7.285
7.274
7.270
7.056
7.051
7.040
6.612
6.592
6.589
6.586





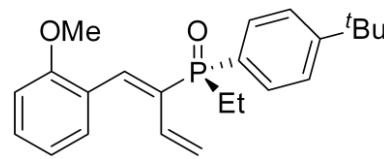


-36.270

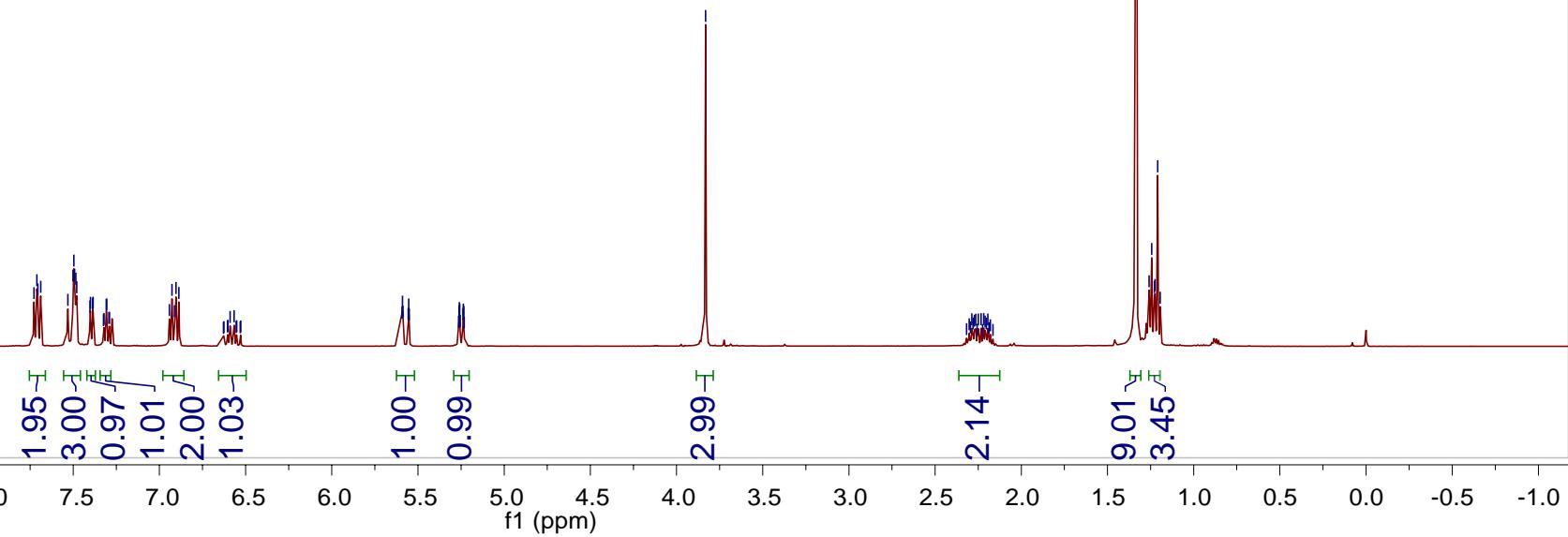
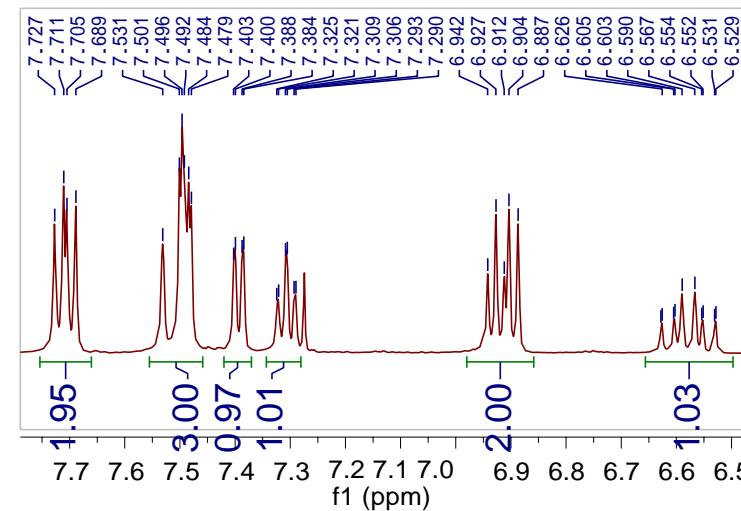
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

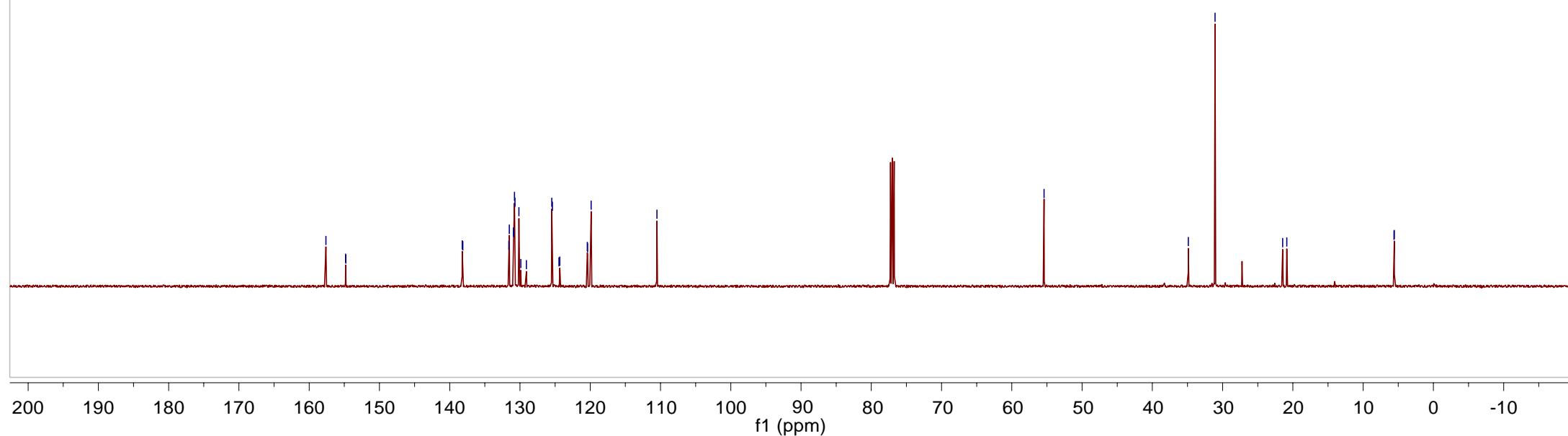
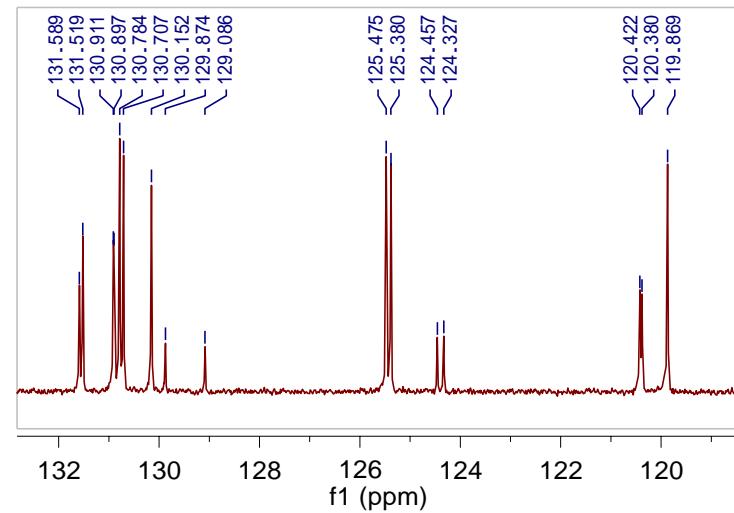
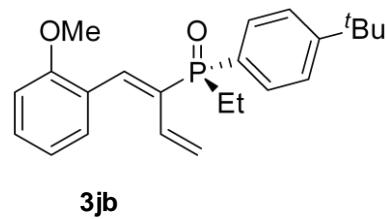
f1 (ppm)

7.727
7.711
7.705
7.689
7.531
7.501
7.496
7.492
7.384
7.479
7.403
7.400
7.306
7.388
7.293
7.290
6.942
6.927
6.605
6.912
6.904
6.887
6.628
6.626
6.603
6.590
6.587
6.554
6.552
6.531
6.529
6.593
6.590
5.593
5.587
5.556
5.553
5.551
5.265
5.262
5.258
5.255
5.239
5.237
5.234
5.232
3.832
2.317
2.302
2.295
2.287
2.280
2.225
2.218
2.210
2.265
2.257
2.249
2.233
2.188
2.179
2.170
2.164
1.334
1.269
1.244
1.228
1.224
1.208
1.194

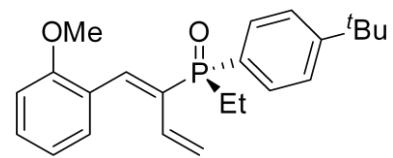


3jb

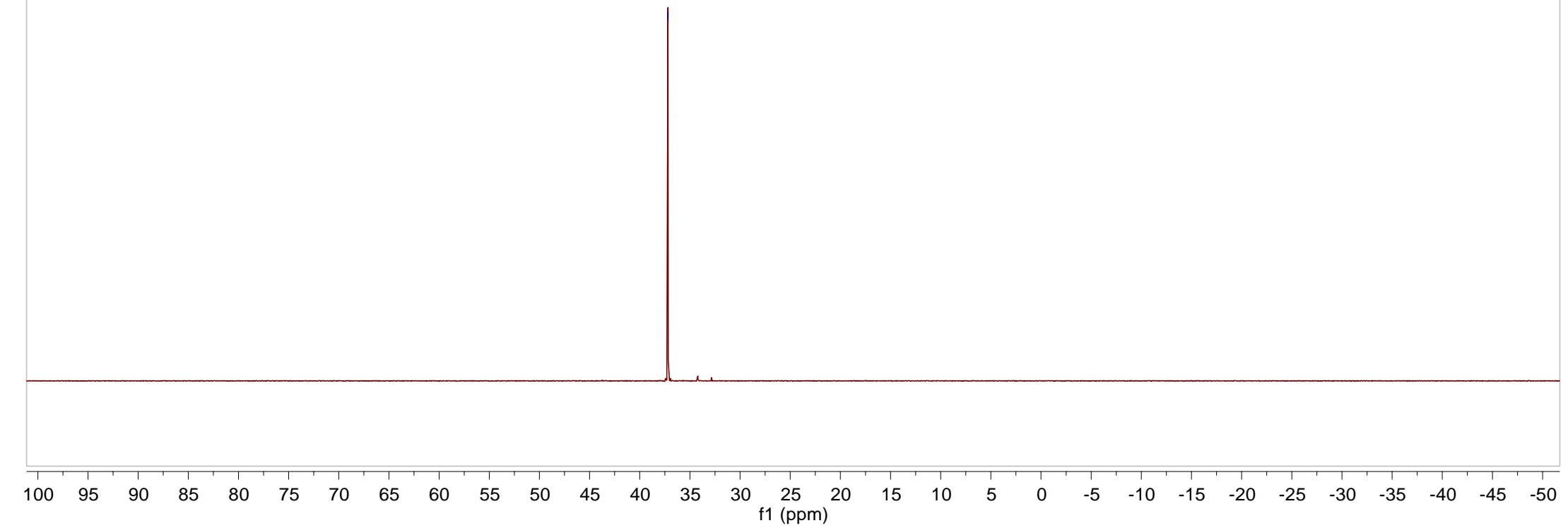


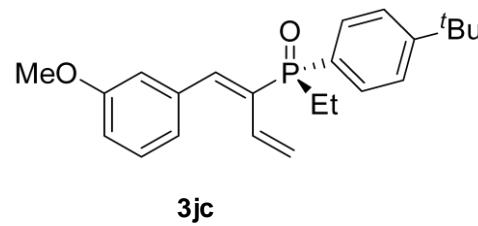


-37.184

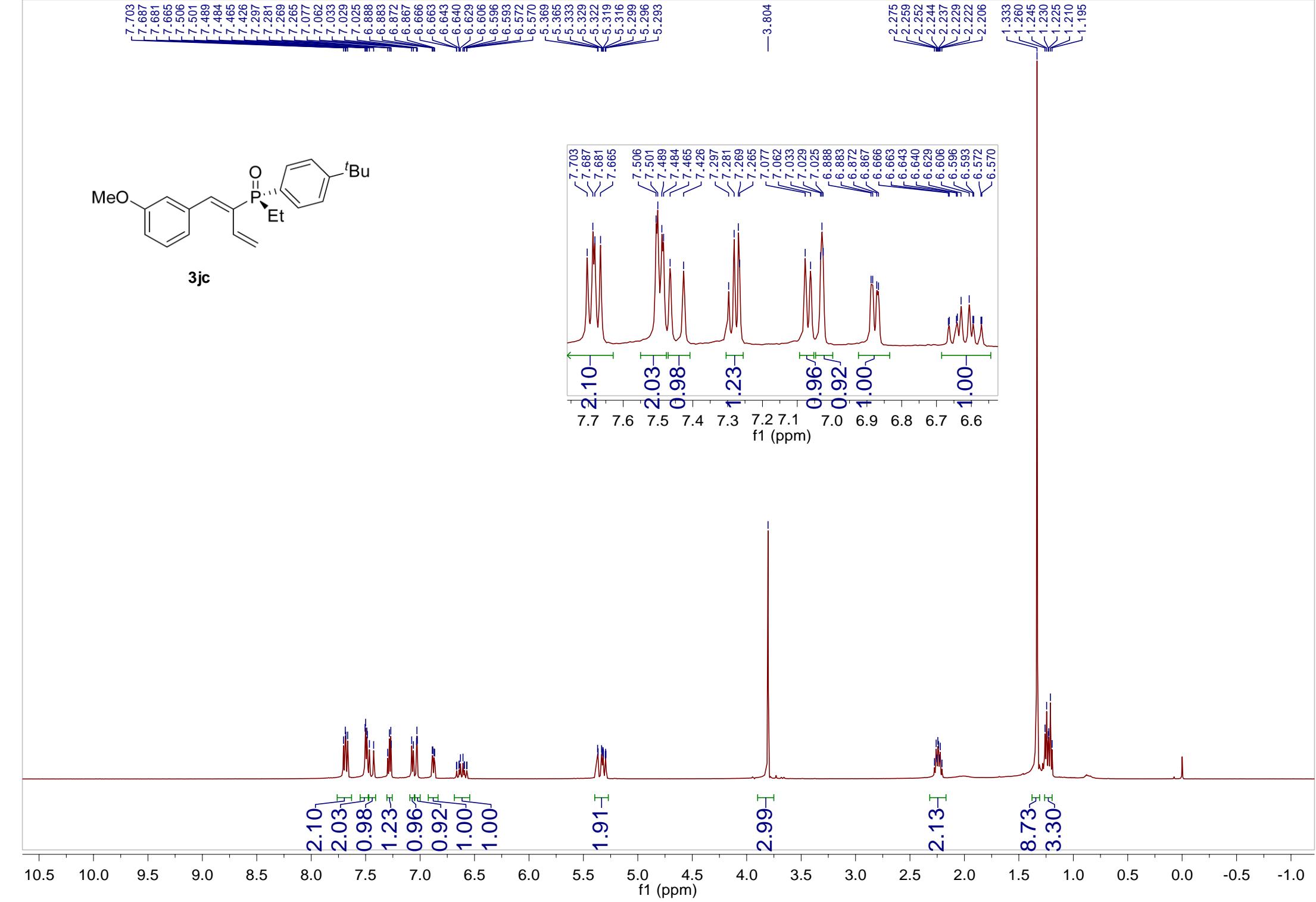


3jb





3jc



-159.375
-155.174
-155.152

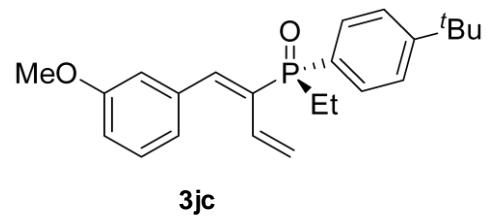
<142.552
<142.491
<136.910
<136.781
<132.355
<131.766
<131.696
<131.650
<130.755
<130.679
<129.967
<129.307
<129.176
<125.714
<125.620
<122.362
<120.829
<120.785
<115.271
<114.573

-55.297

-34.990
-31.129

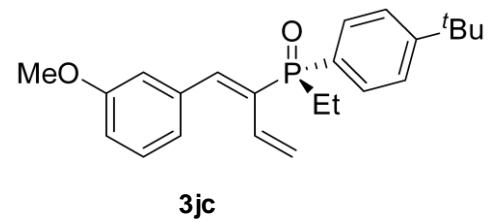
<20.550
<19.963

<5.523
<5.484



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

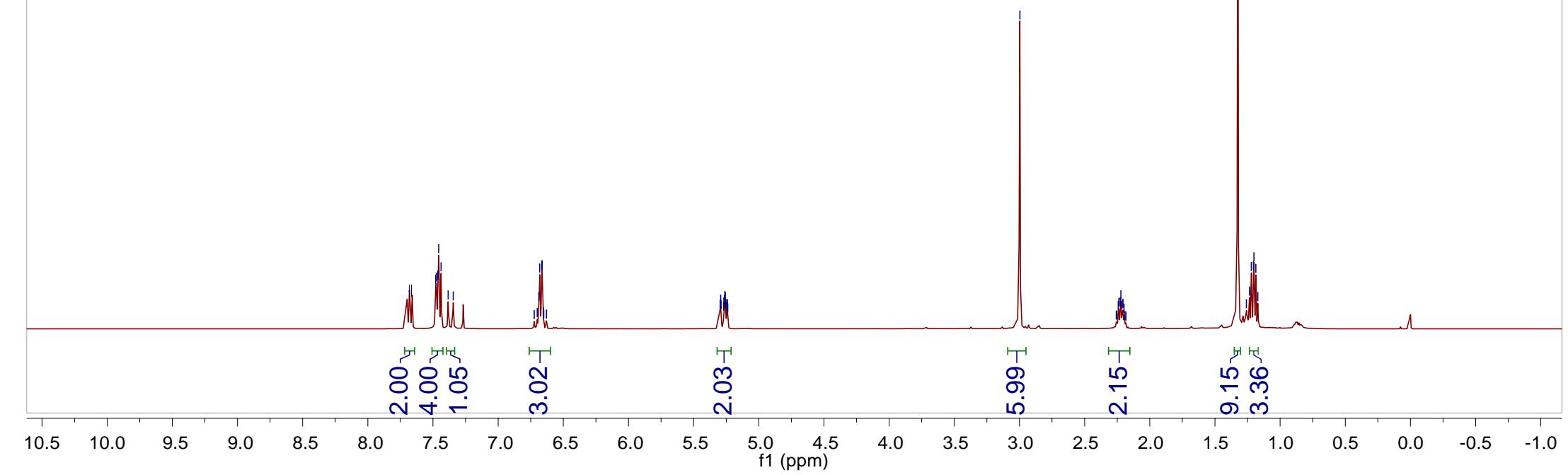
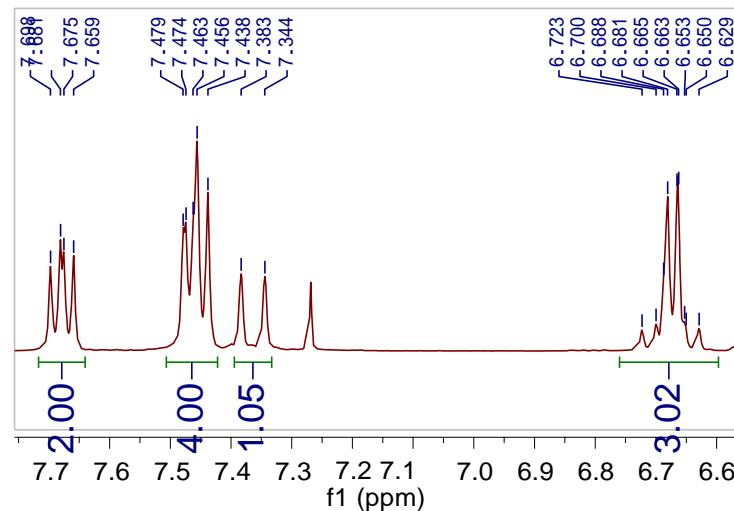
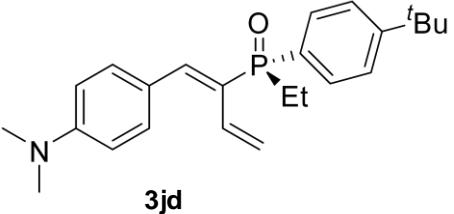
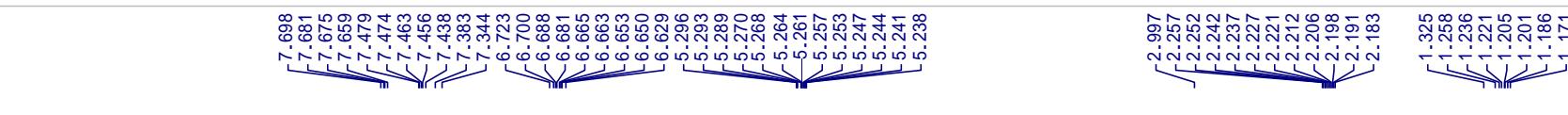
f1 (ppm)

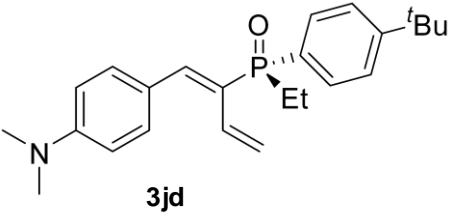


-35.565

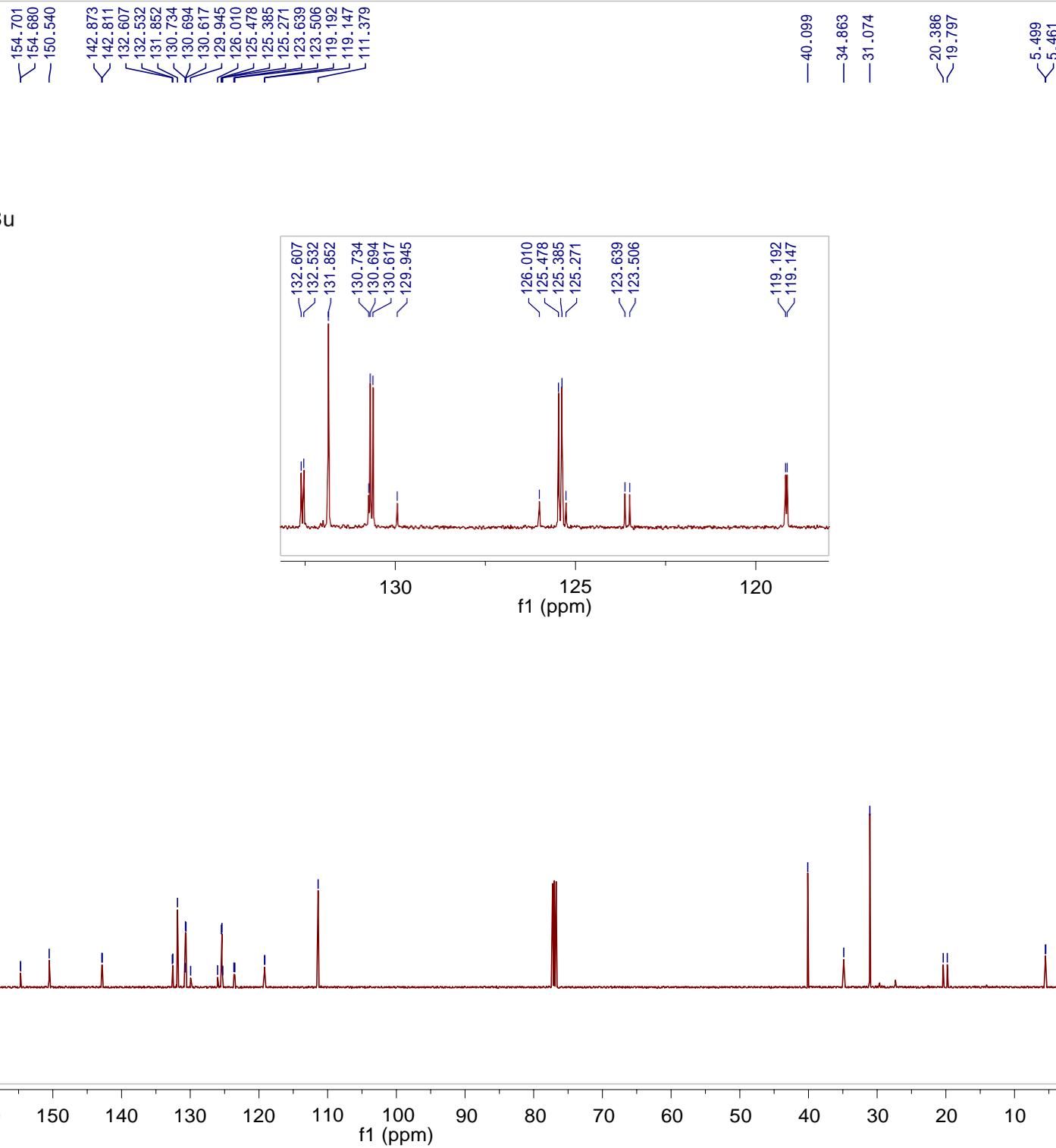
f1 (ppm)

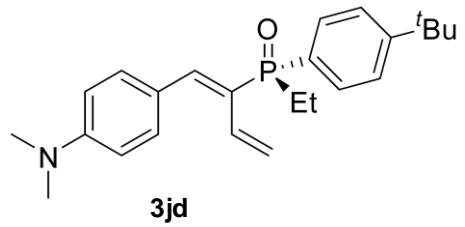
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50





3jd

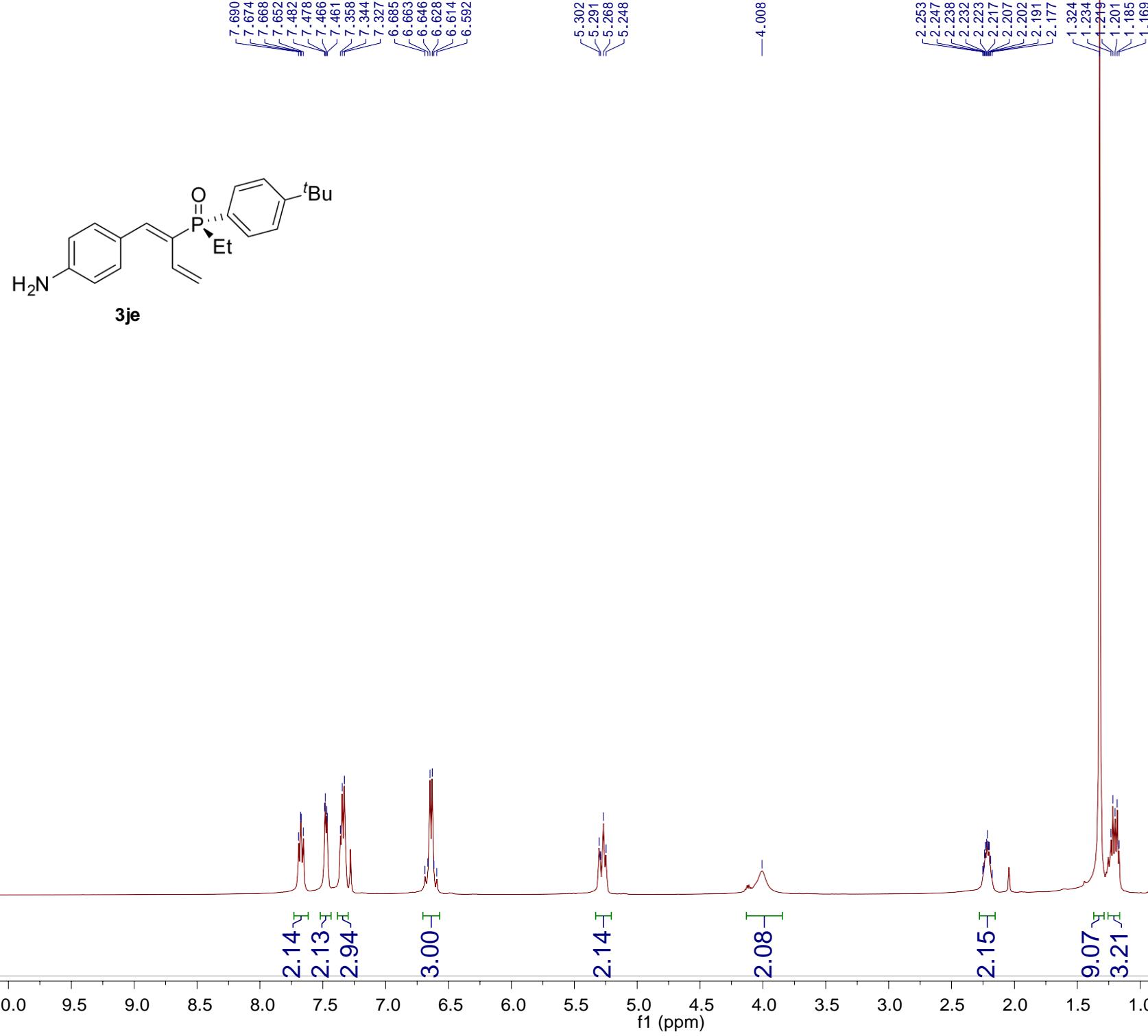


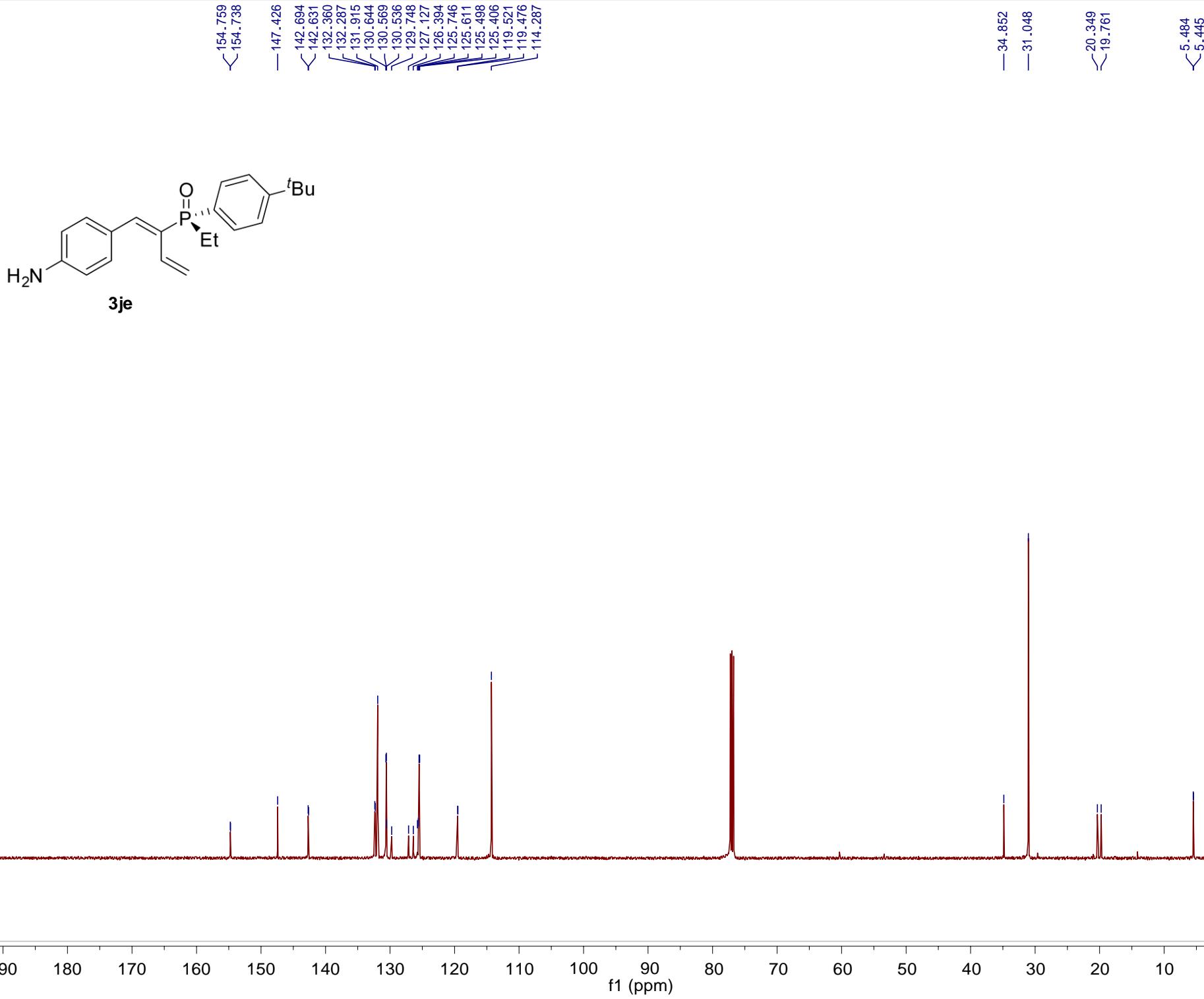


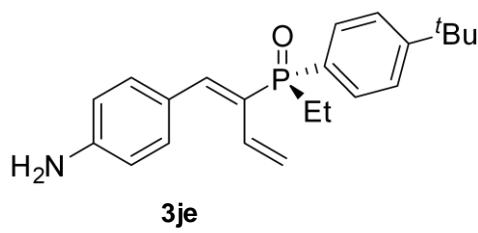
-36.336

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

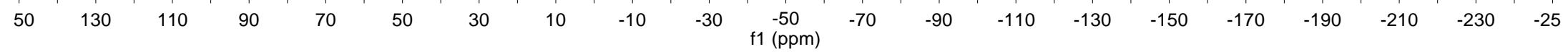
f1 (ppm)

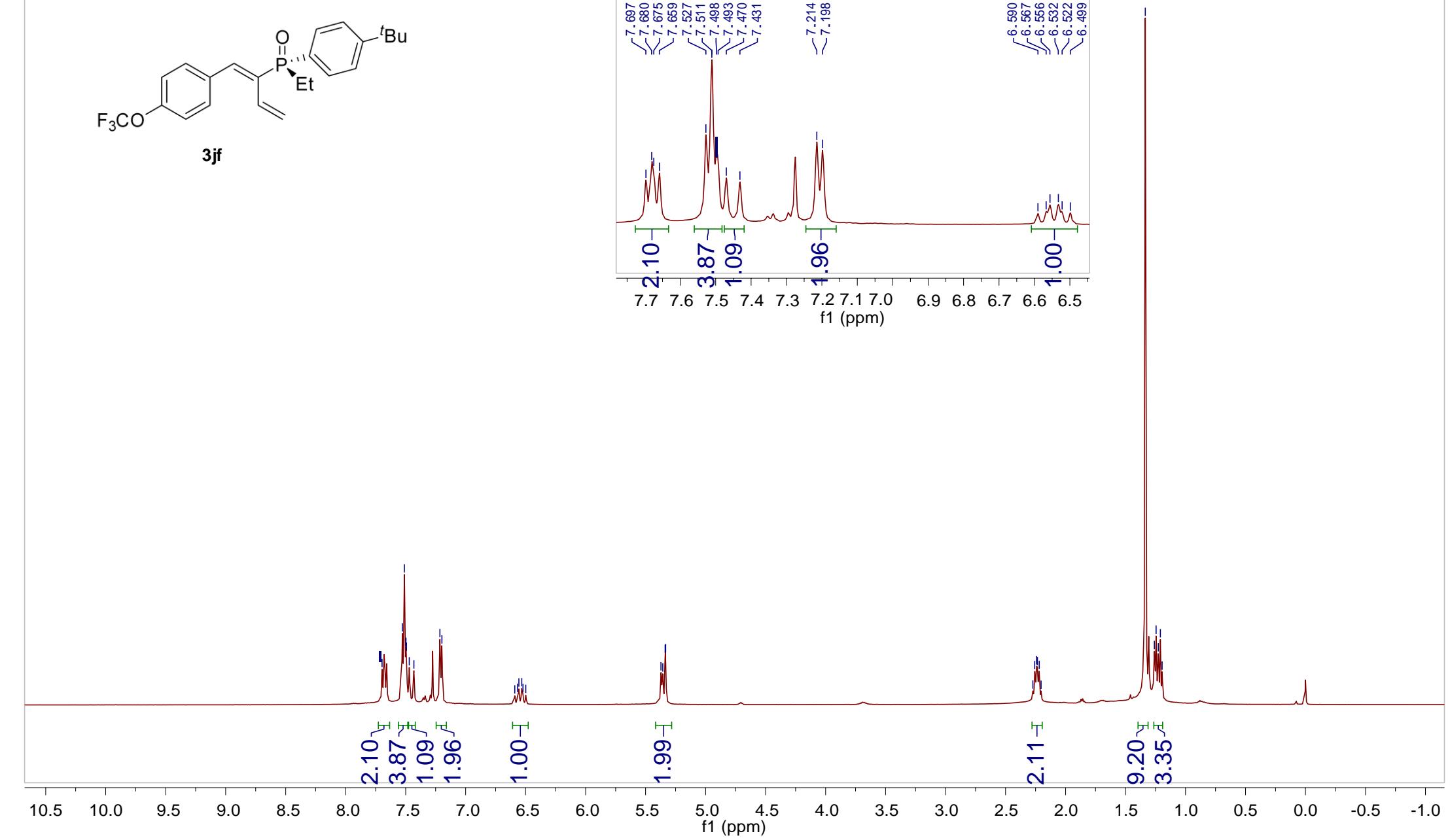
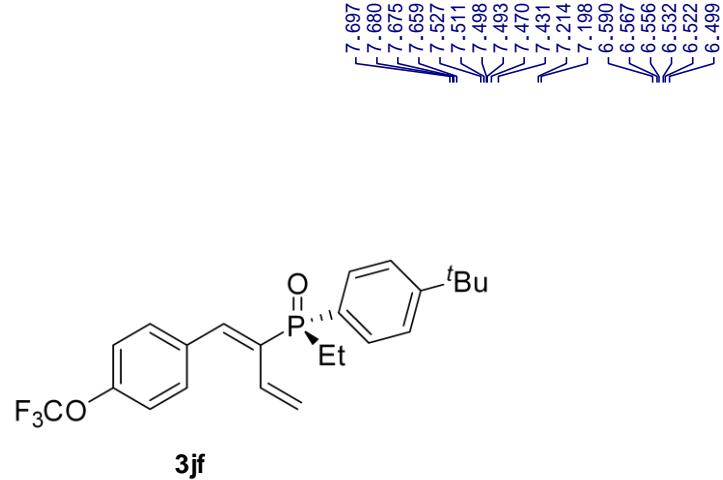


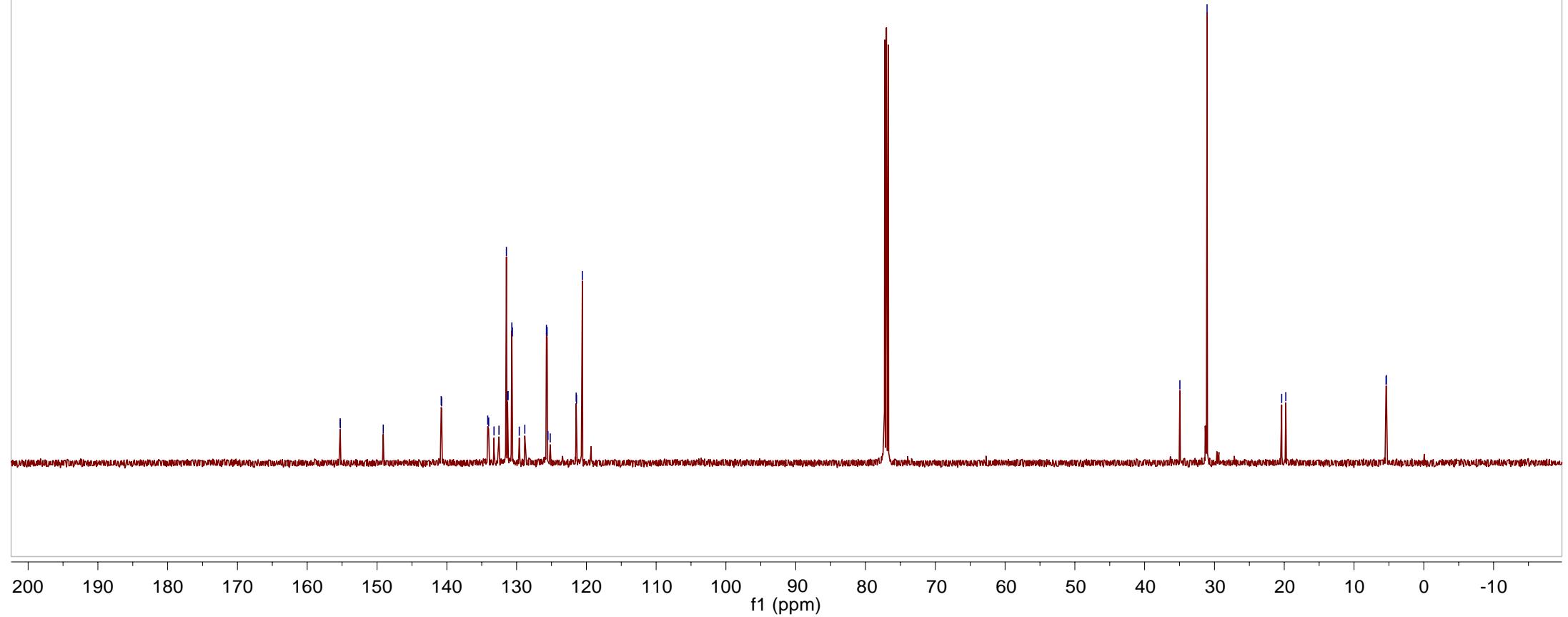
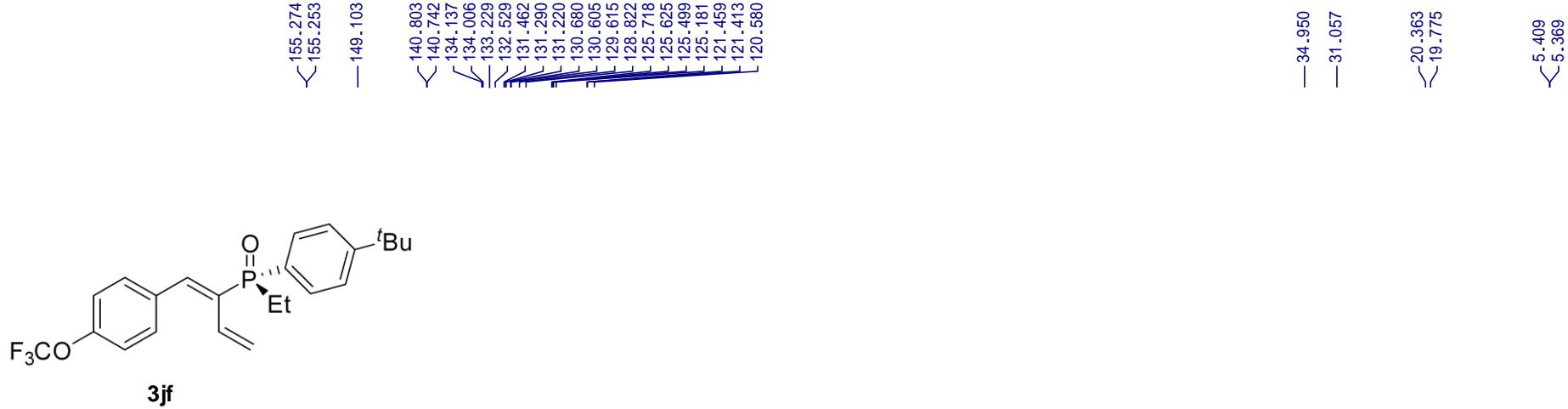


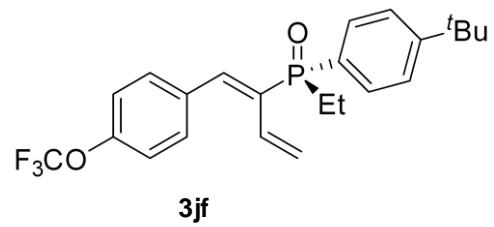


-36.133





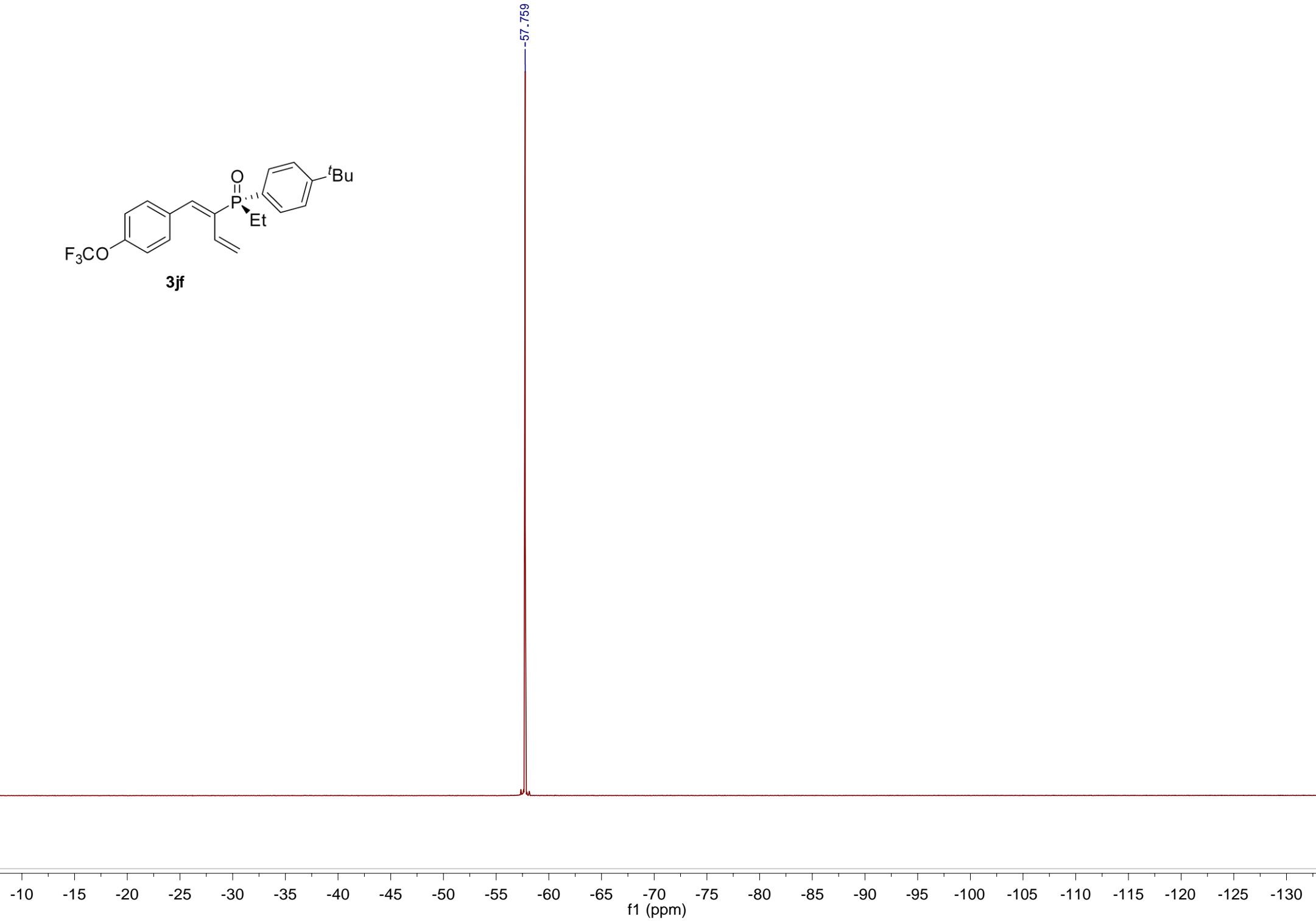
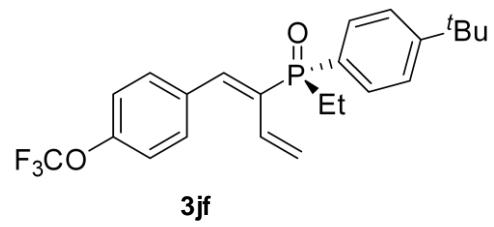


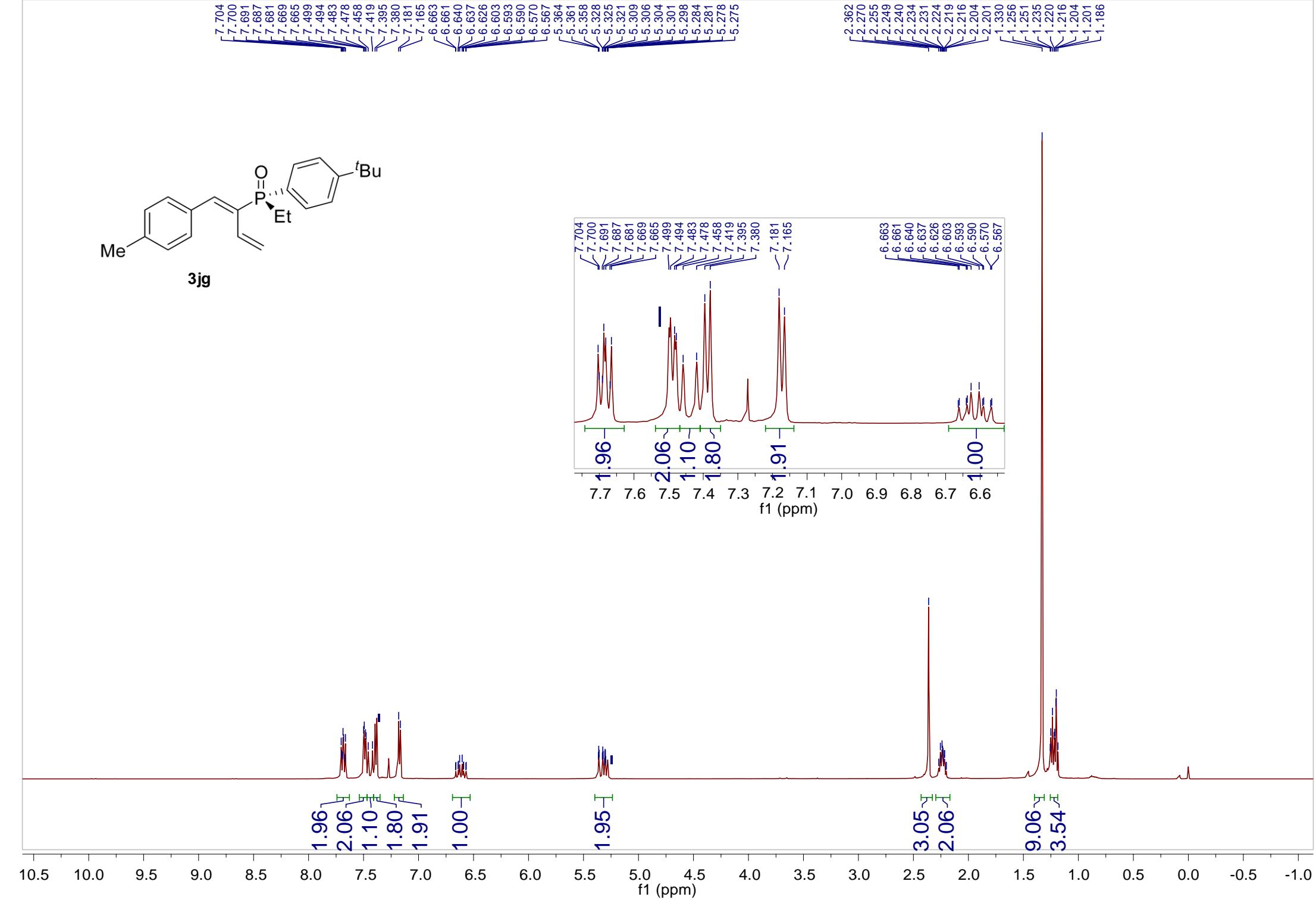
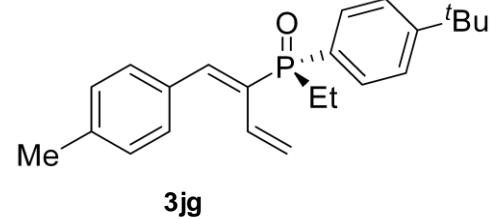


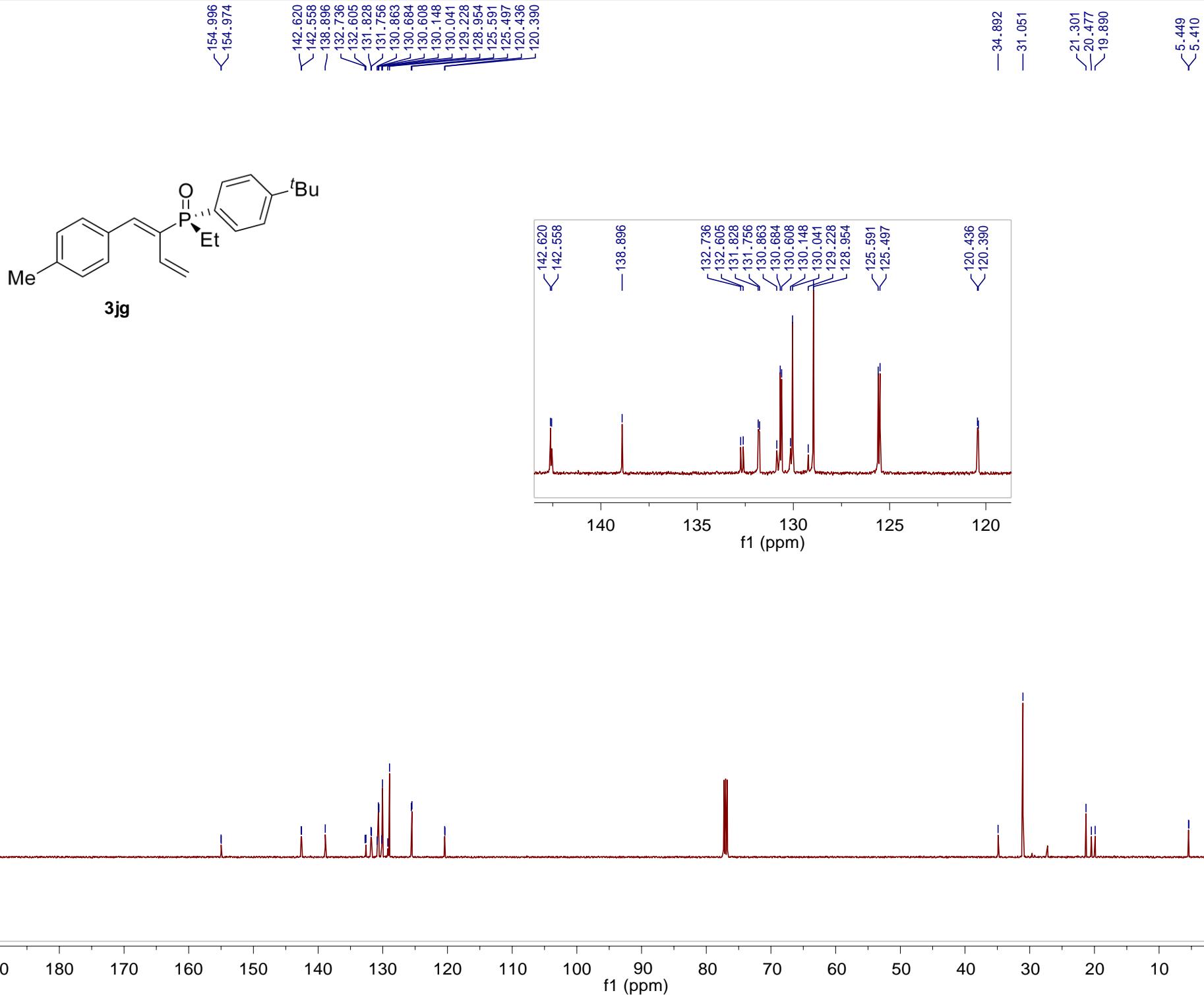
-35.238

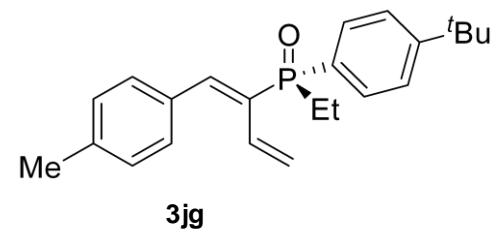
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)





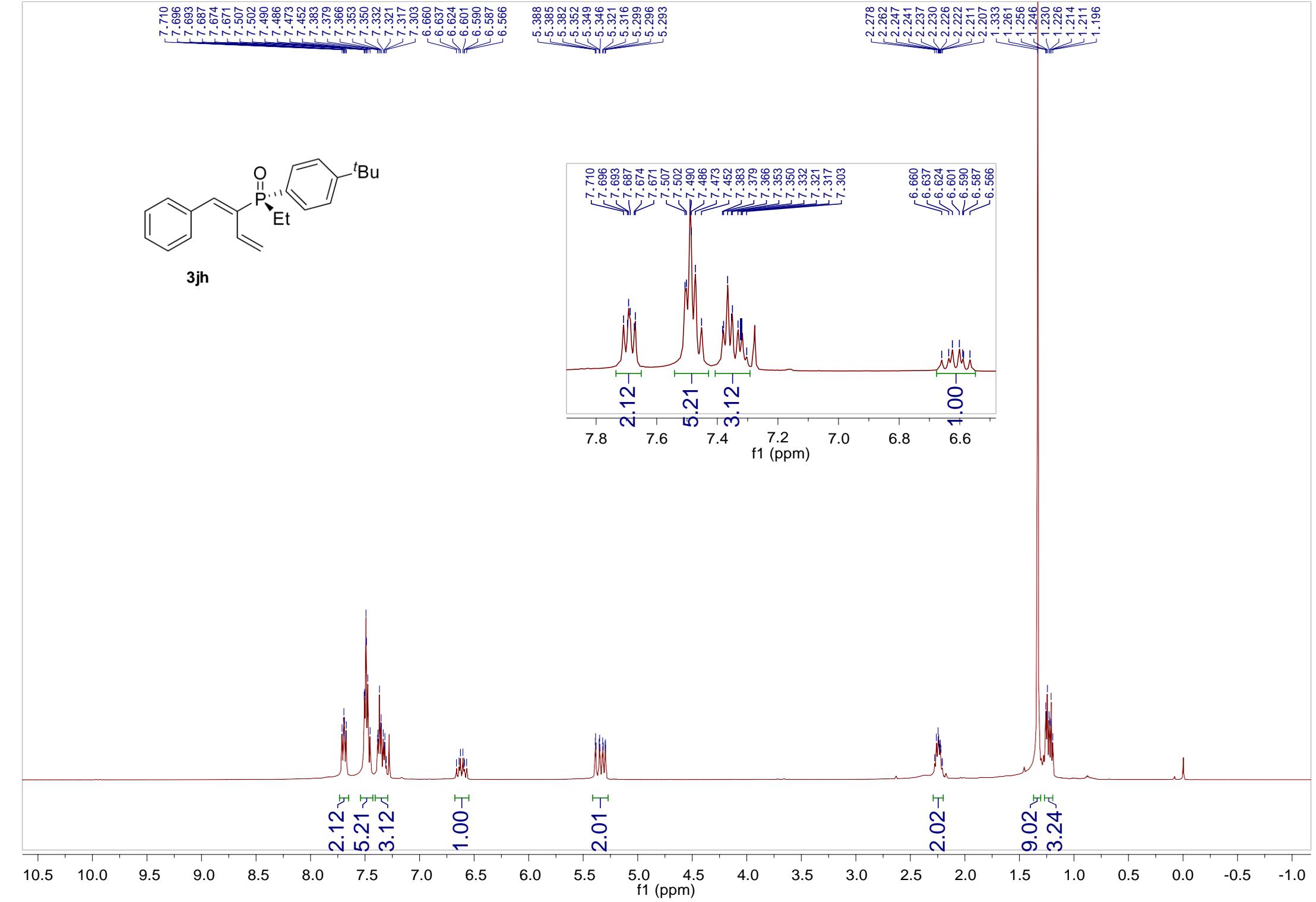
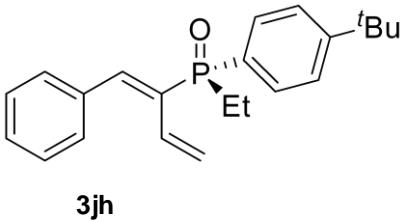


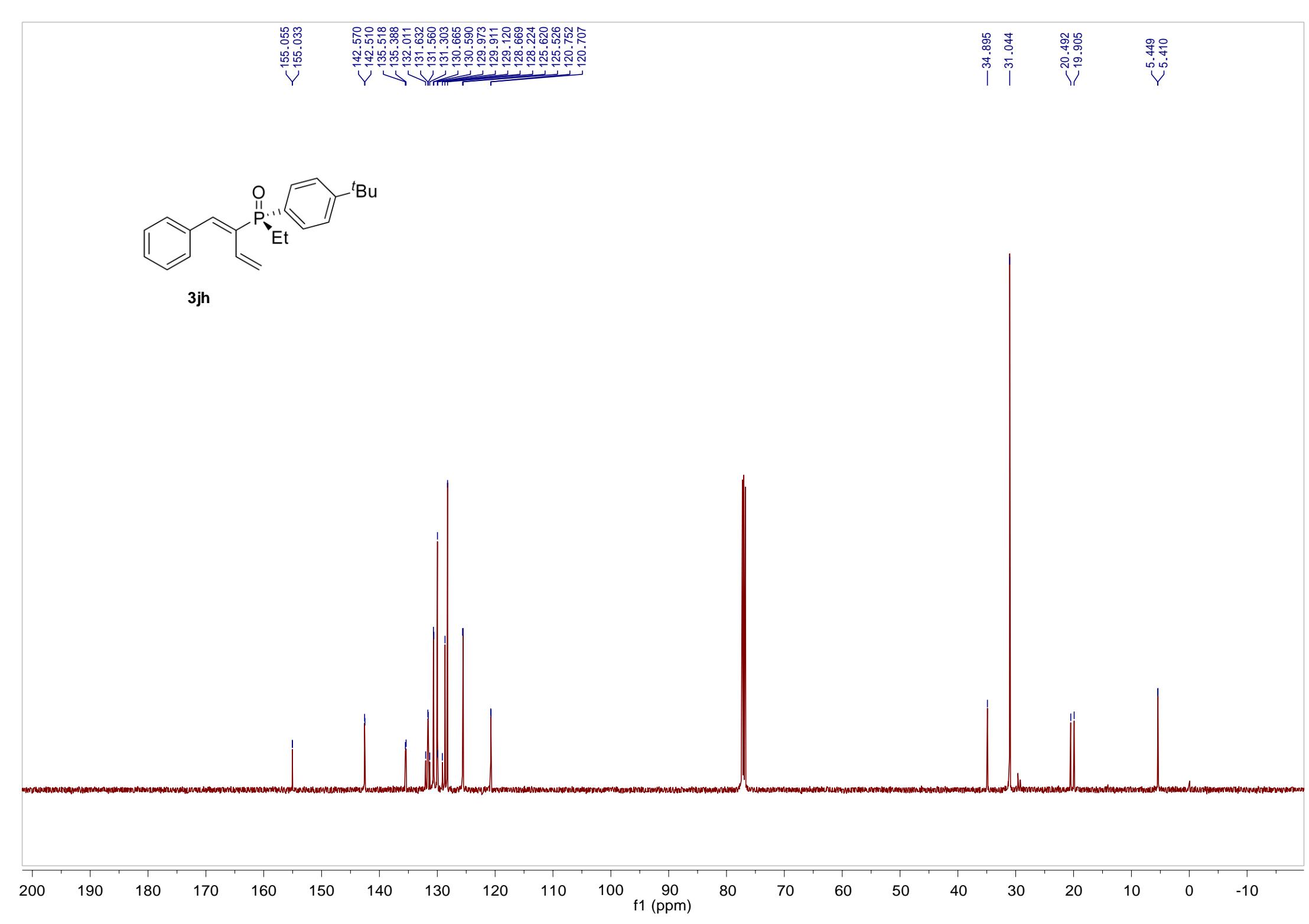


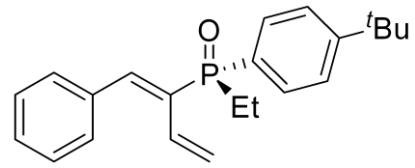
-35.881

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

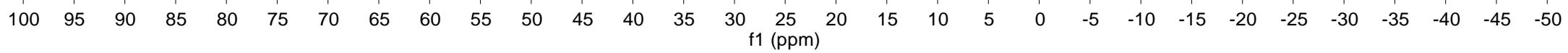


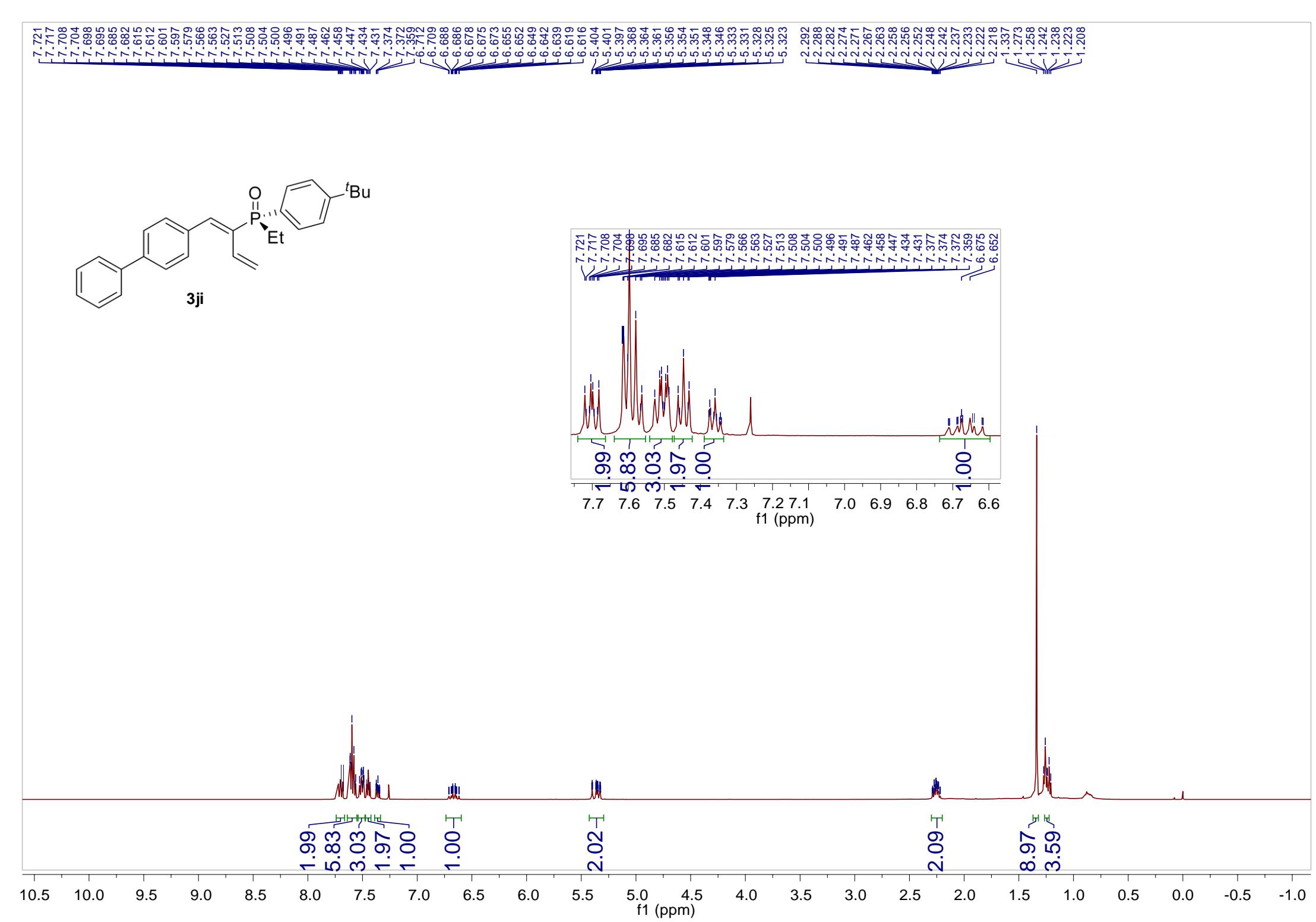


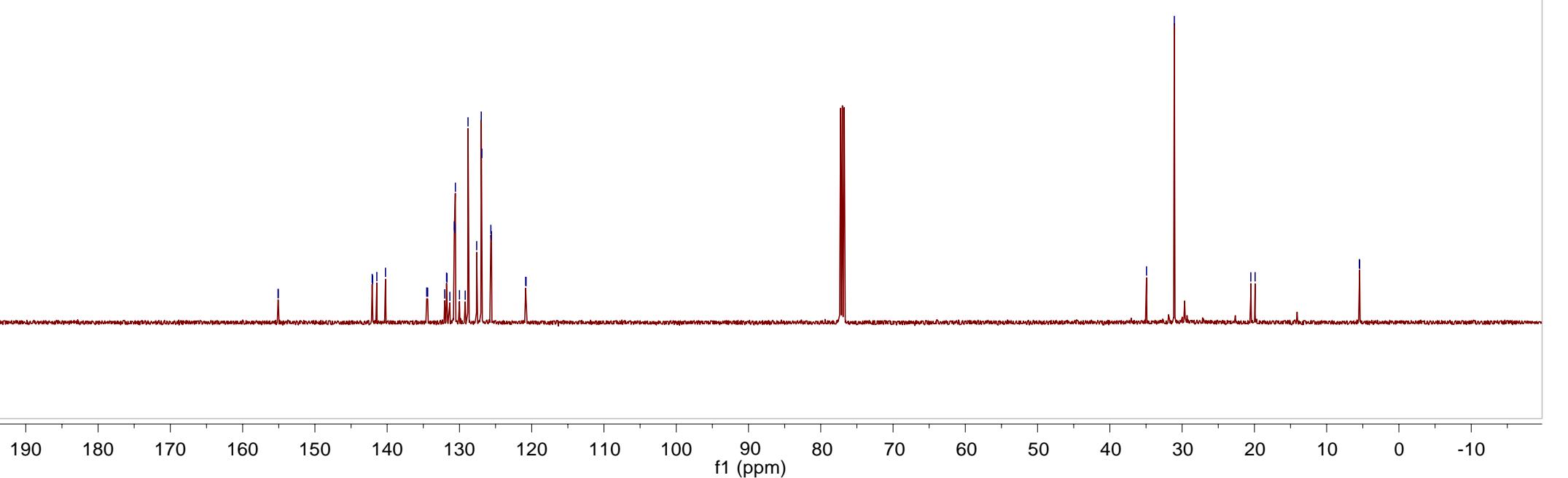
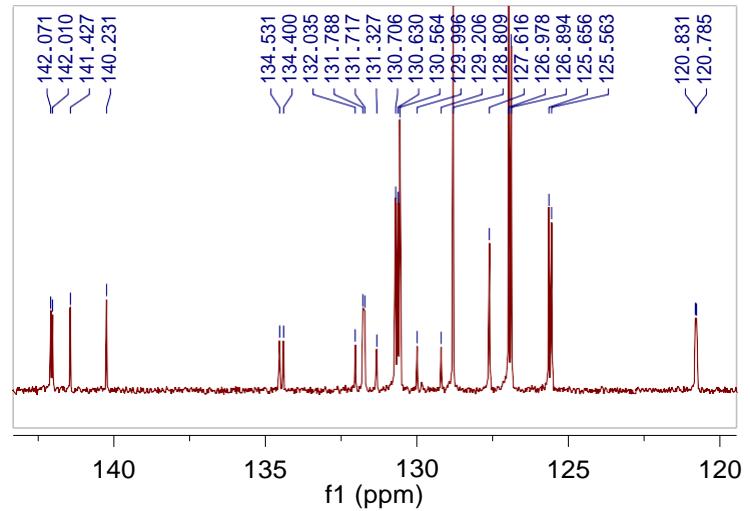
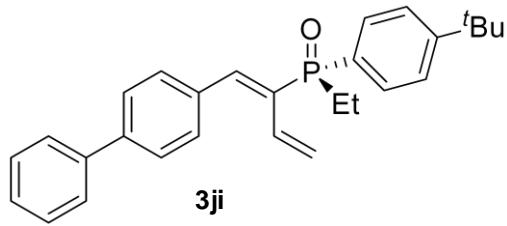


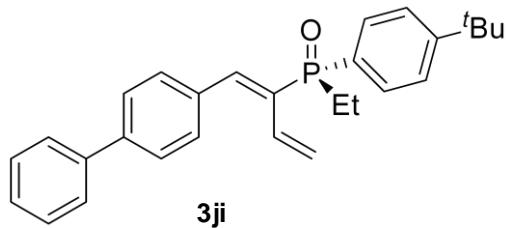
3jh

-35.629





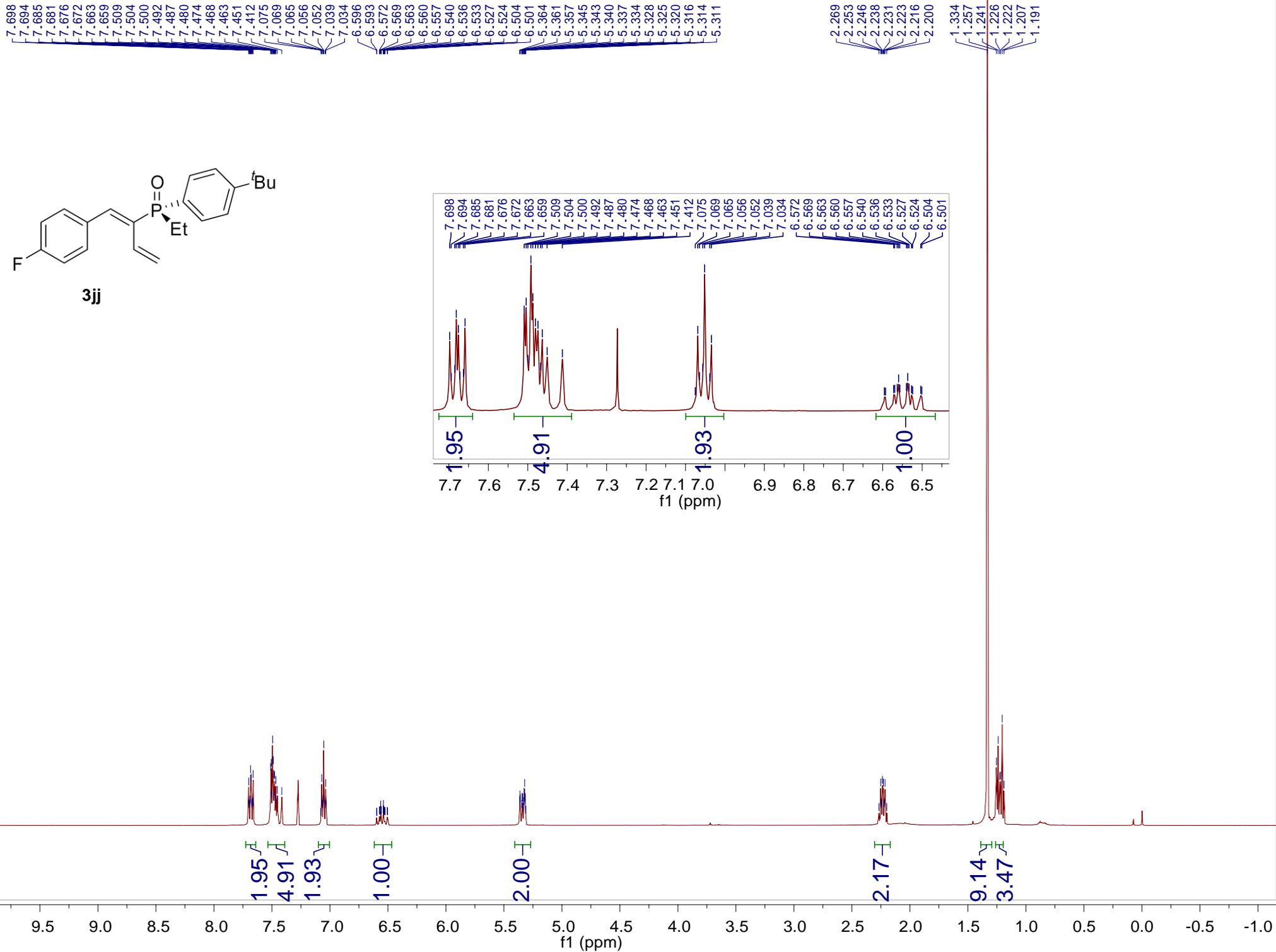


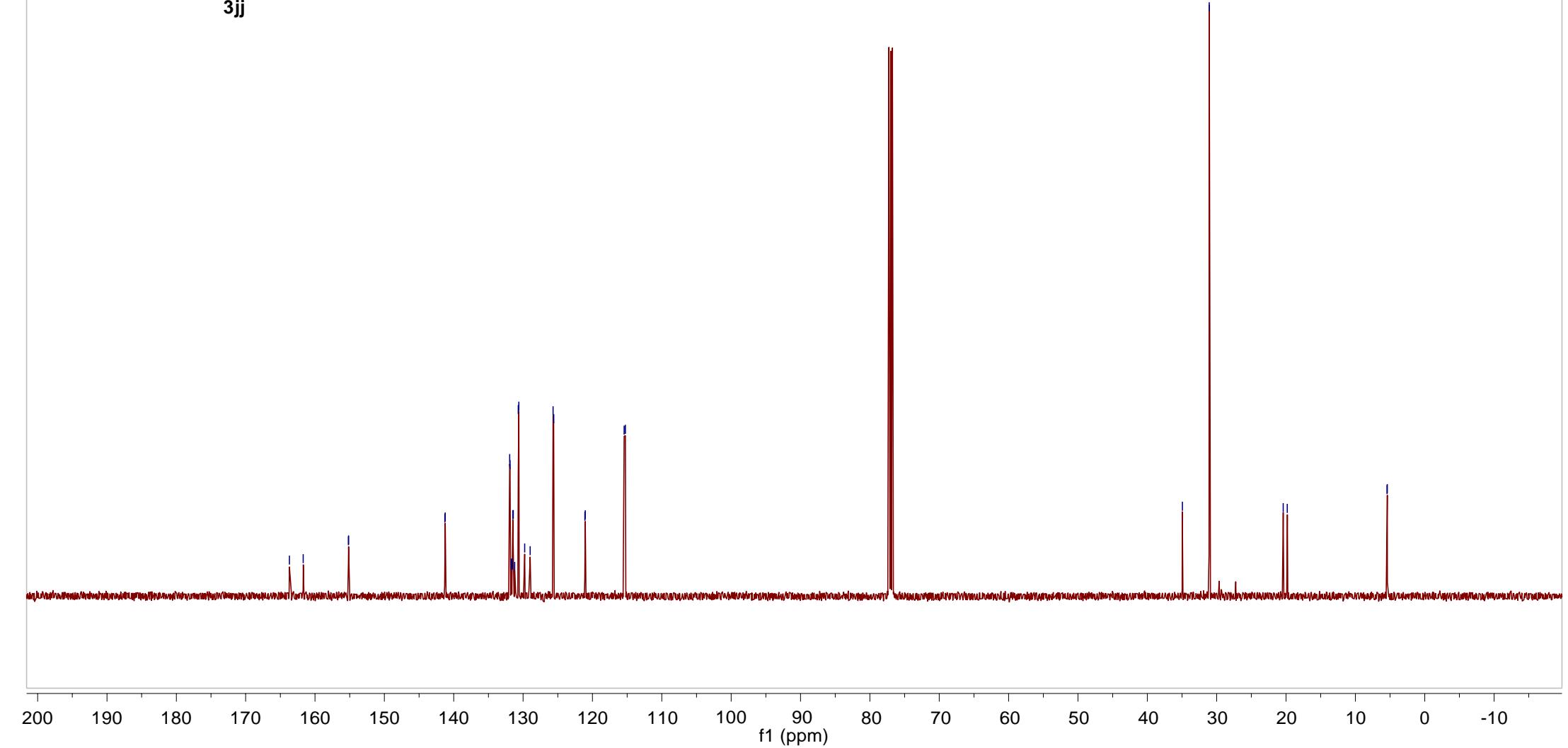
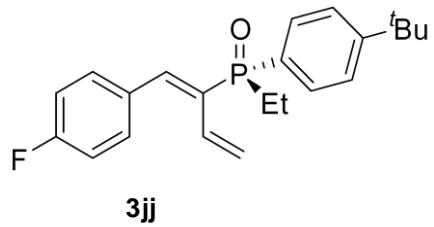


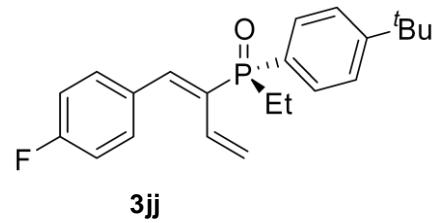
-35.546

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

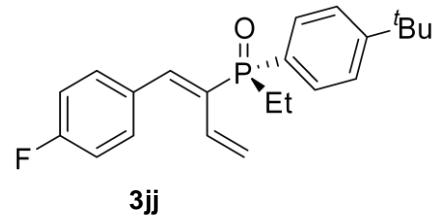






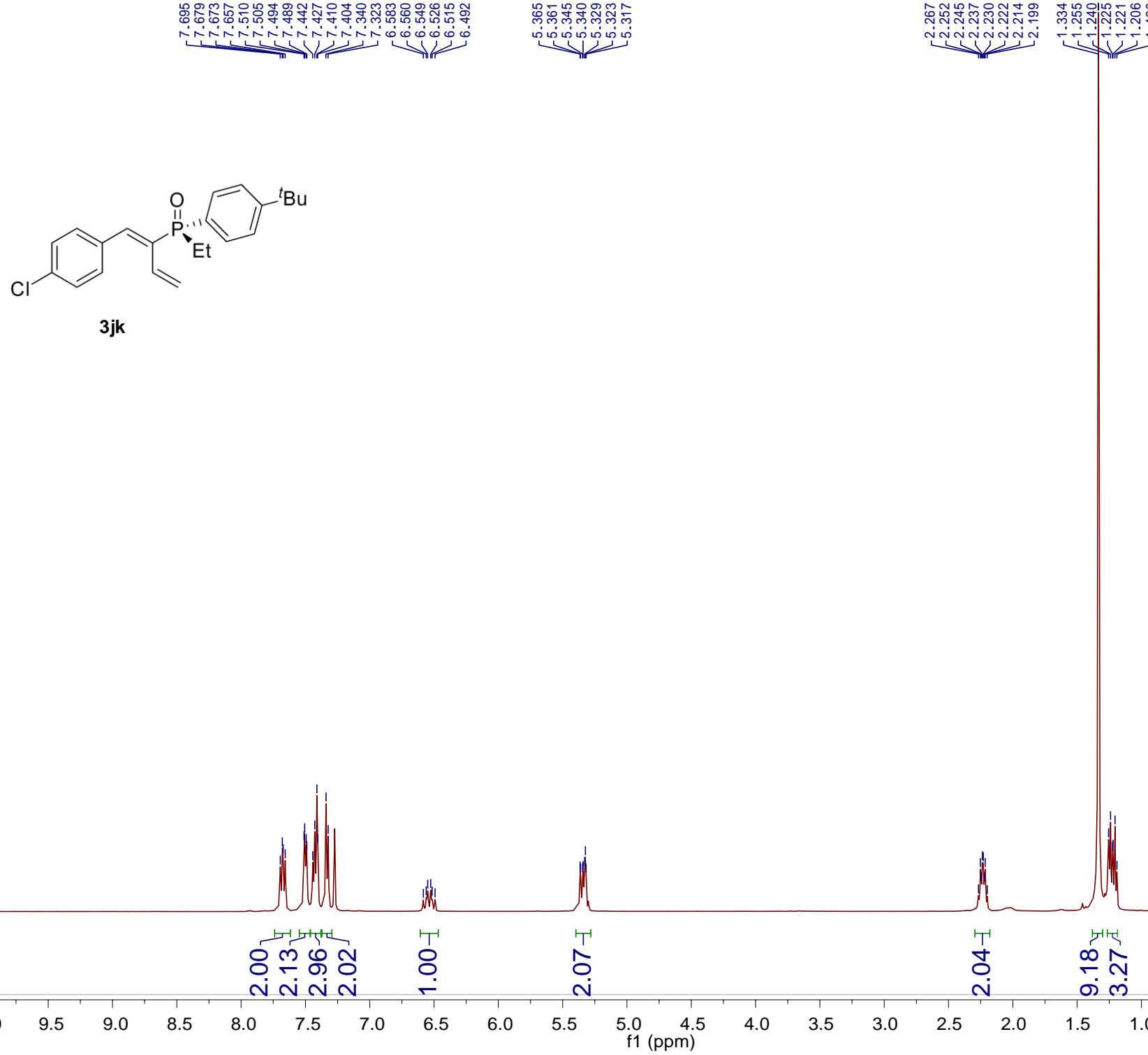
-35.455

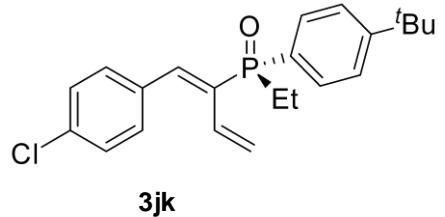
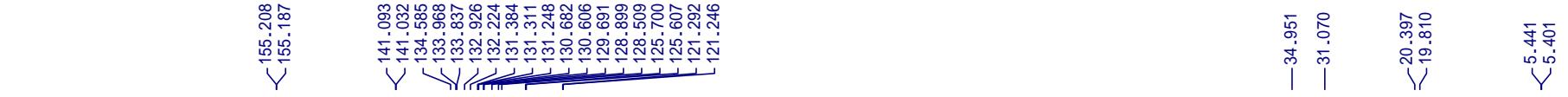
-111.580

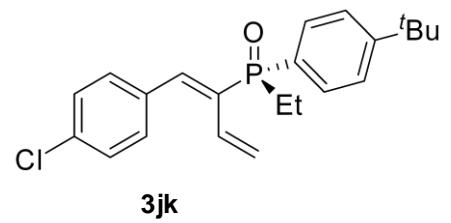


-10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130

f1 (ppm)



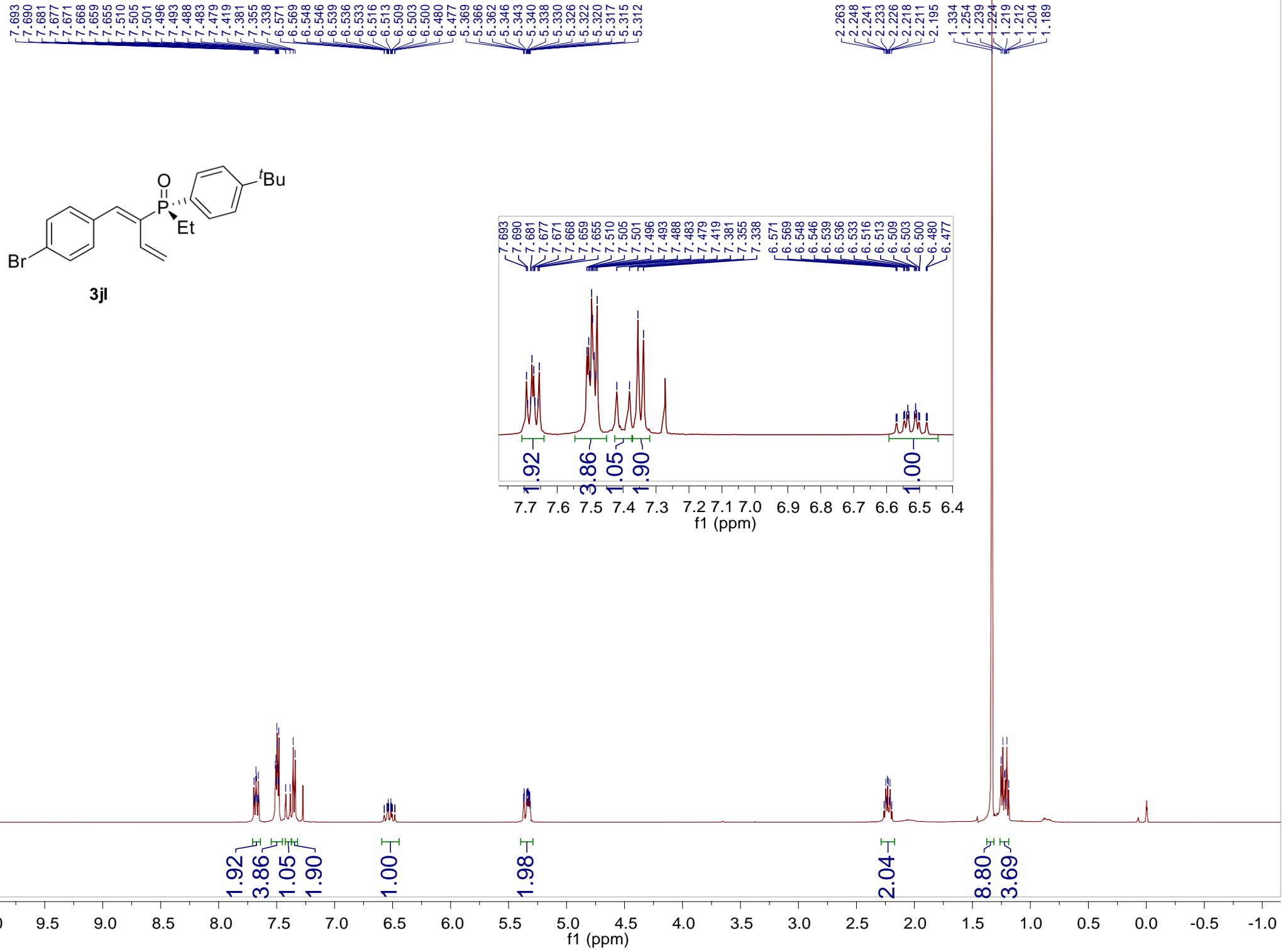


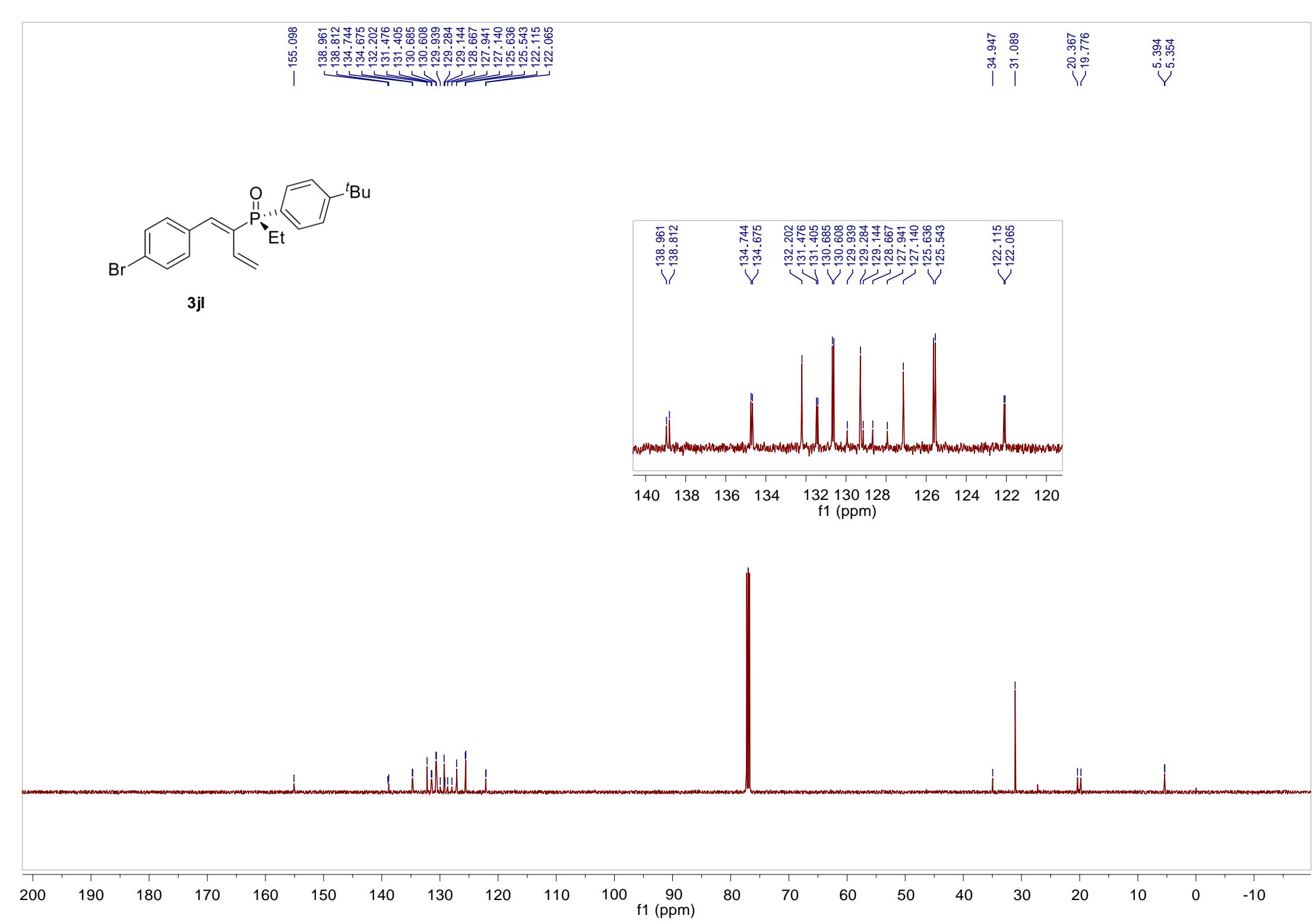


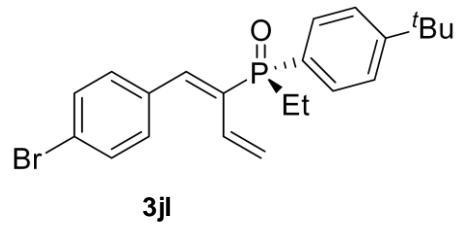
—35.402

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)



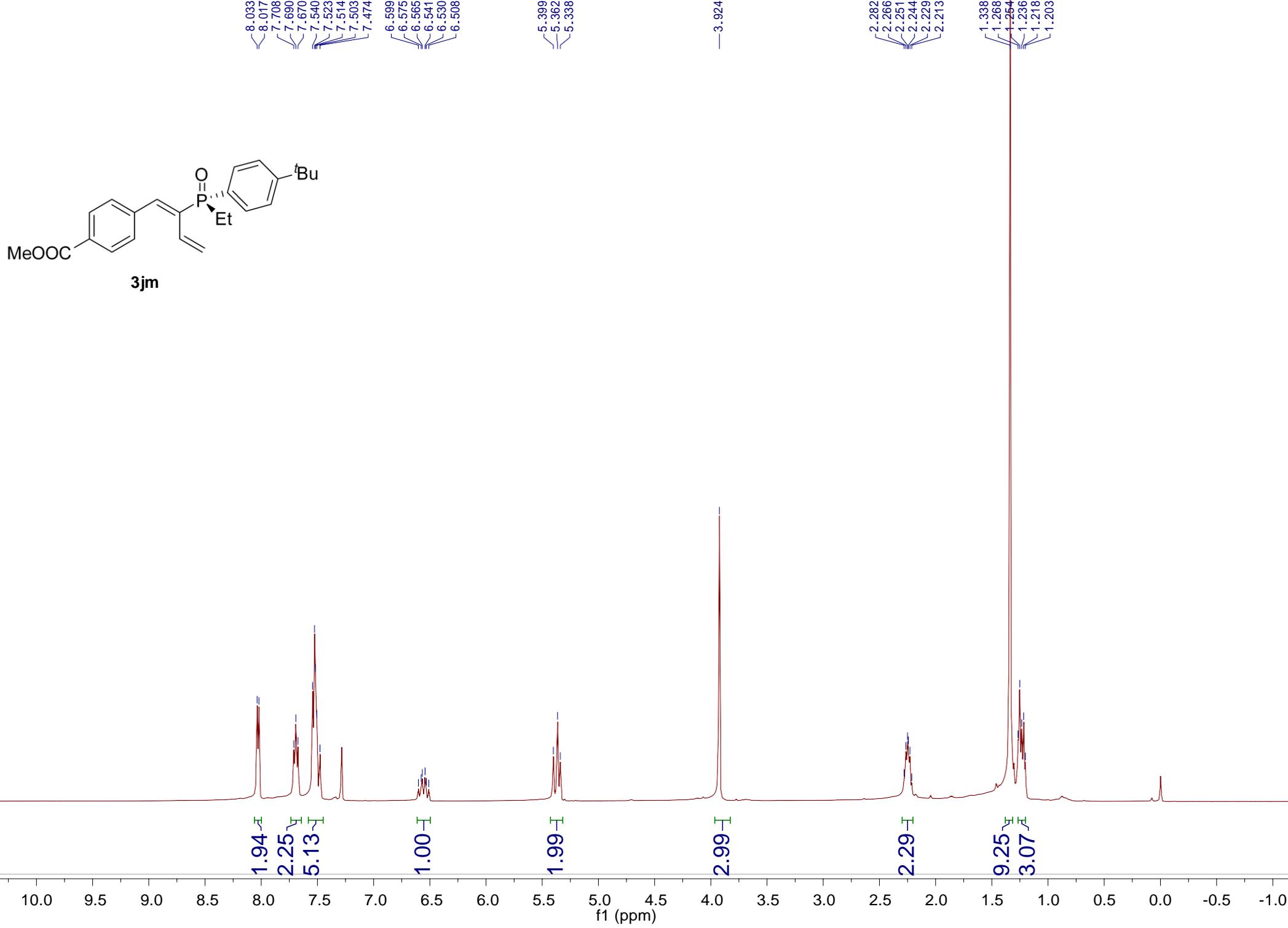




-35.188

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)



Chemical Shift (ppm)

— 166.531

< 155.295

< 155.274

141.175

141.115

< 139.979

< 139.850

134.756

134.063

< 131.237

131.167

< 130.702

130.627

129.849

129.804

129.516

129.454

128.724

125.724

125.631

121.670

121.623

— 52.163

— 34.952

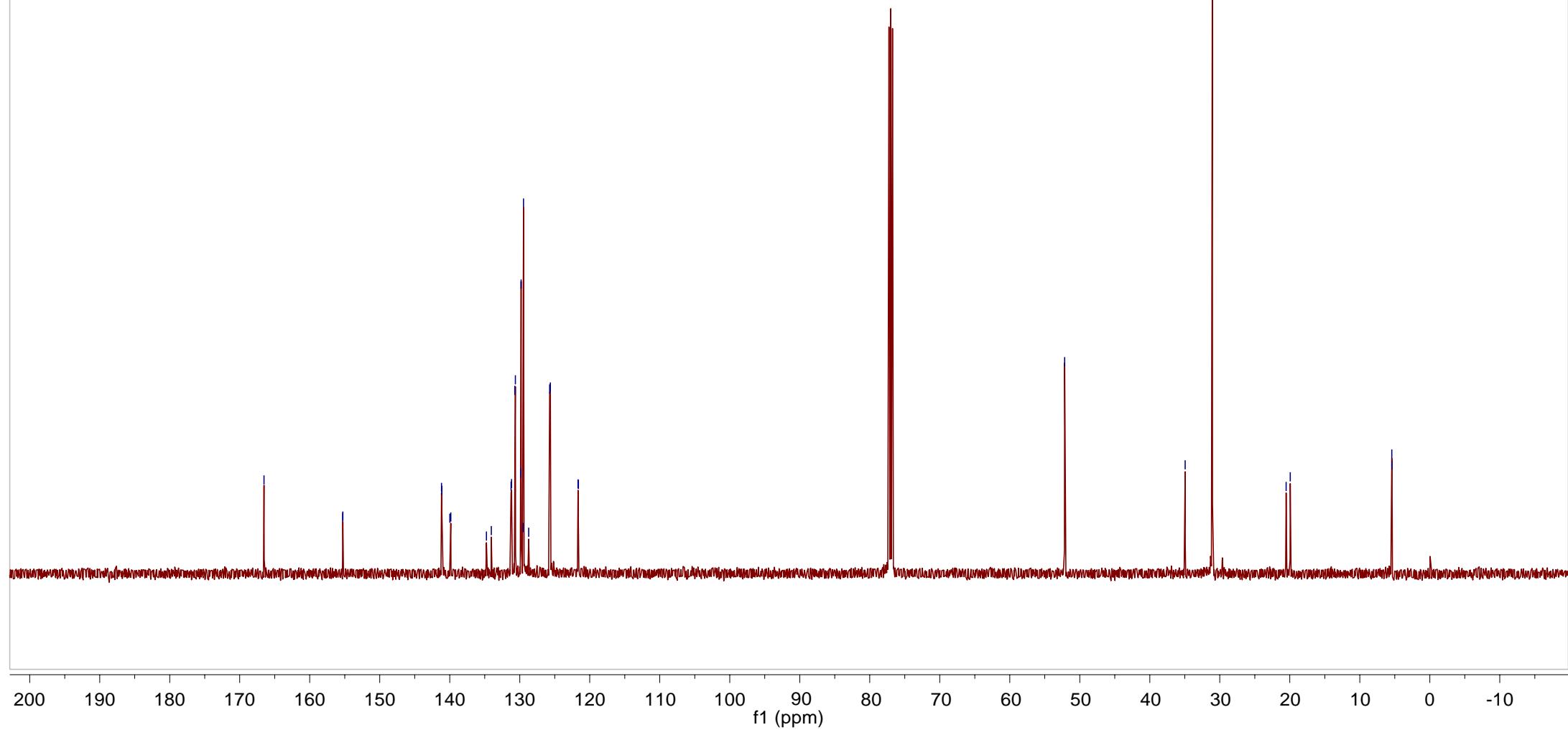
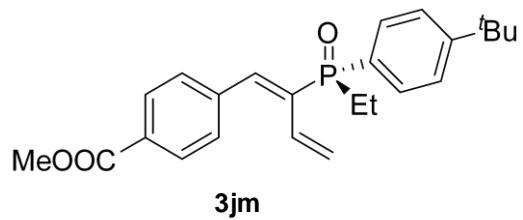
— 31.058

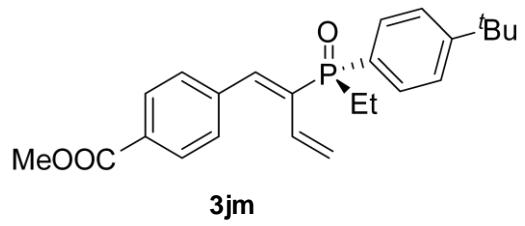
< 20.524

< 19.937

< 5.425

< 5.385

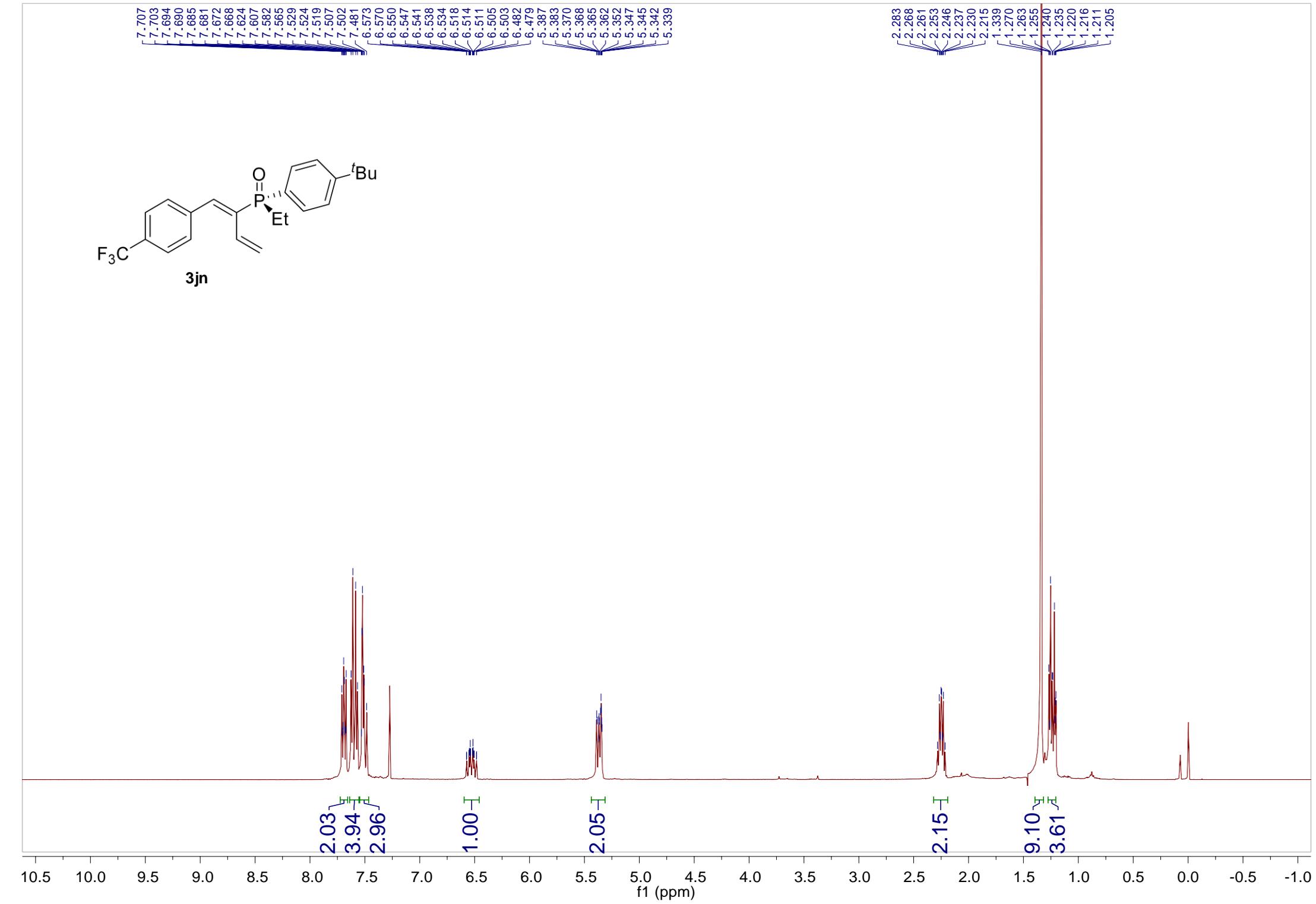
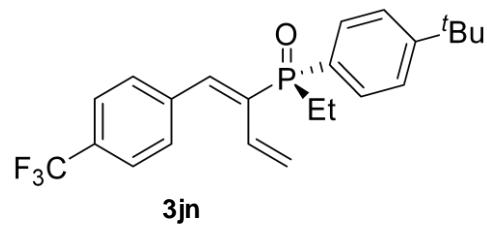




35.169

100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50

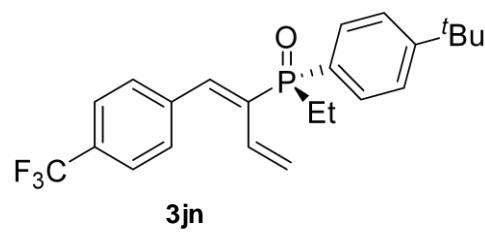
f1 (ppm)





190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

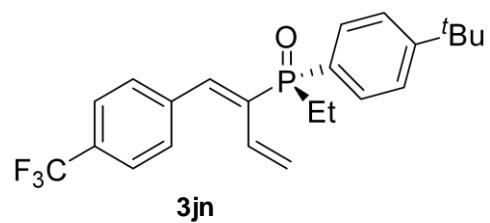
f1 (ppm)



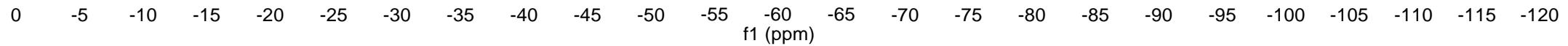
35.008

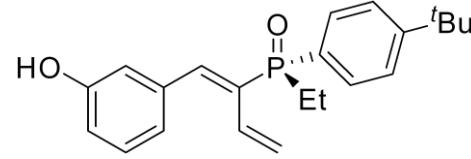
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

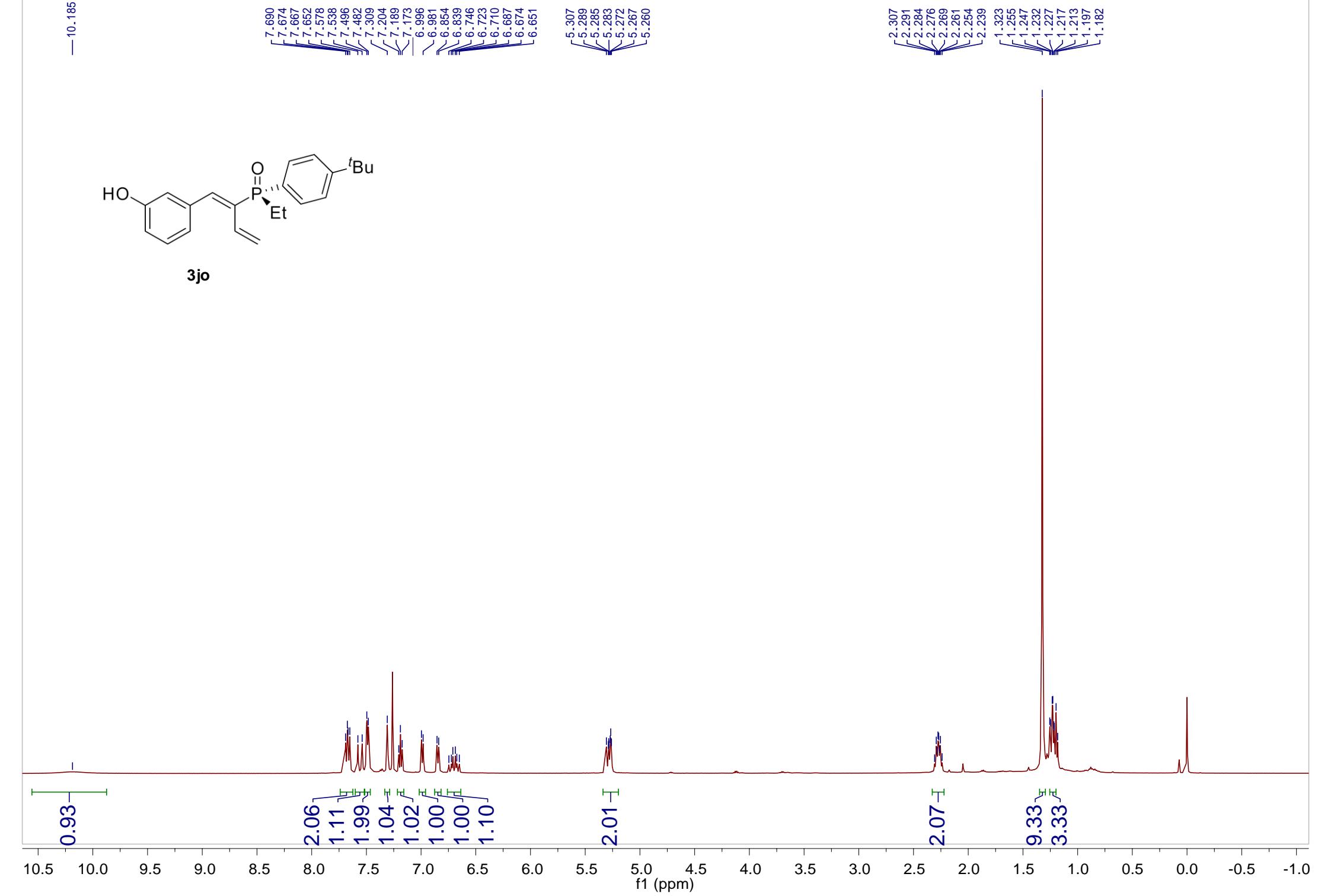


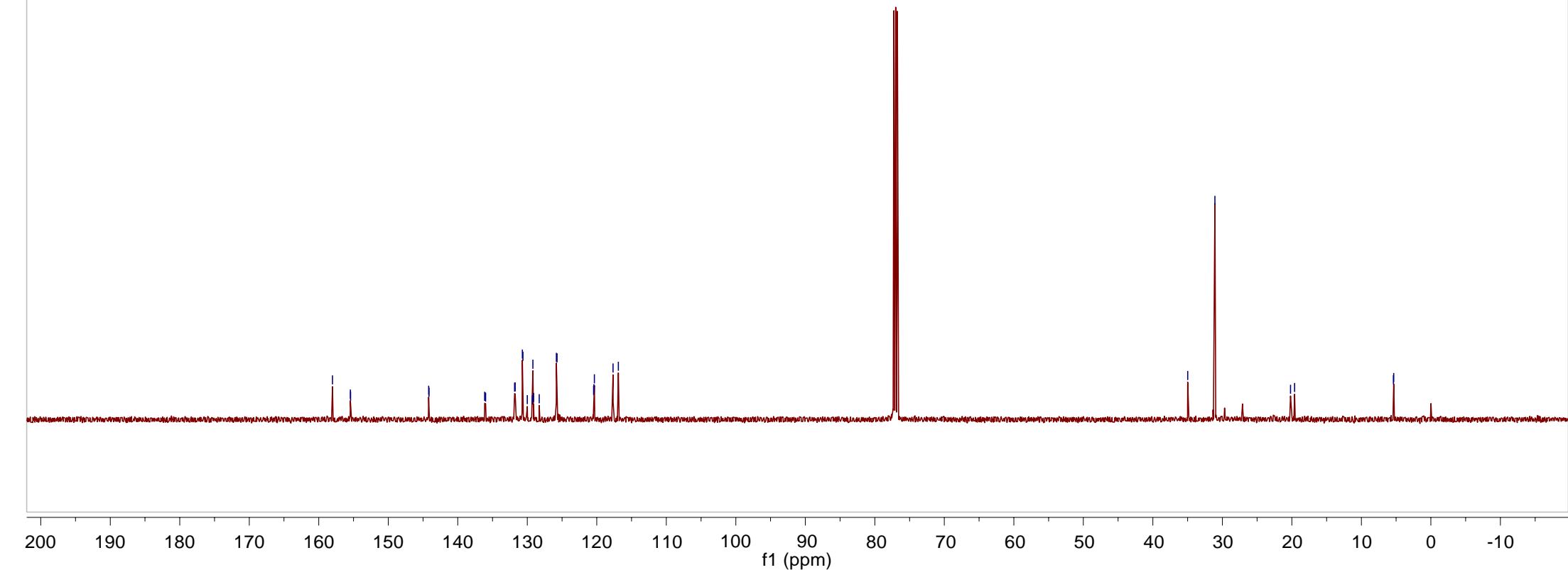
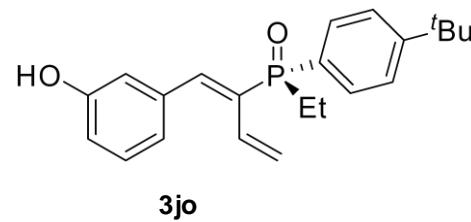
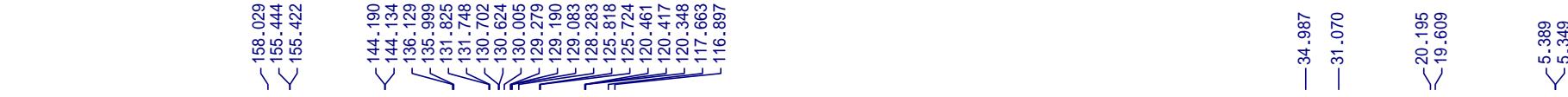
-62.759

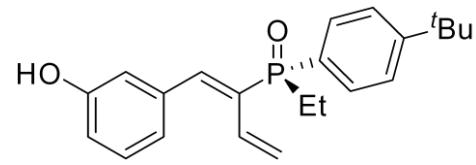




3jo



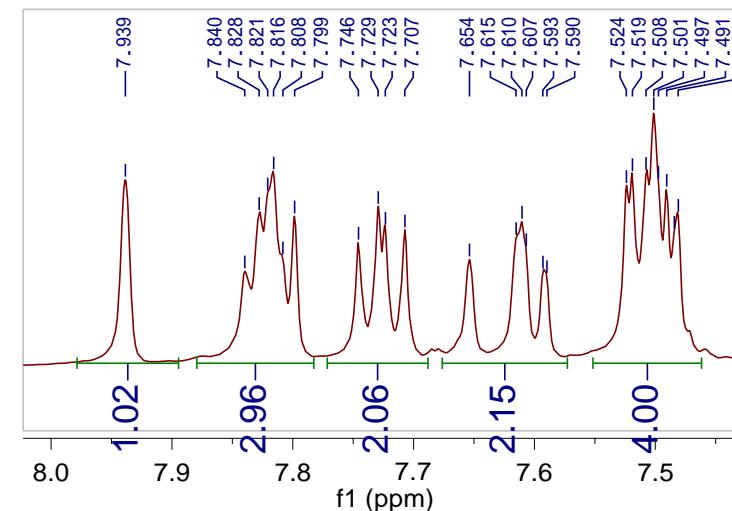
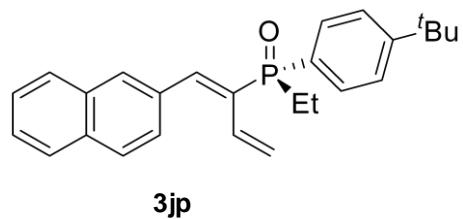


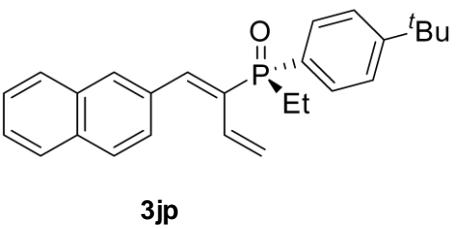


3jo

-37.942

7.939
 7.840
 7.828
 7.821
 7.816
 7.808
 7.799
 7.746
 7.729
 7.723
 7.707
 7.654
 7.615
 7.590
 7.524
 7.519
 7.508
 7.501
 7.497
 7.491
 7.484
 7.481
 7.607
 7.593
 7.581
 7.564
 7.550
 7.534
 7.524
 7.519
 7.508
 7.501
 7.497
 7.491
 7.484
 7.481
 6.734
 6.731
 6.711
 6.709
 6.698
 6.675
 6.664
 6.662
 6.641
 6.639
 5.430
 5.427
 5.424
 5.394
 5.391
 5.388
 5.362
 5.358
 5.340
 5.337
 5.334





< 155.115
< 155.094

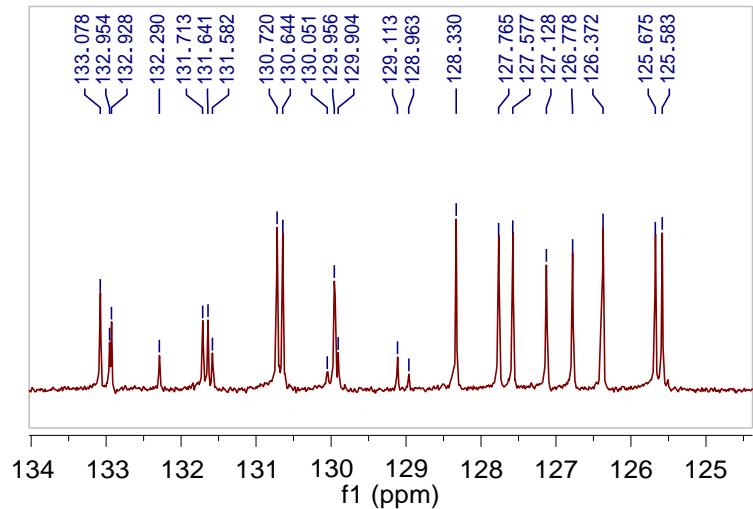
< 142.614
< 142.552
< 133.078
— 132.954
— 132.928
— 132.290
— 131.713
— 131.641
— 131.582
— 130.720
— 130.644
— 130.051
— 129.956
— 129.904
— 129.113
— 128.963
— 128.330
— 127.765
— 127.577
— 127.128
— 126.778
— 126.372
— 125.675
— 125.583
— 120.980
— 120.934

— 34.928
— 31.066

< 20.558

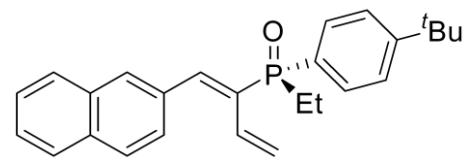
< 19.972

< 5.486
< 5.447



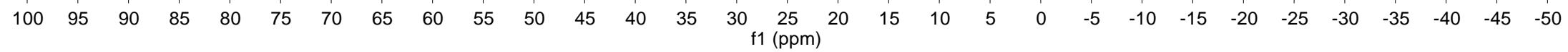
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

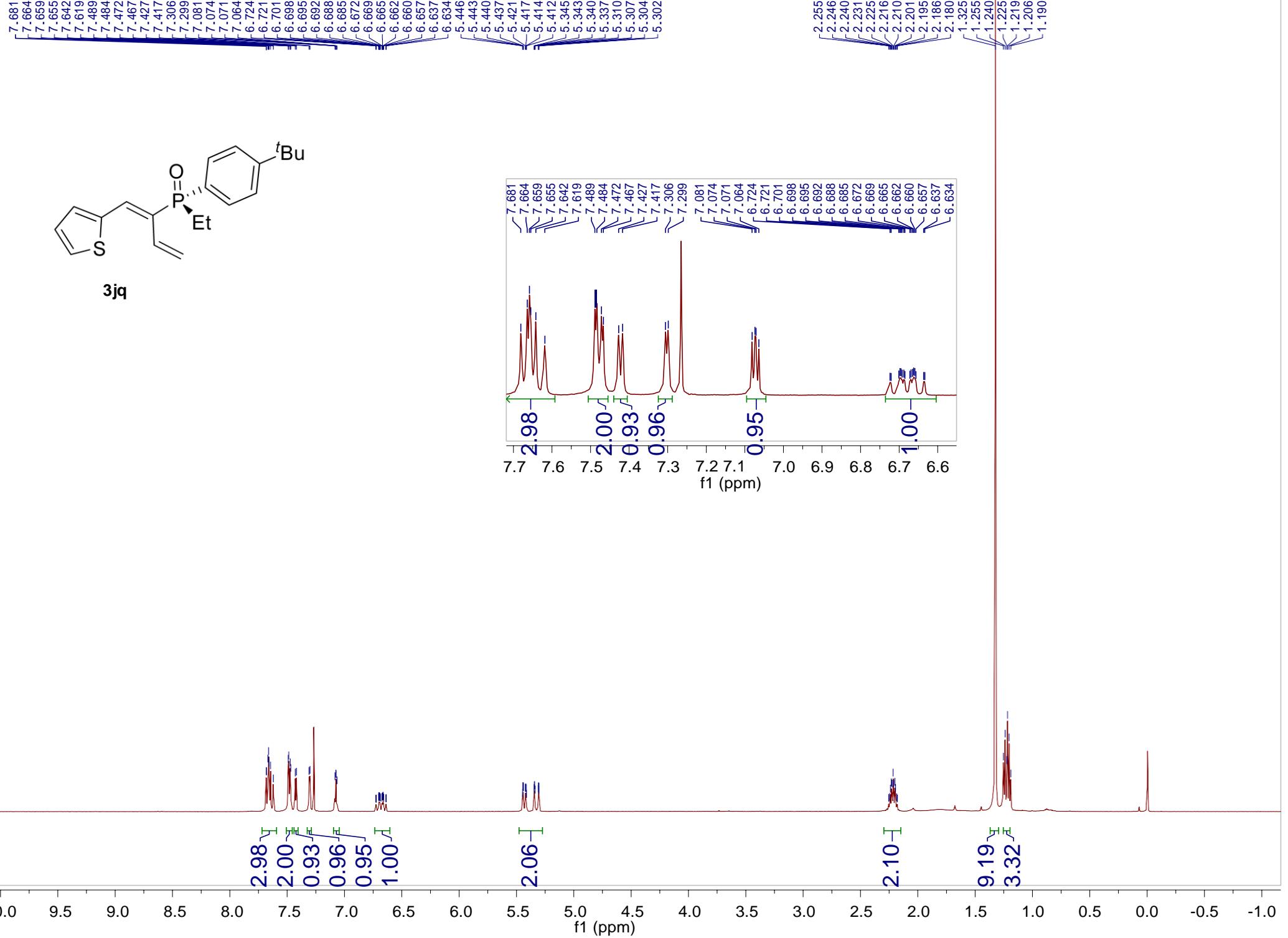
f1 (ppm)

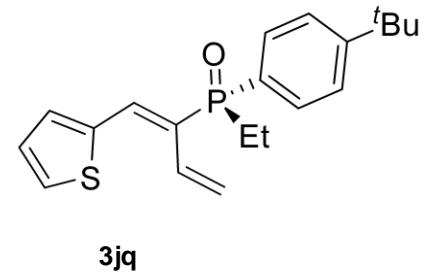


3jp

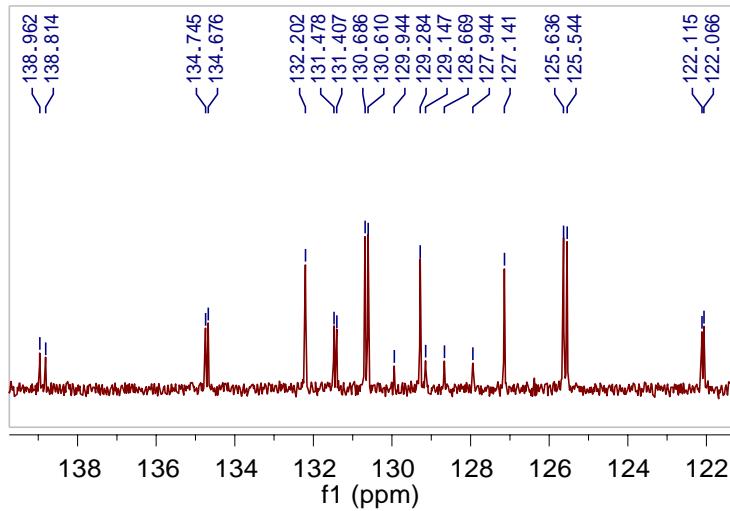
-35.681







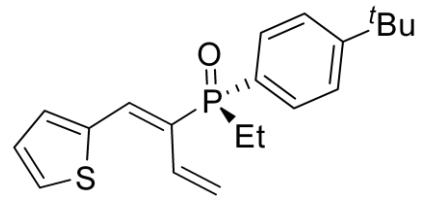
<155.121
 <155.098
 138.962
 138.814
 134.745
 134.676
 132.202
 131.478
 131.407
 130.686
 130.610
 129.944
 129.284
 129.147
 128.669
 127.944
 127.141
 125.636
 125.544
 122.115
 122.066



00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

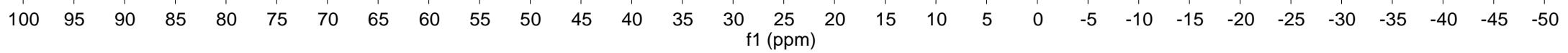
f1 (ppm)

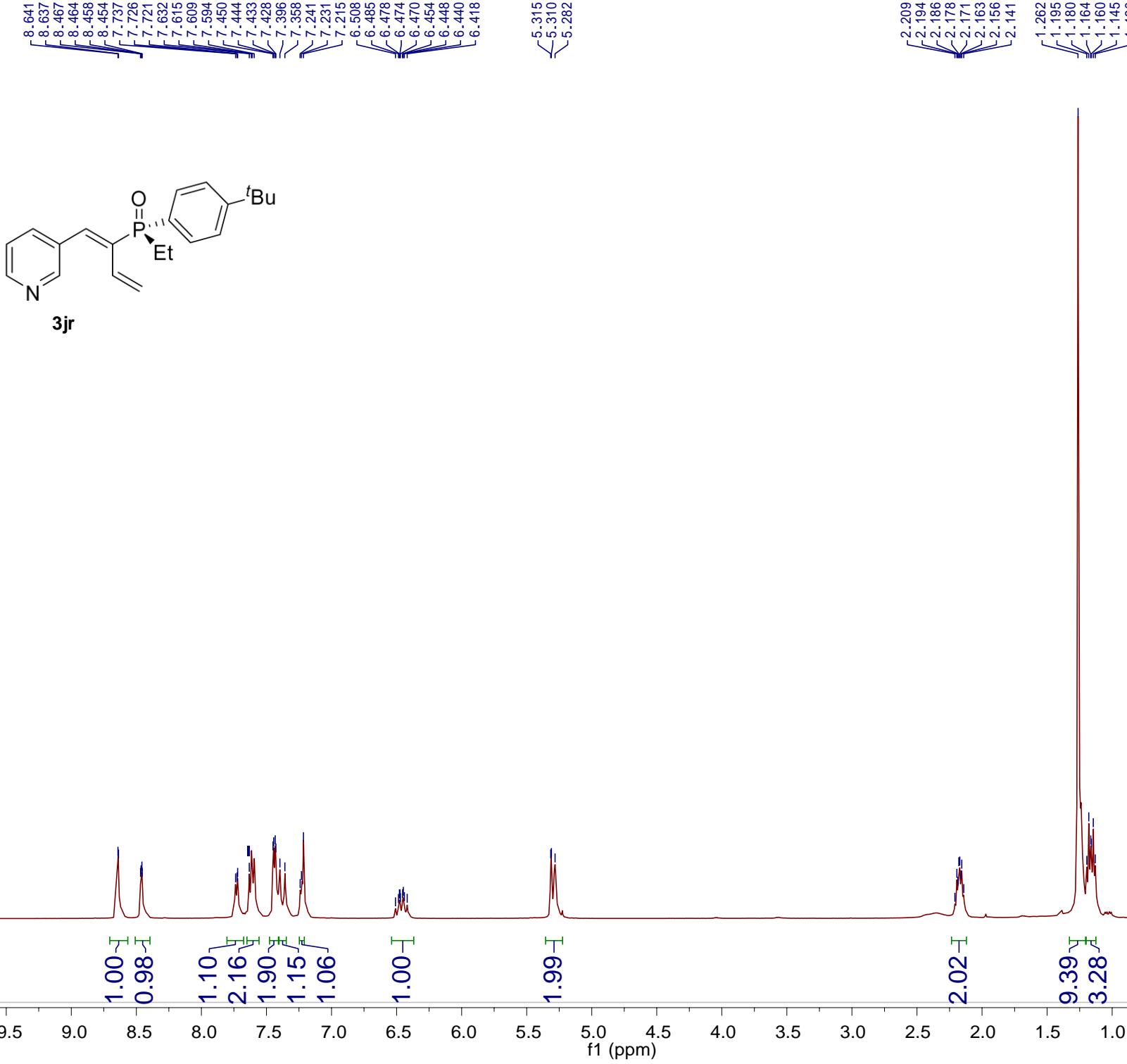
—34.949
 —31.089
 <20.368
 <19.776
 <5.395
 <5.355

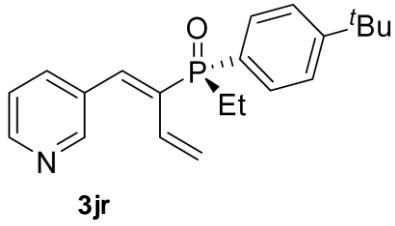


3jq

-34.934





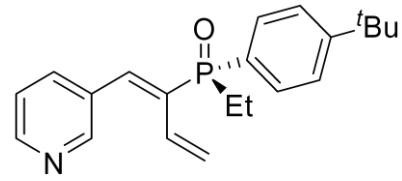


< 155.340
 < 155.319
 — 150.708
 — 149.294
 — 138.616
 — 138.555
 — 136.749
 — 135.031
 — 134.339
 — 131.362
 — 131.234
 — 130.922
 — 130.851
 — 130.639
 — 130.363
 — 129.250
 — 128.456
 — 125.738
 — 125.644
 — 123.113
 — 121.965
 — 121.918

— 34.932
 — 31.022
 — 20.317
 < 19.729
 < 5.366
 < 5.325

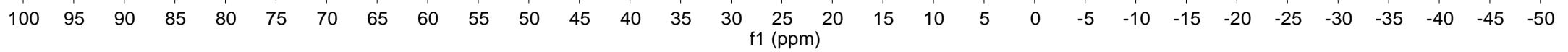
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

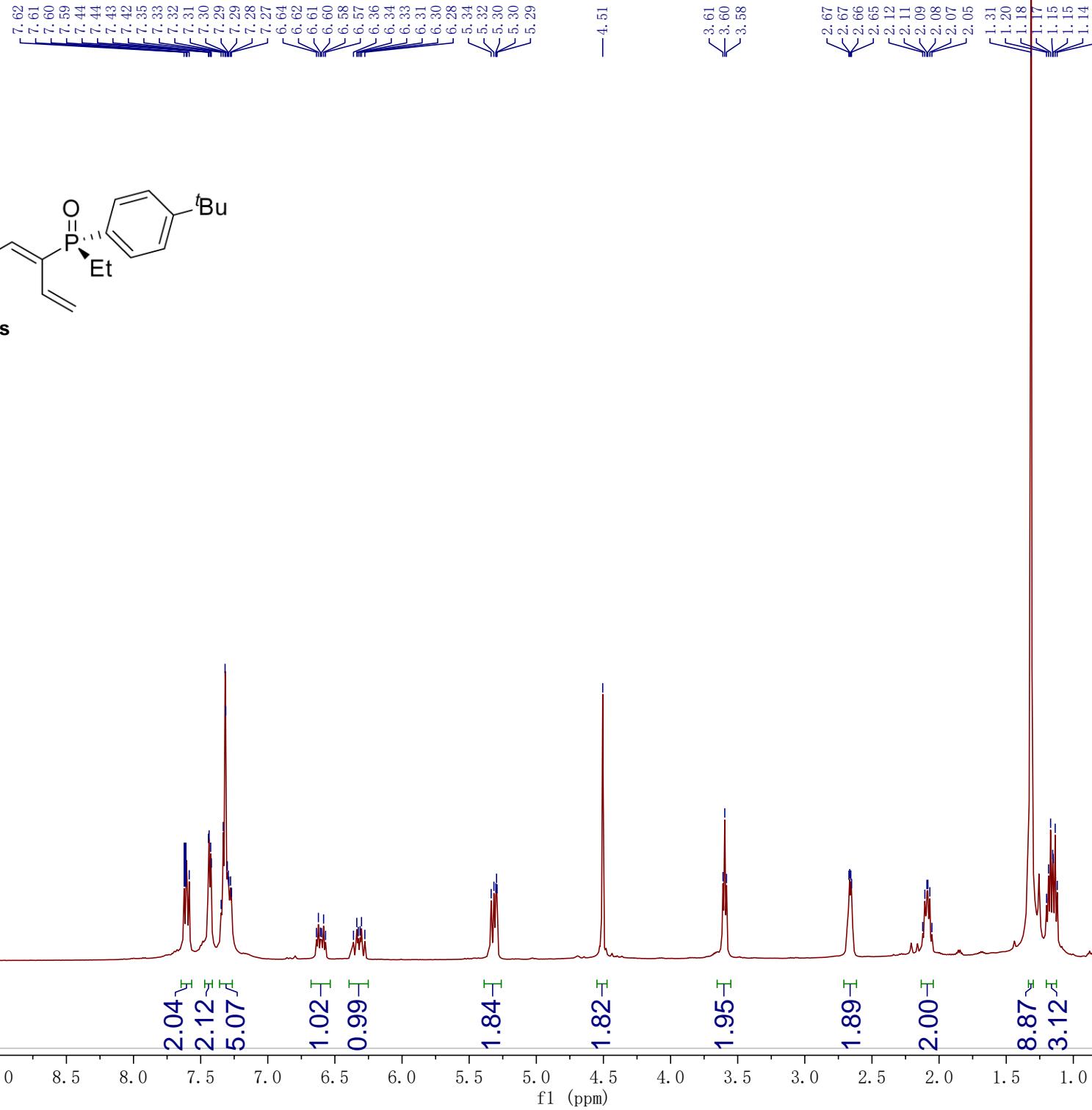
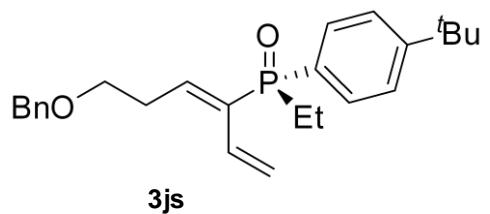
f1 (ppm)

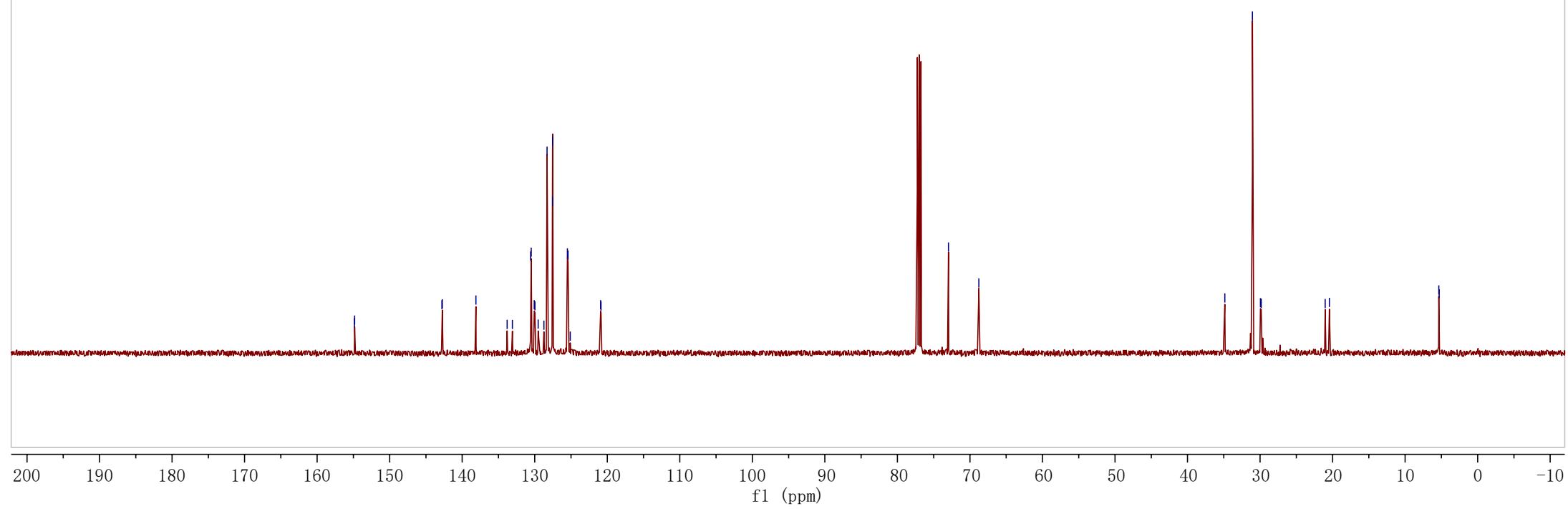
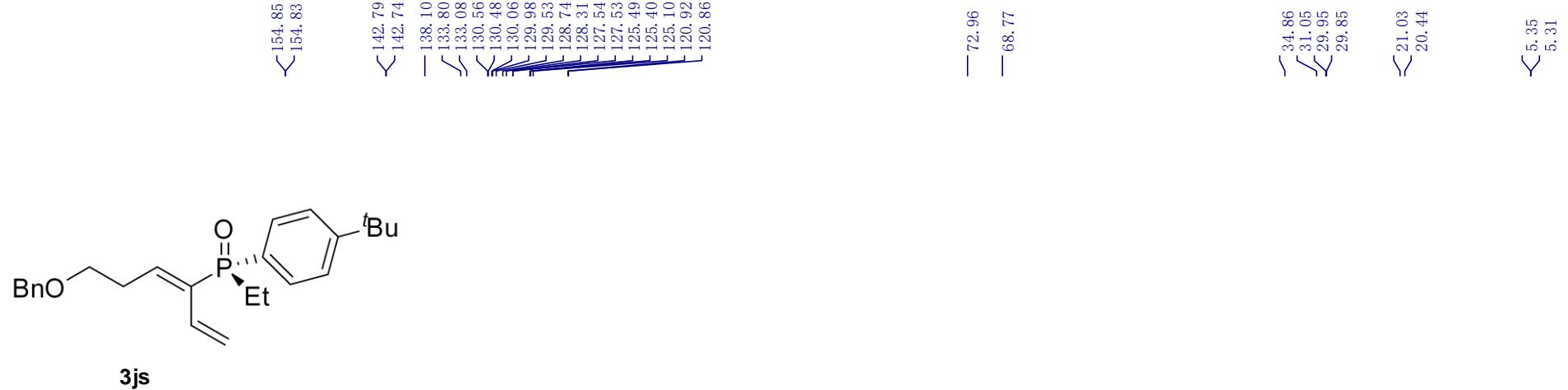


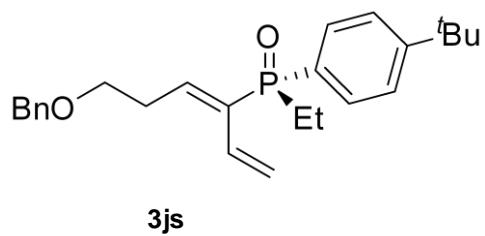
3jr

-34.897

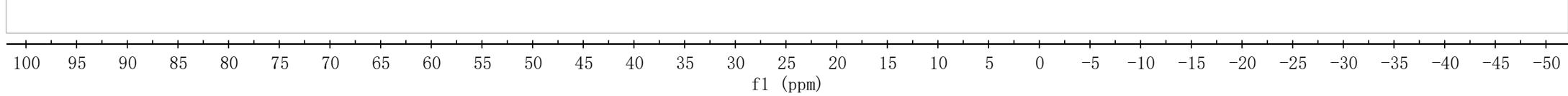




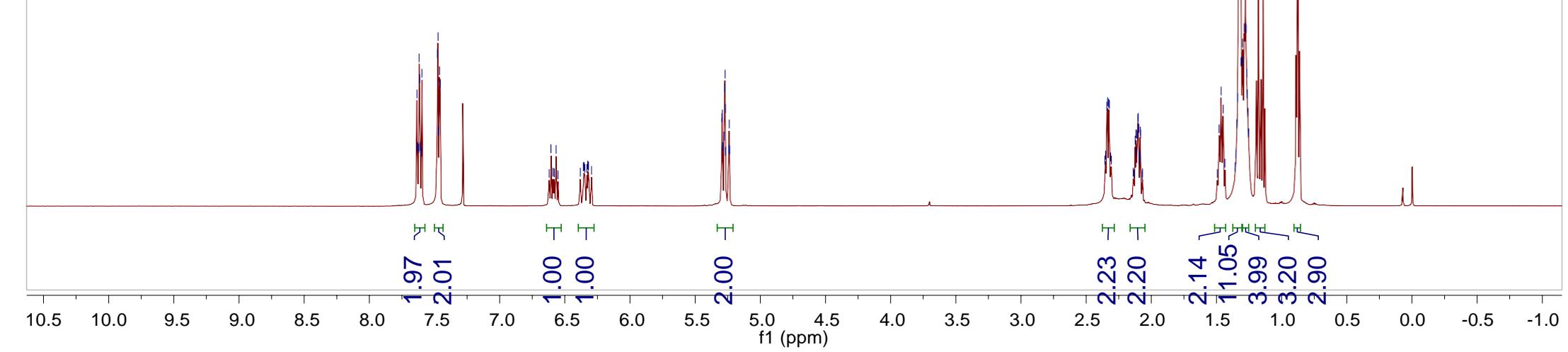
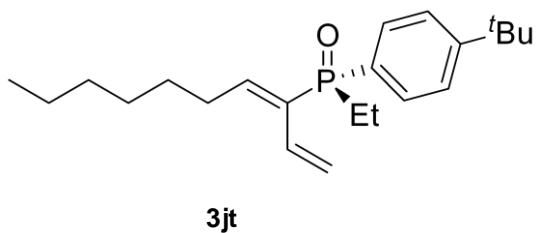


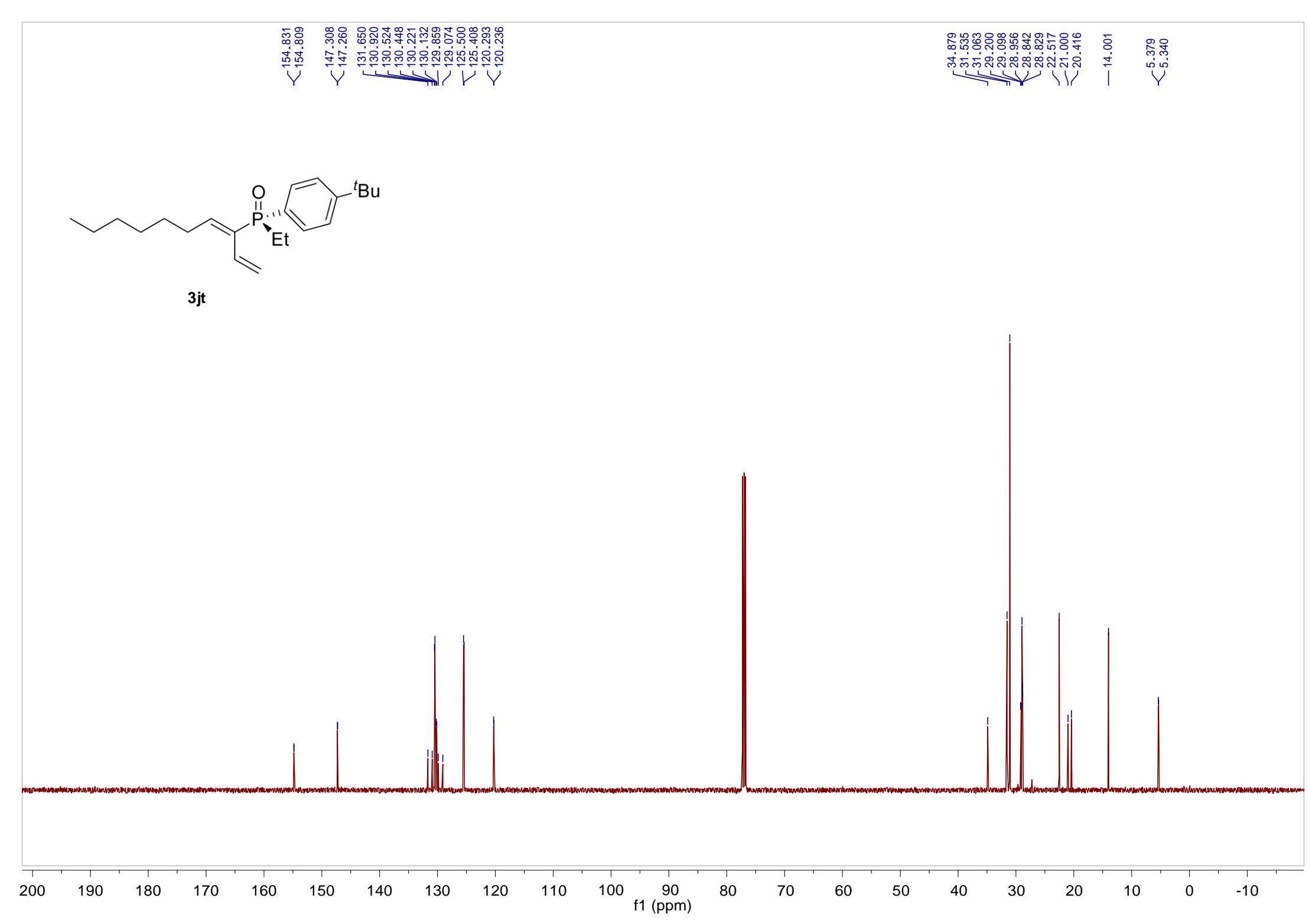


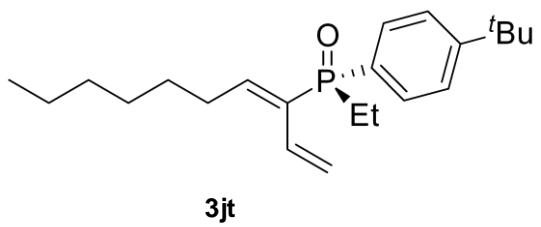
—34.29



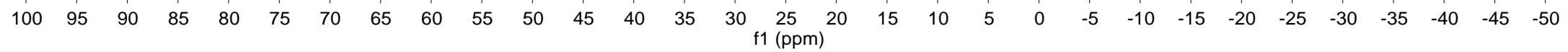
7.632
7.629
7.620
7.616
7.610
7.607
7.598
7.594
7.476
7.471
7.467
7.459
7.454
6.619
6.604
6.589
6.565
6.550
6.380
6.316
6.293
6.293
5.290
5.288
5.277
5.273
5.270
5.267
5.265
5.242
5.238
5.235
2.358
2.352
2.343
2.337
2.328
2.322
2.313
2.307
2.140
2.134
2.125
2.119
2.116
2.110
2.104
2.101
2.098
2.094
2.089
2.086
2.083
2.071
2.068
2.068
1.495
1.481
1.466
1.451
1.359
1.353
1.346
1.340
1.332
1.324
1.312
1.312
1.304
1.301
1.289
1.280
1.274
1.269
1.266
1.259
1.255

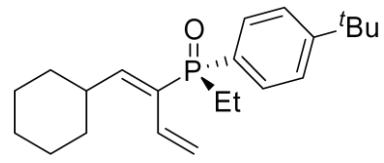




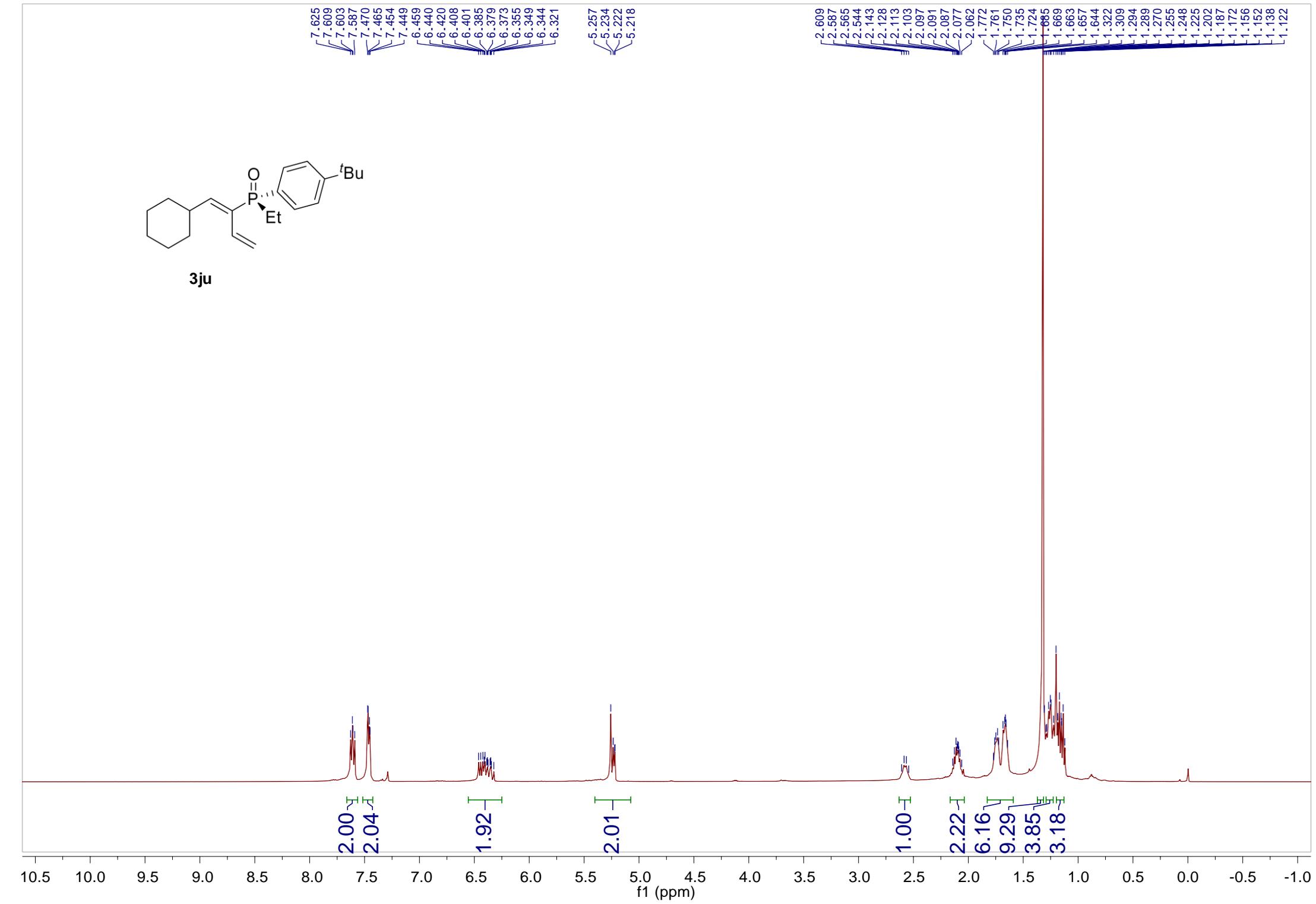


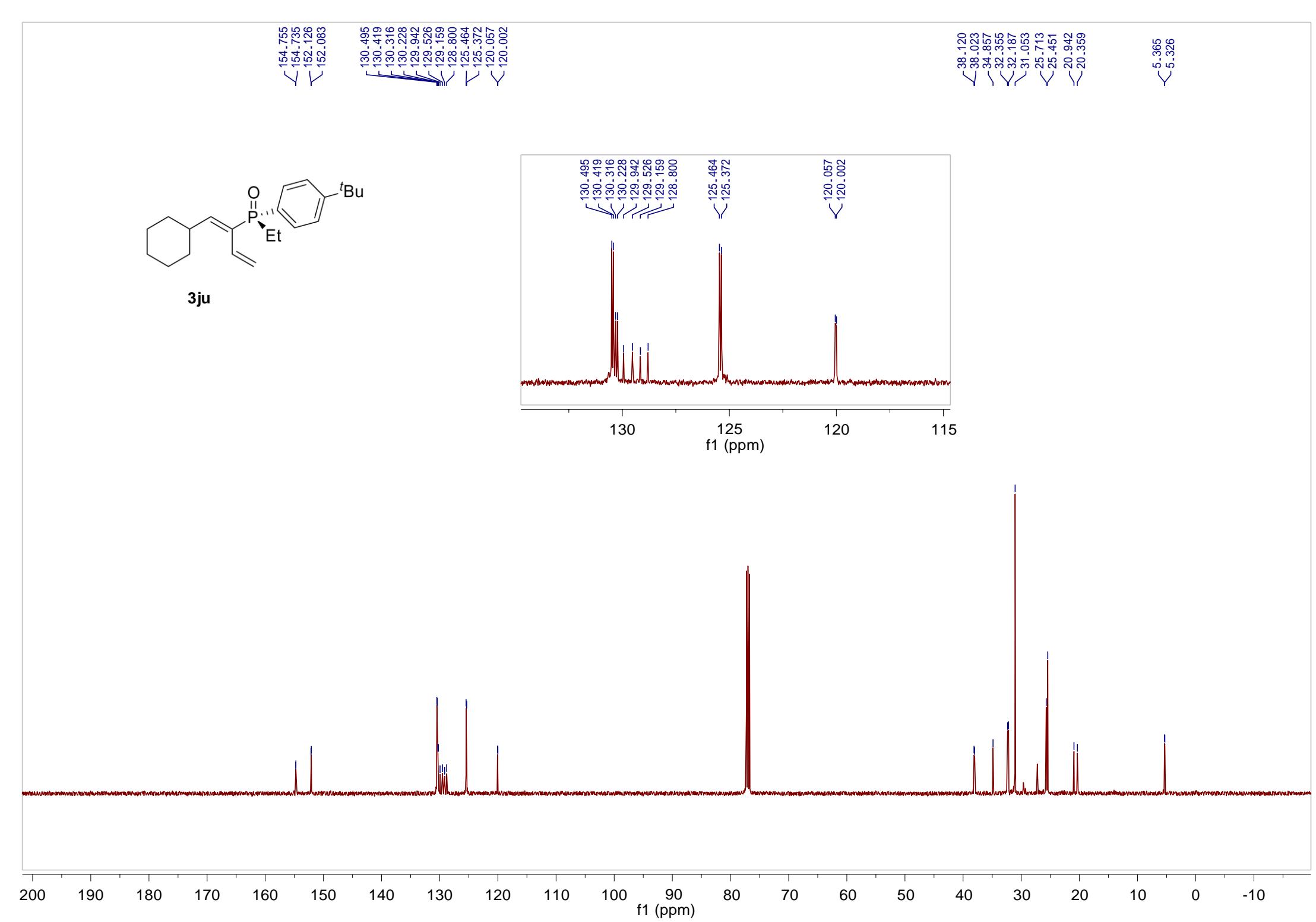
-34.292

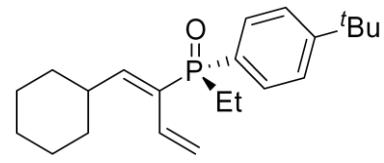




3ju

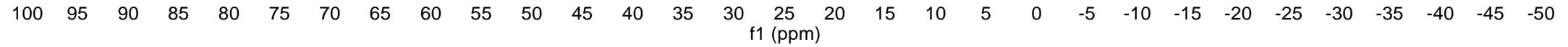






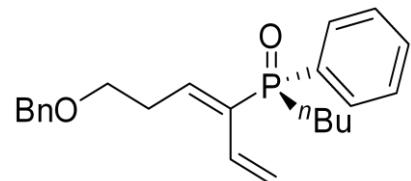
3ju

—34.284

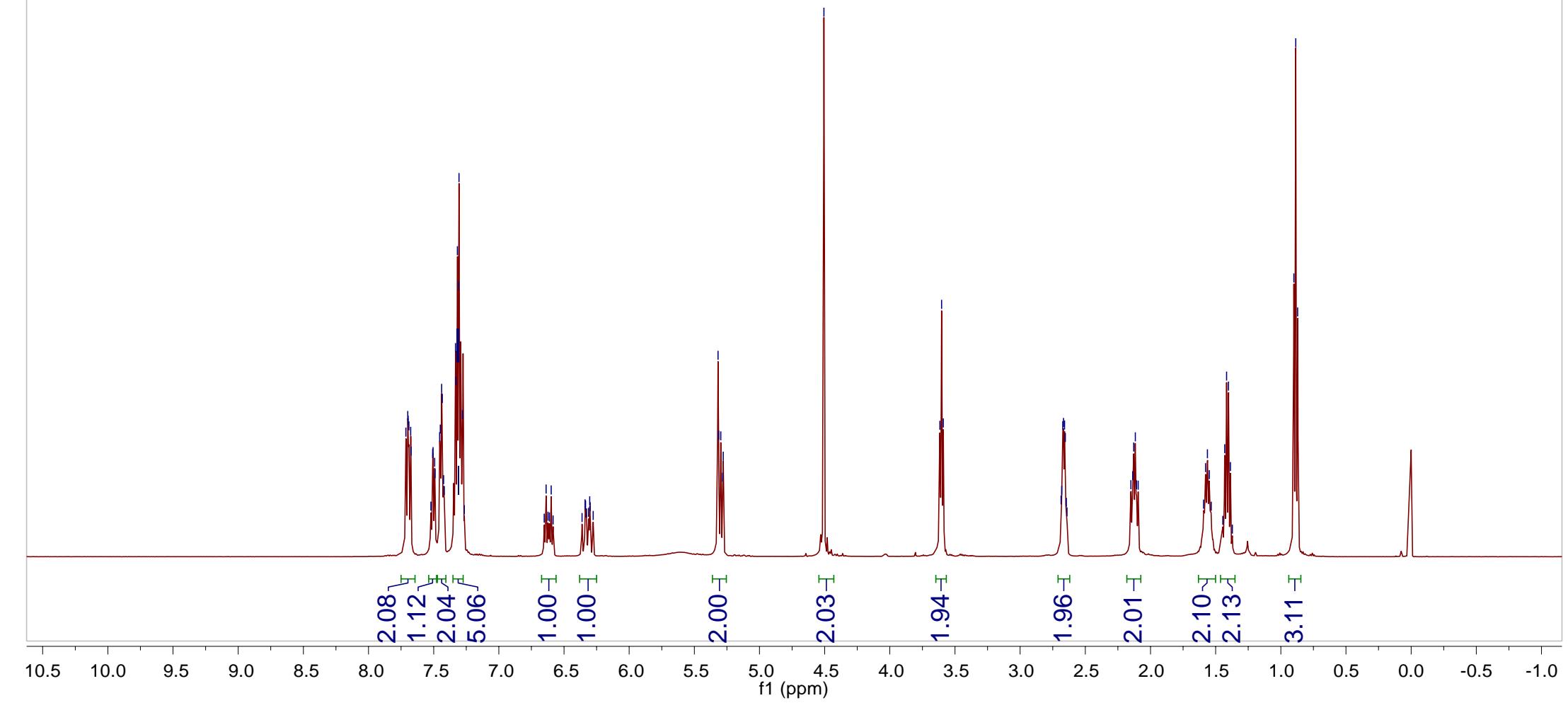


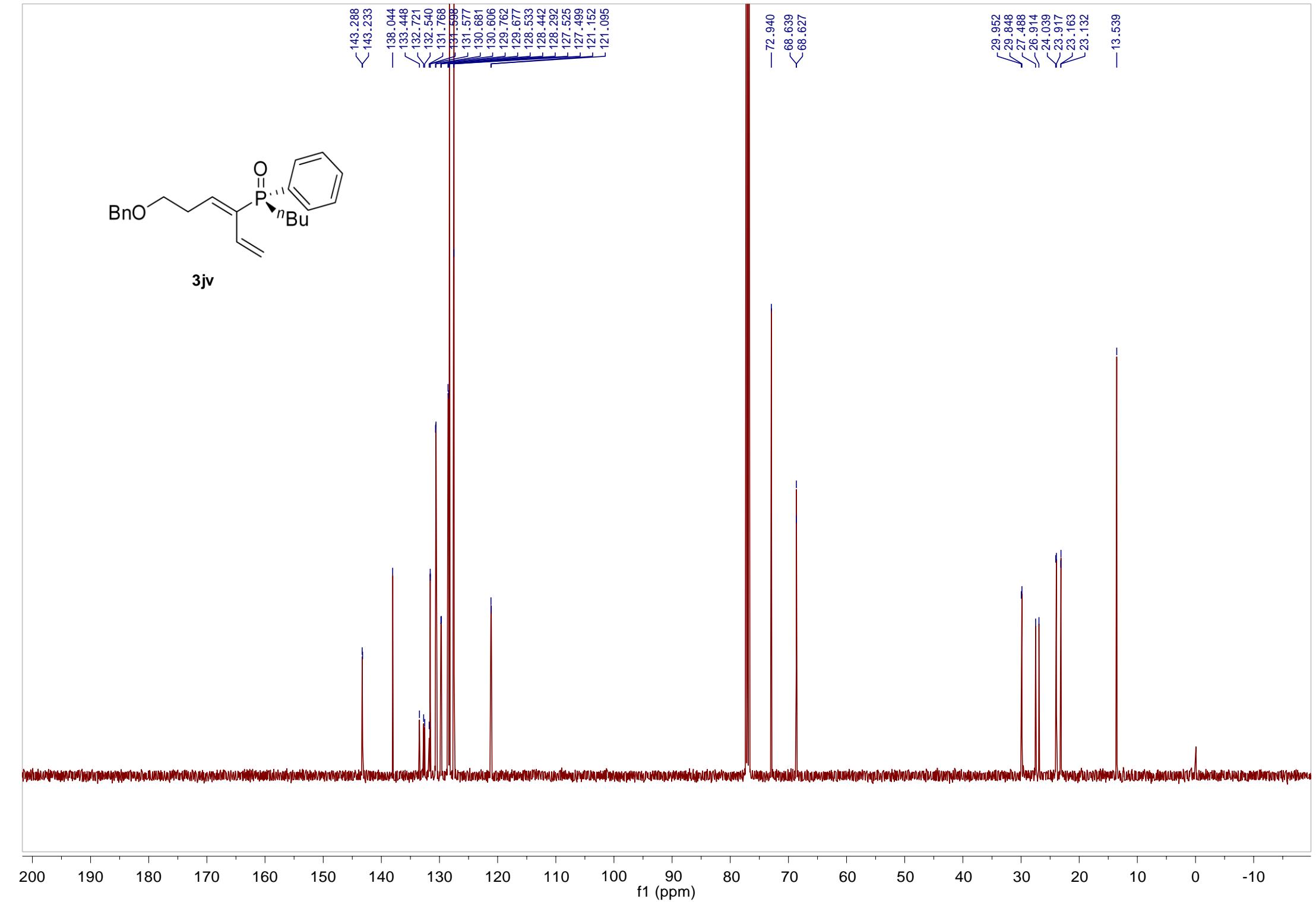
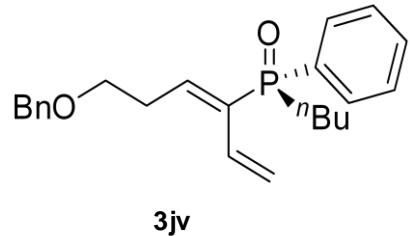
7.713
7.699
7.696
7.690
7.676
7.673
7.521
7.508
7.505
7.492
7.434
7.424
7.489
7.419
7.449
7.439
7.346
7.332
7.329
7.318
7.309
7.305
7.295
7.292
7.279
7.215
7.265
6.637
6.623
6.612
6.598
6.584
6.362
6.338
6.335
6.326
6.311
6.303
6.299
6.276
5.318
5.313
5.297
5.283
5.279

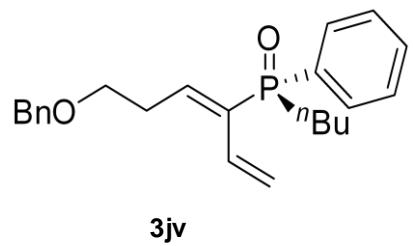
3.616
3.603
3.590
2.686
2.681
2.673
2.67
2.667
2.659
2.654
2.646
2.640
2.150
2.137
2.129
2.117
2.108
2.095
1.593
1.577
1.563
1.549
1.534
1.445
1.431
1.416
1.401
1.387
1.372
0.900
0.885
0.871



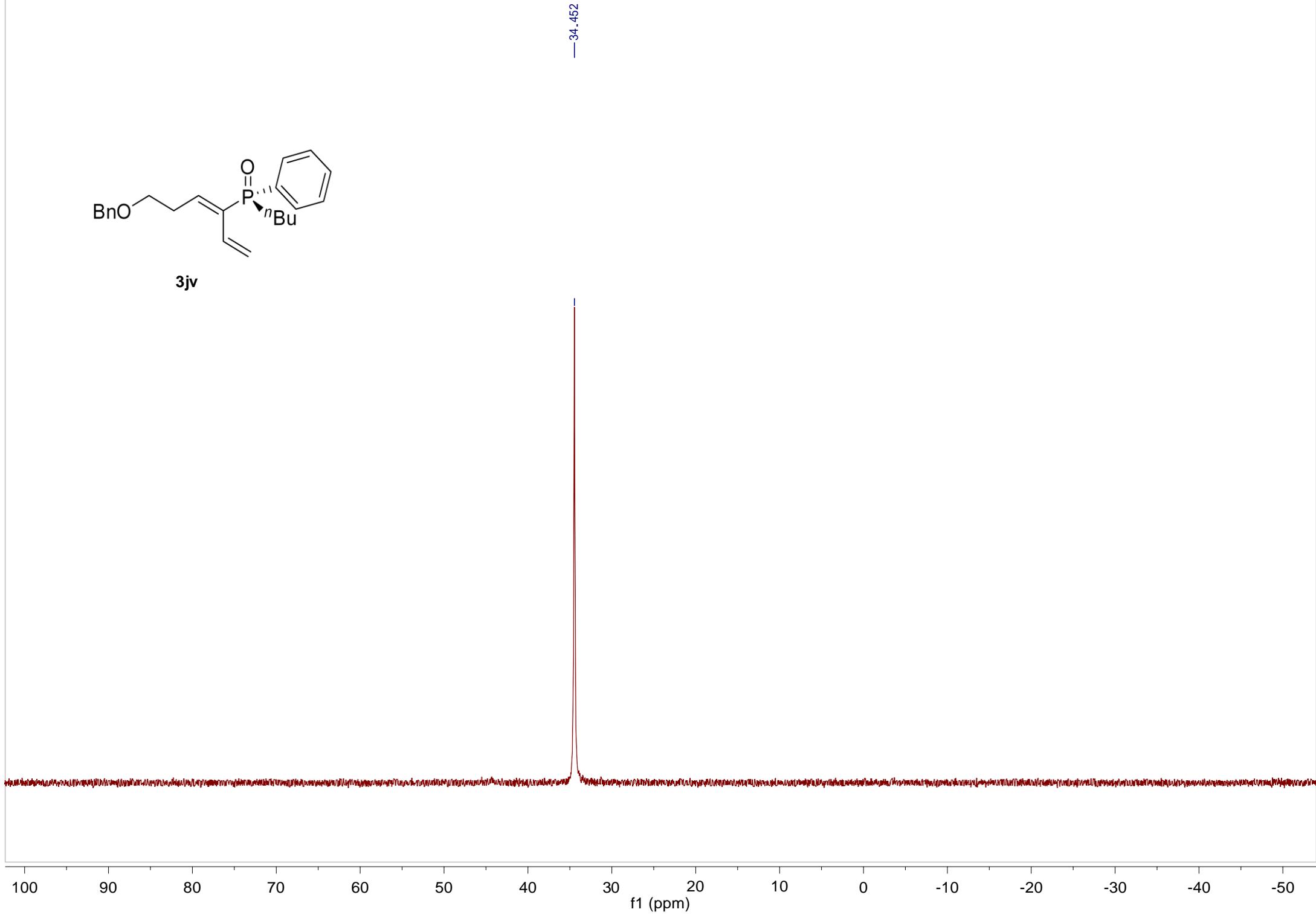
3jv

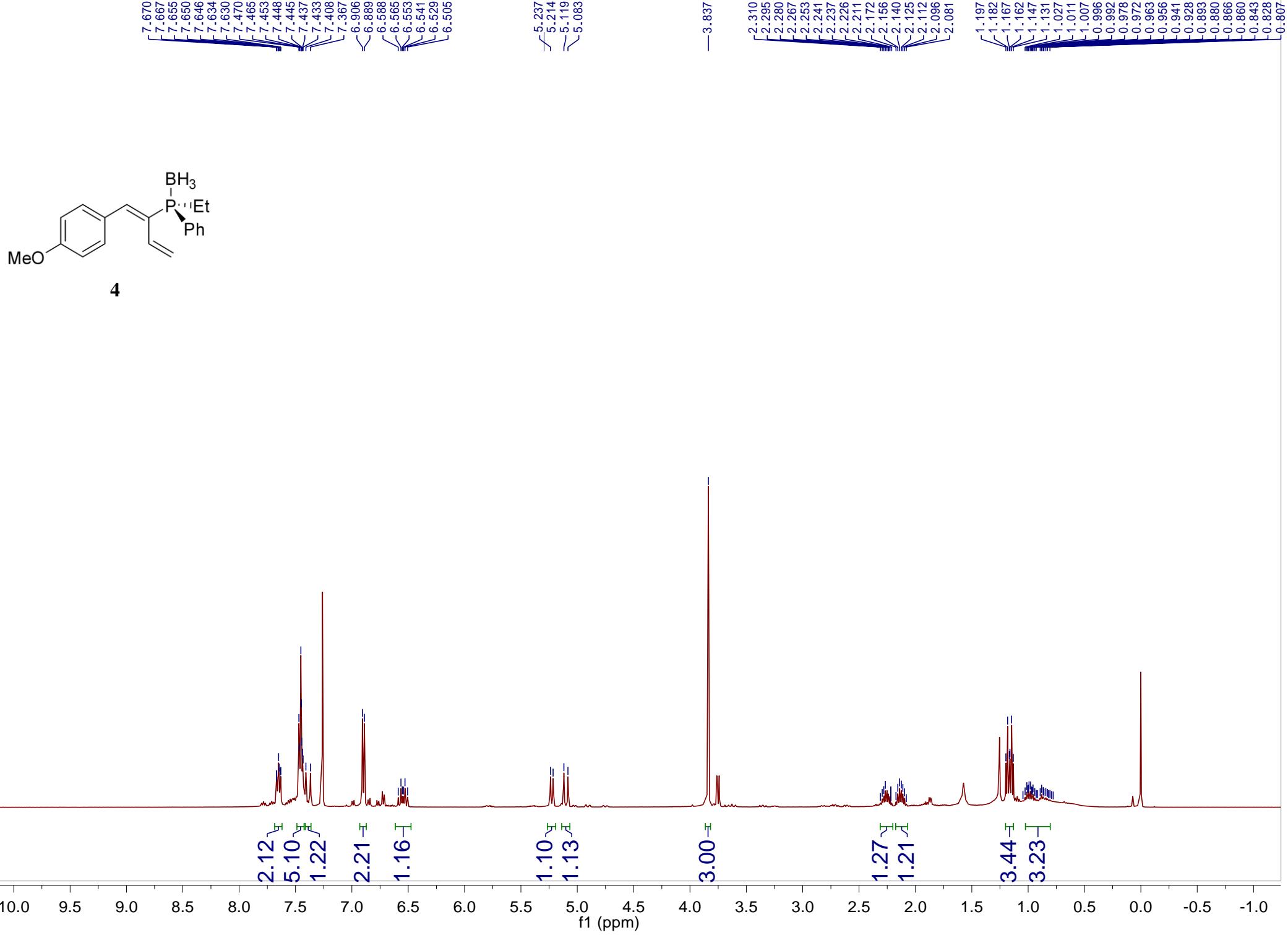


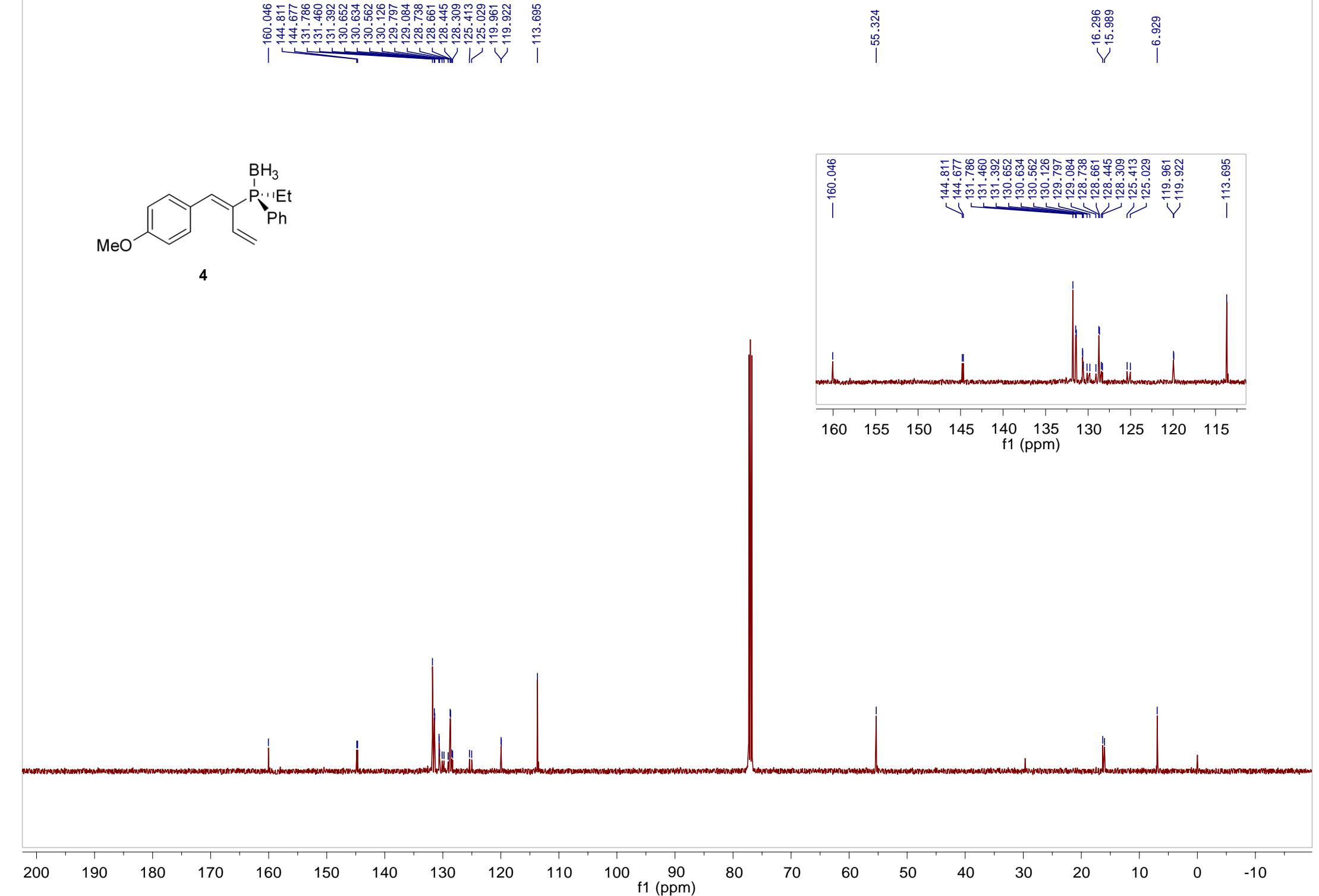
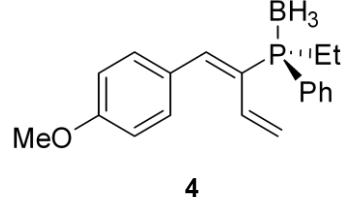


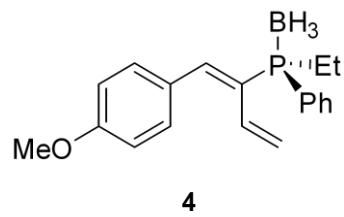


—34.452

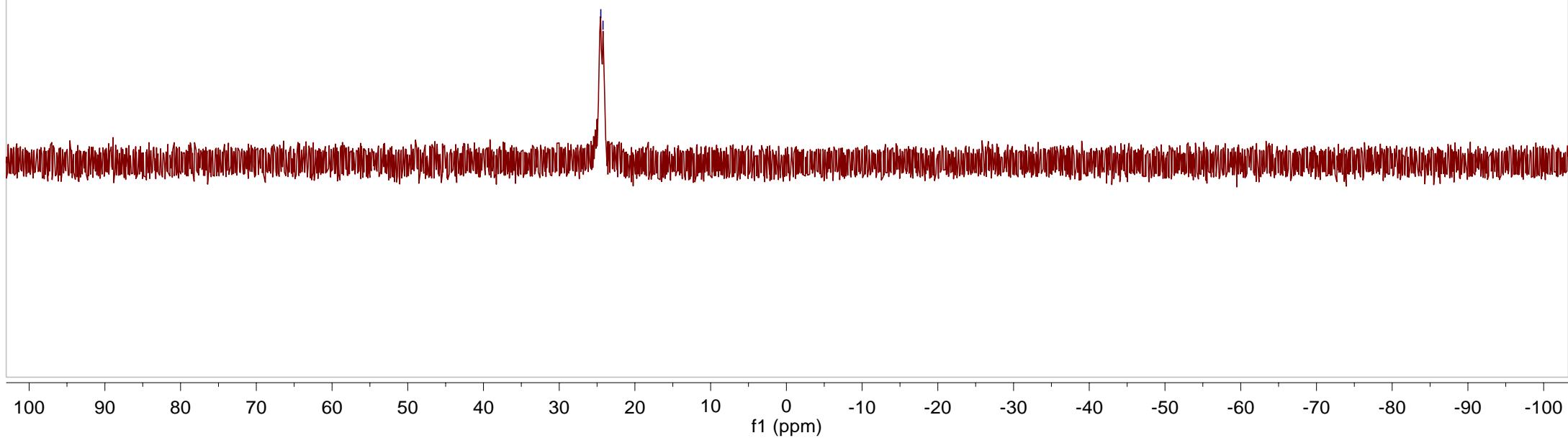


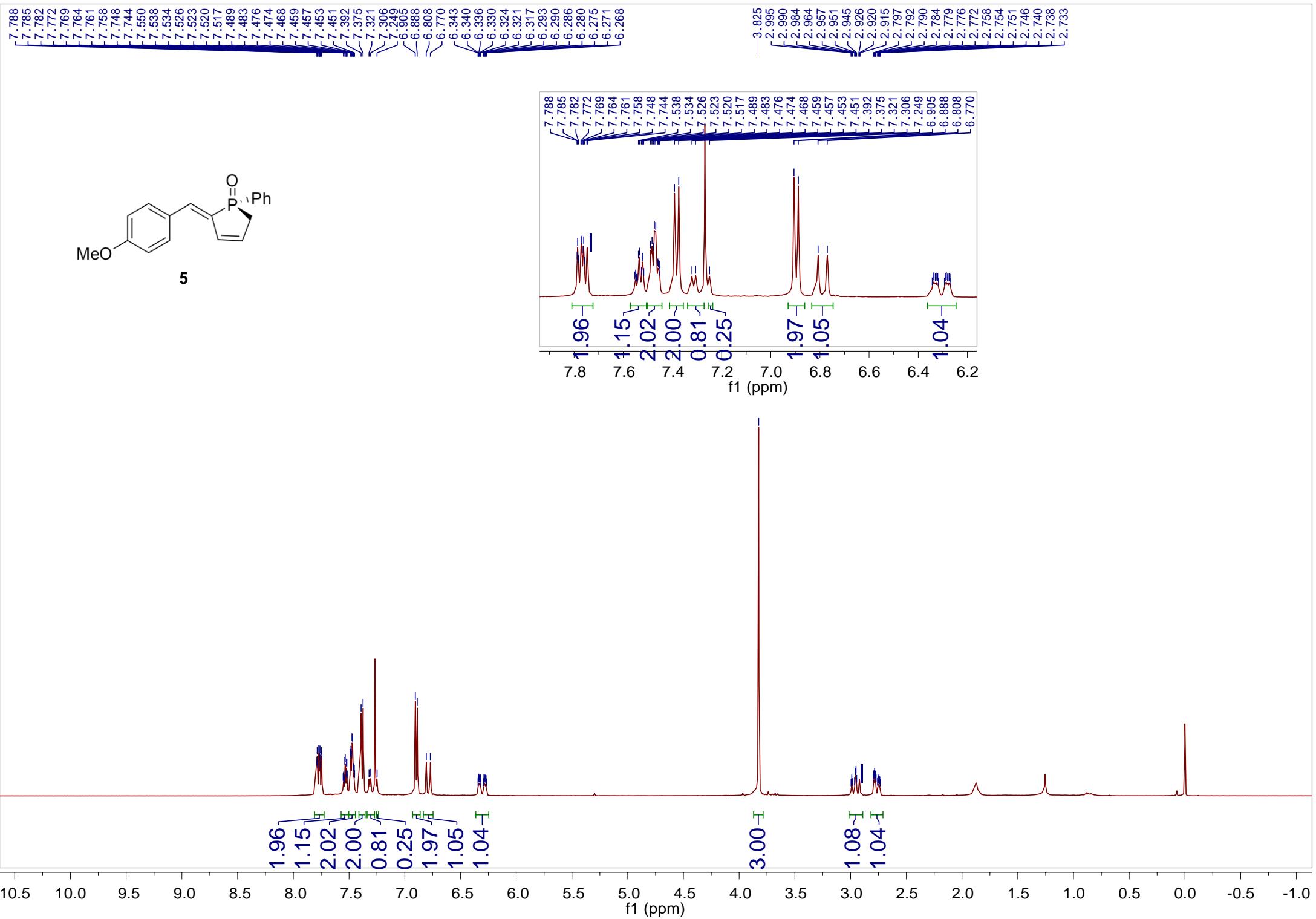






24.502
24.214





1.96

1.15

2.02

2.00

0.25

0.81

1.97

1.05

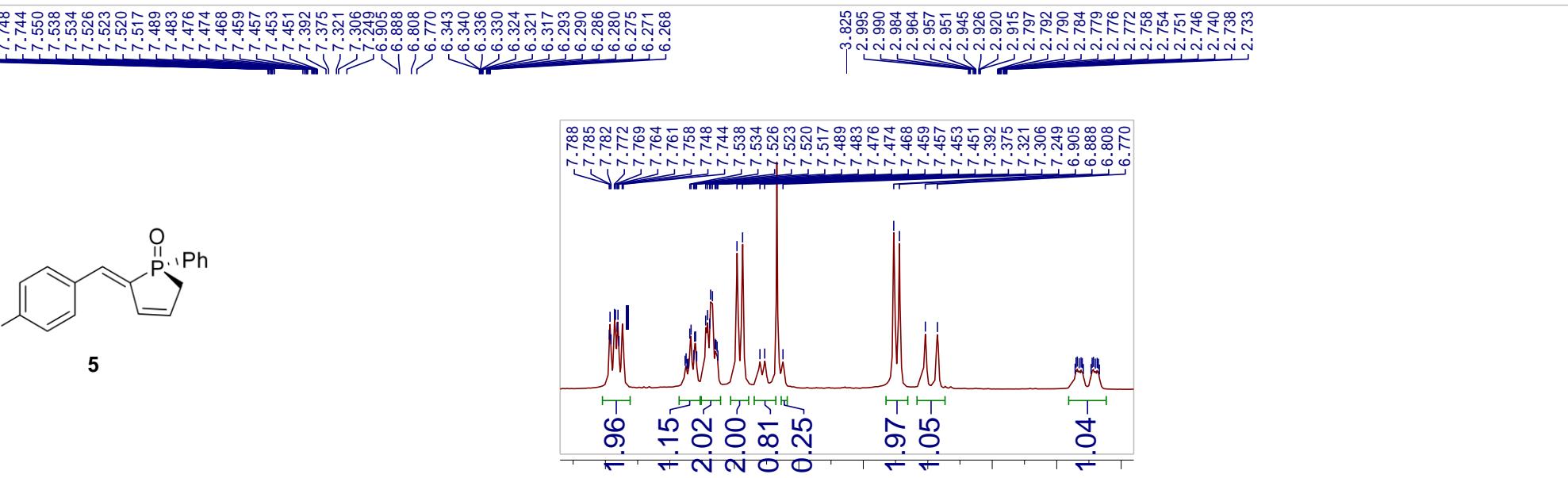
1.04

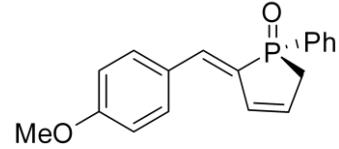
3.00

1.08

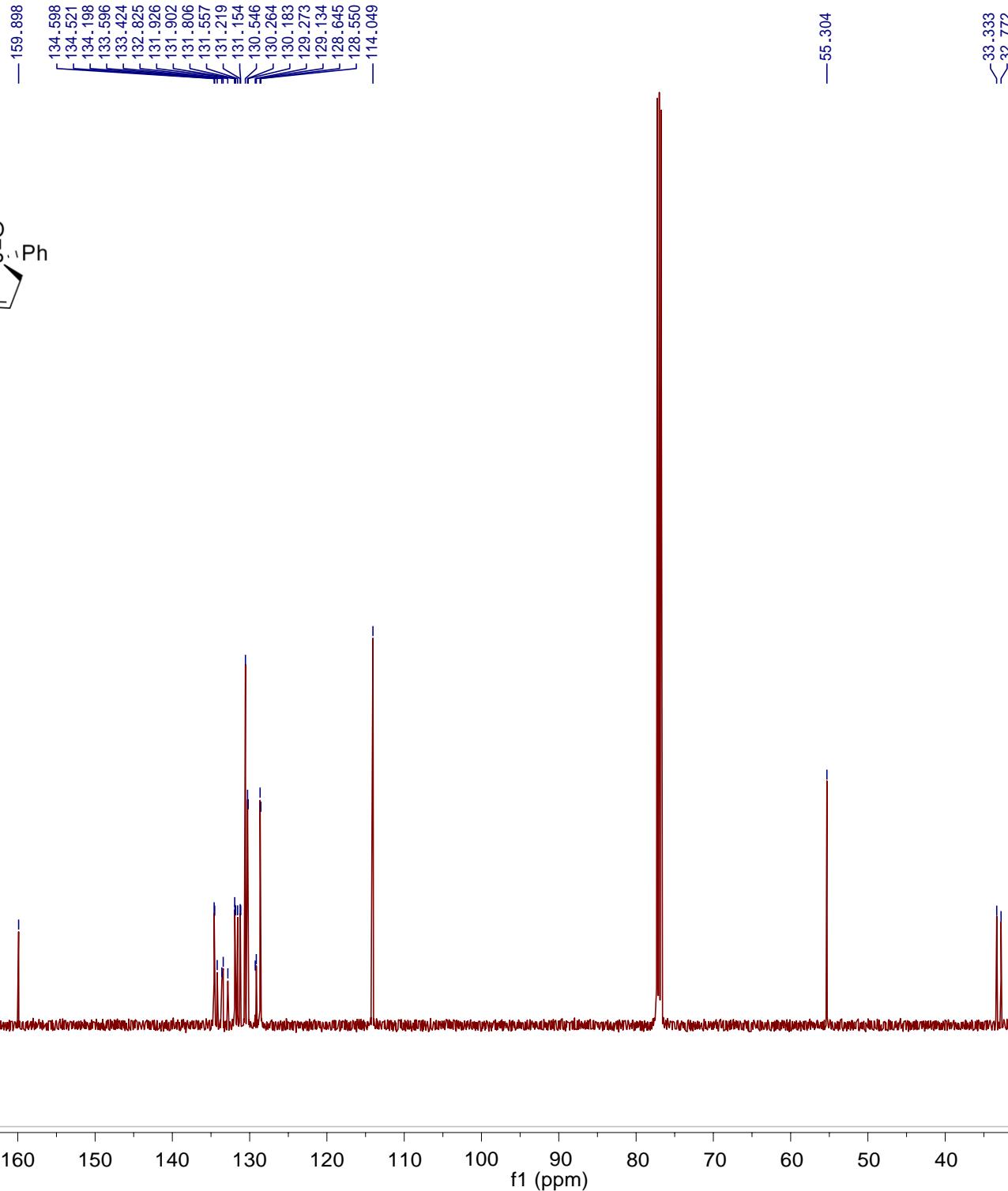
1.04

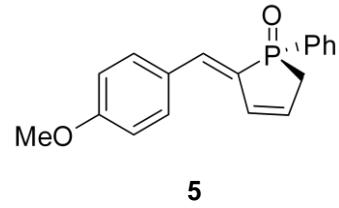
5





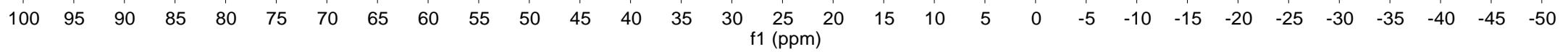
5





5

-45.359



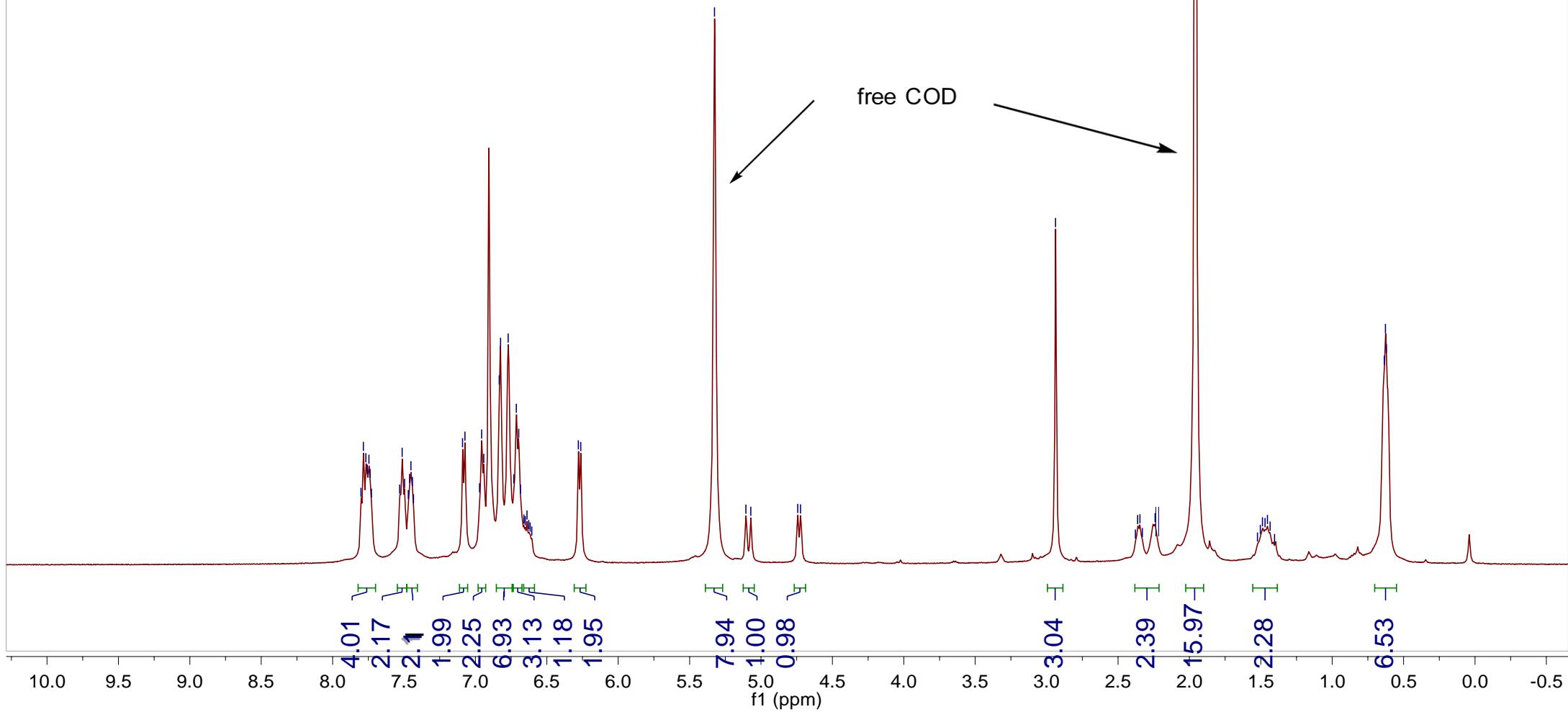
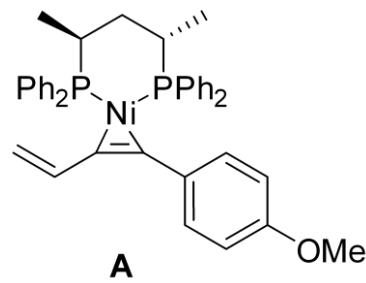
7.801
7.784
7.766
7.756
7.745
7.737
7.727
7.530
7.513
7.495
7.469
7.433
7.408
7.373
7.341
7.309
7.277
7.241
7.209
7.177
7.144
7.113
6.941
6.833
6.823
6.770
6.730
6.713
6.696
6.684
6.660
6.650
6.638
6.626
6.616
6.605
6.278
6.262

-5.325
5.105
5.071
4.742
4.723

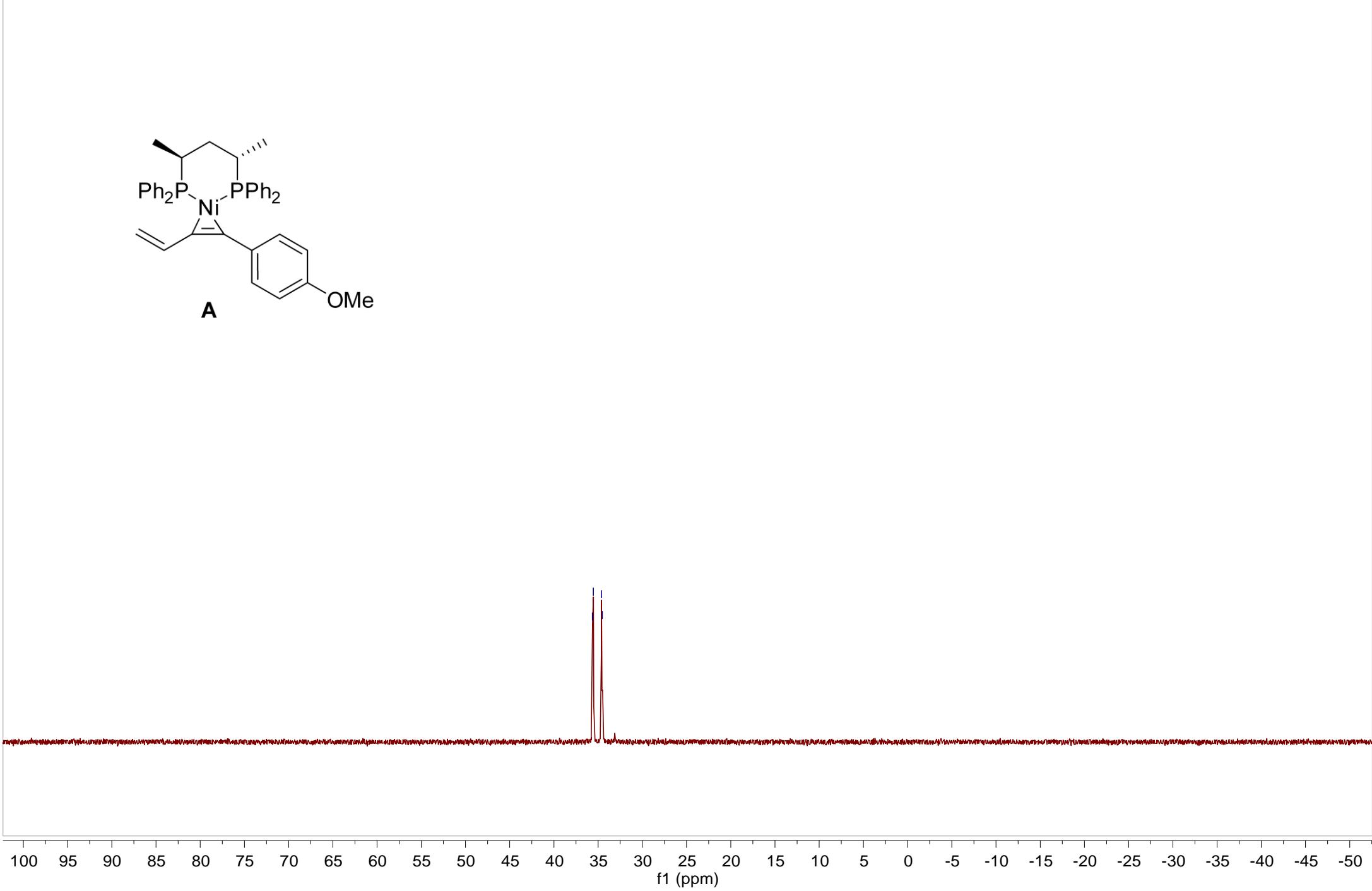
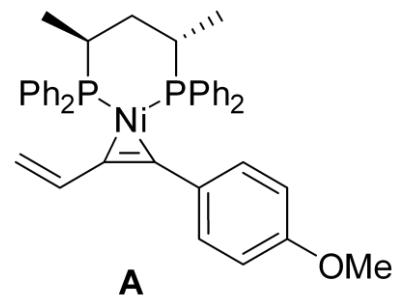
-2.937
2.377
2.362
2.345
2.329
2.271
2.256
2.240
2.223
1.558

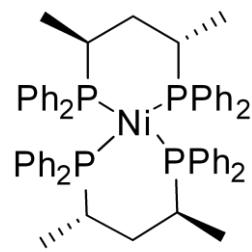
1.523
1.503
1.488
1.469
1.453
1.435
1.404

0.635
0.627
0.620

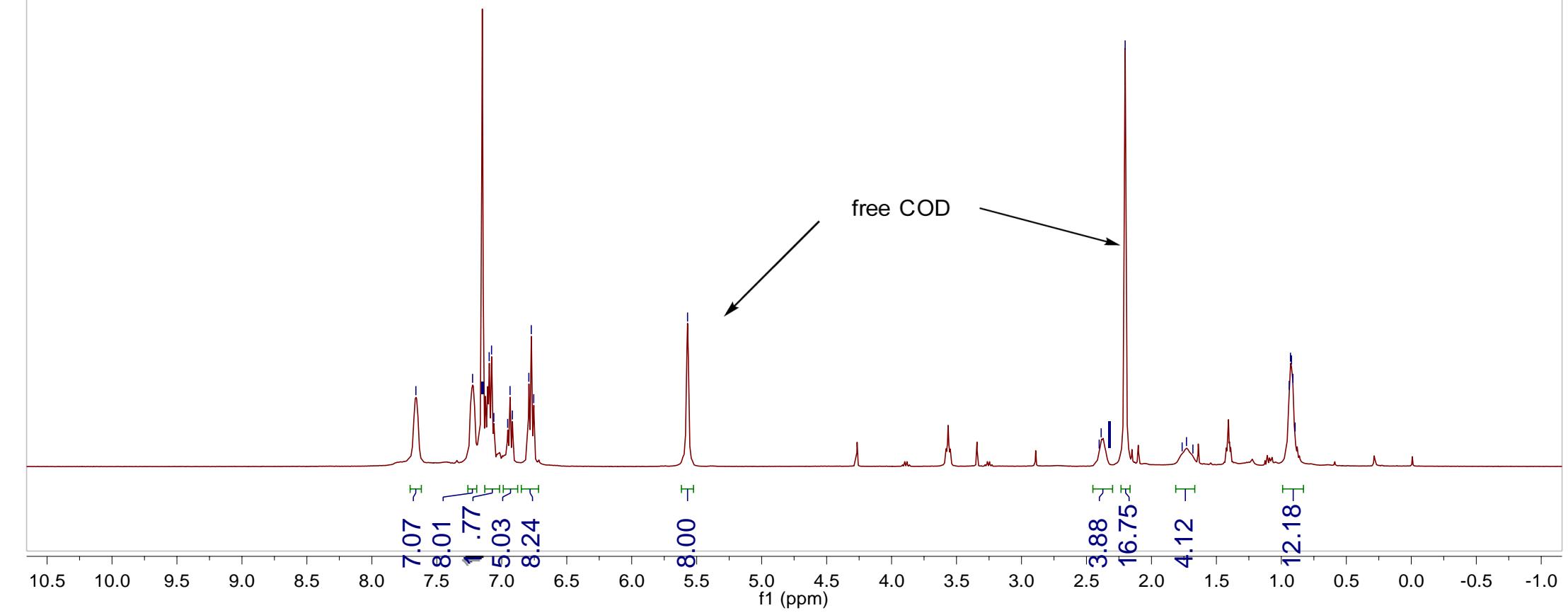
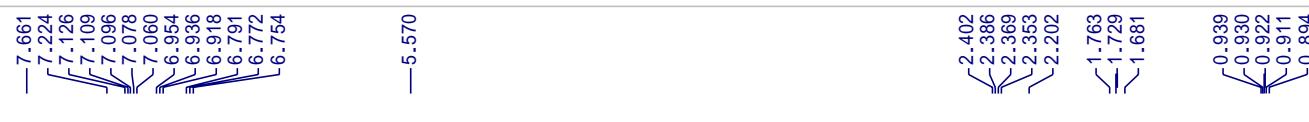


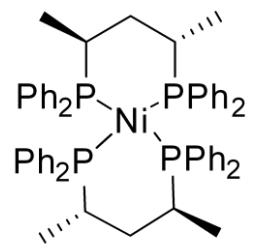
-35.635
-35.535
-34.619
-34.520





B



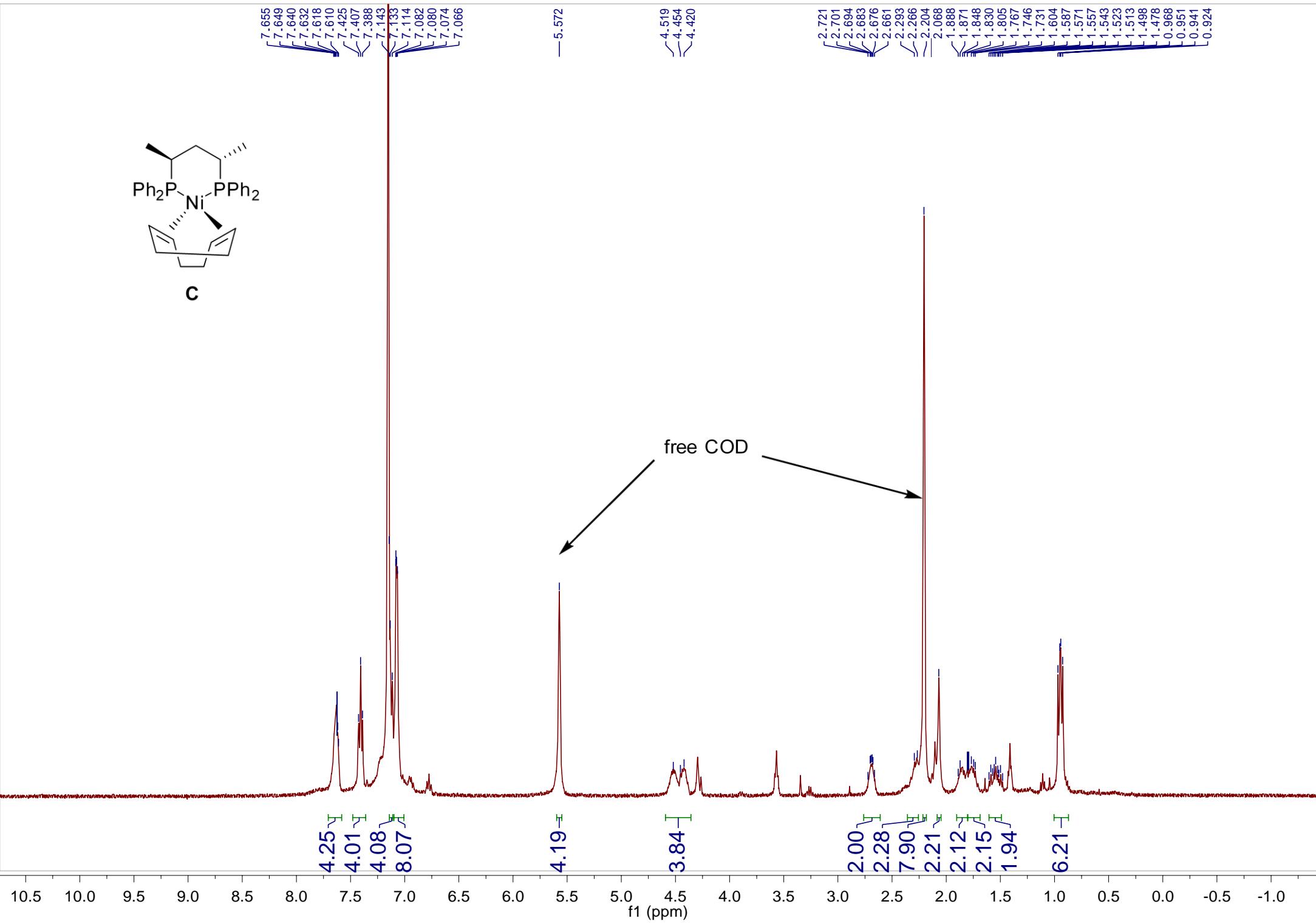
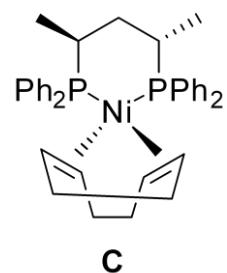


B

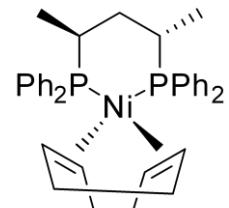
-28.036

100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50

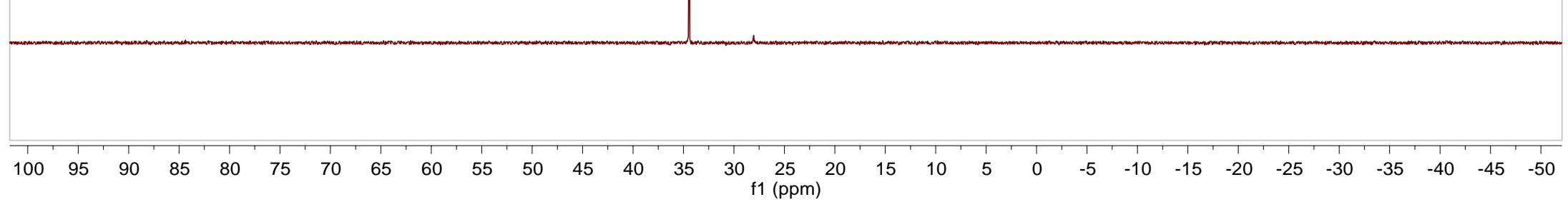
f1 (ppm)

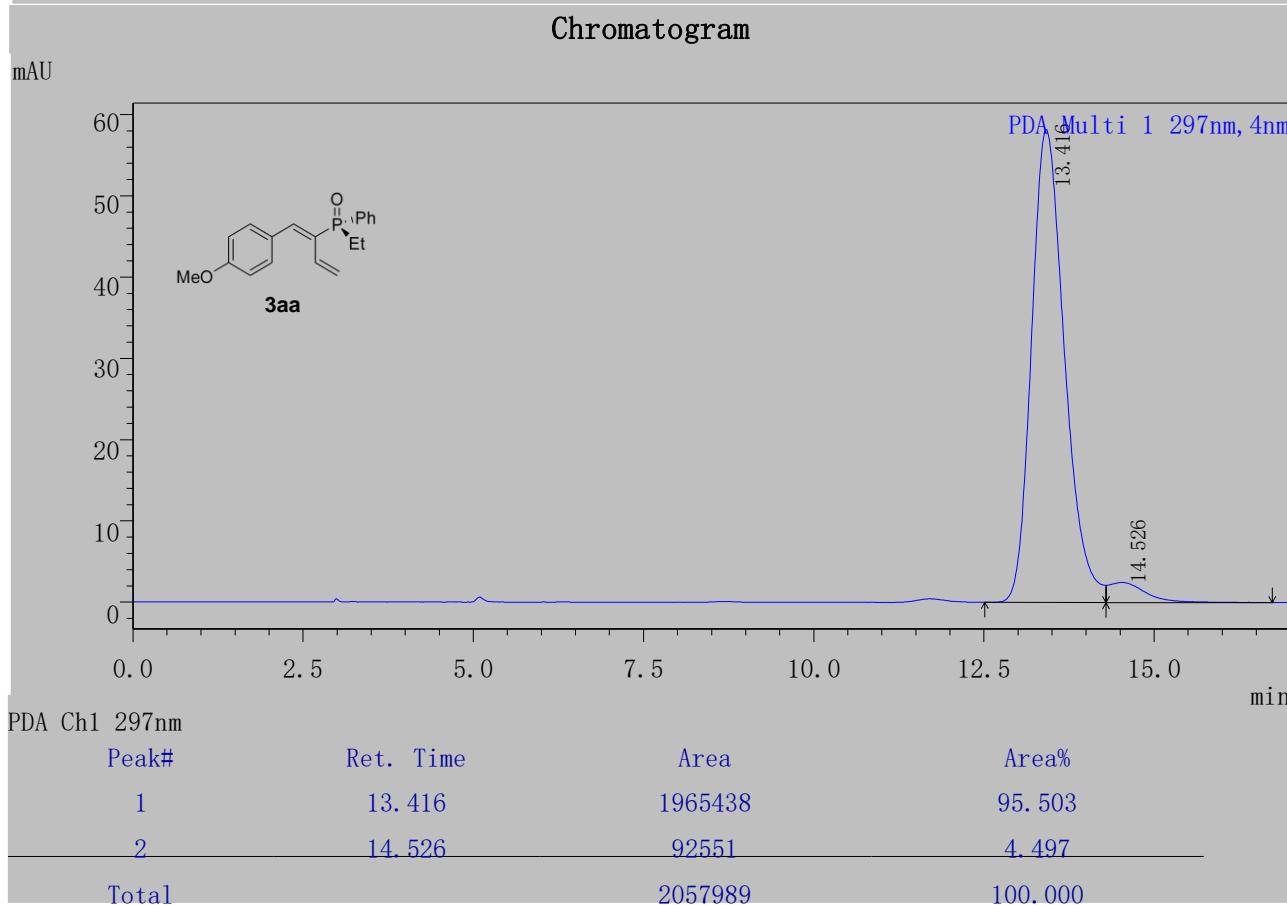
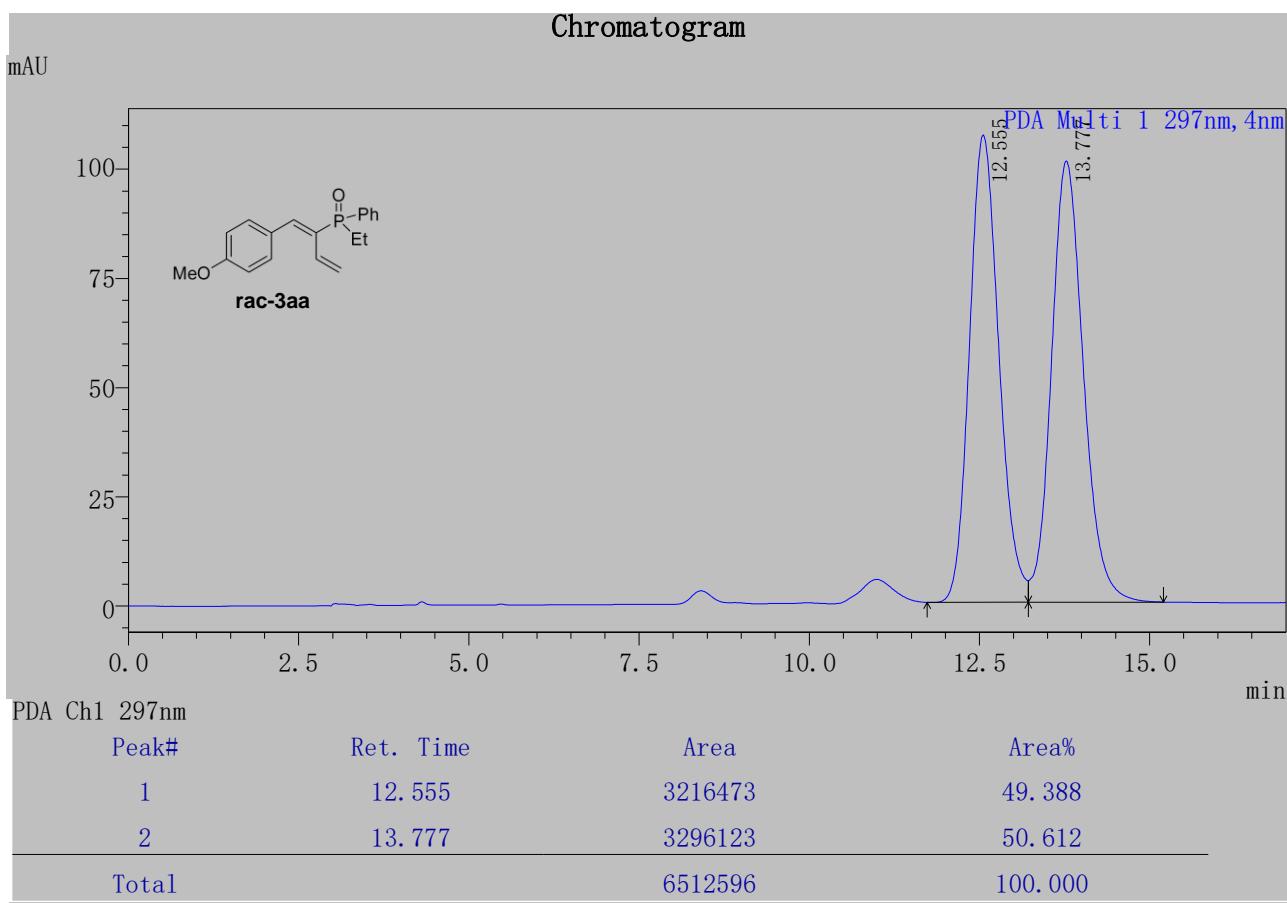


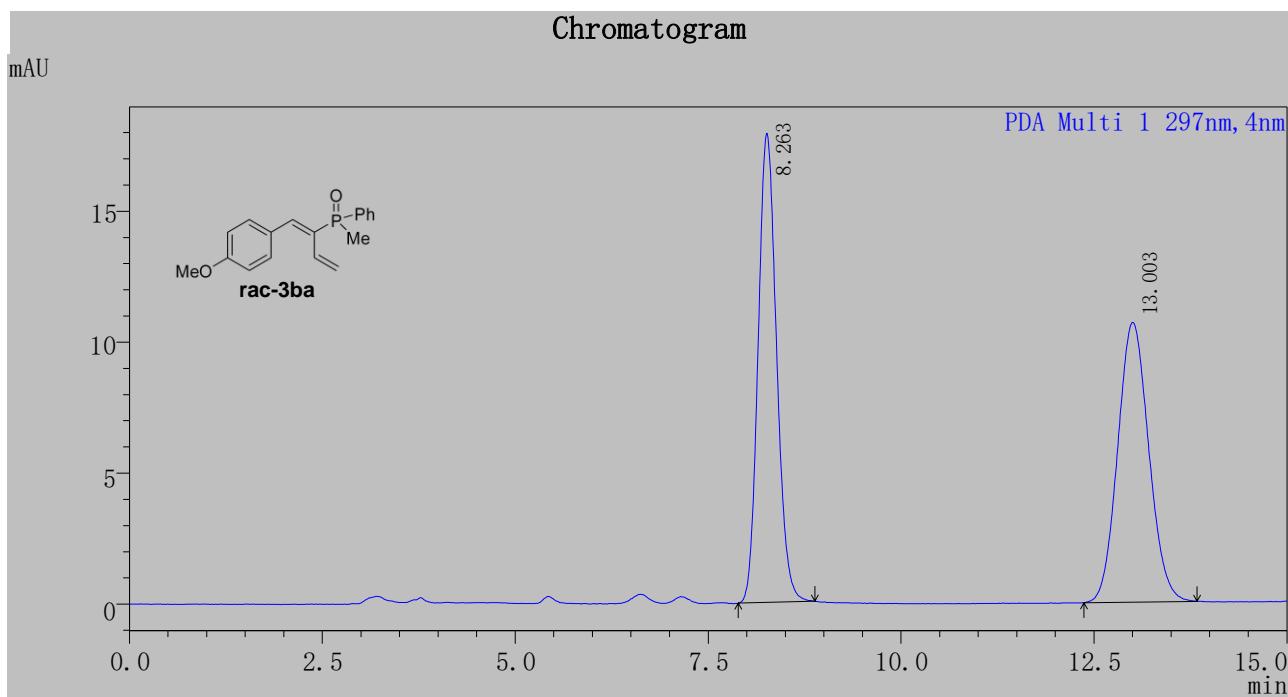
-34.422



C

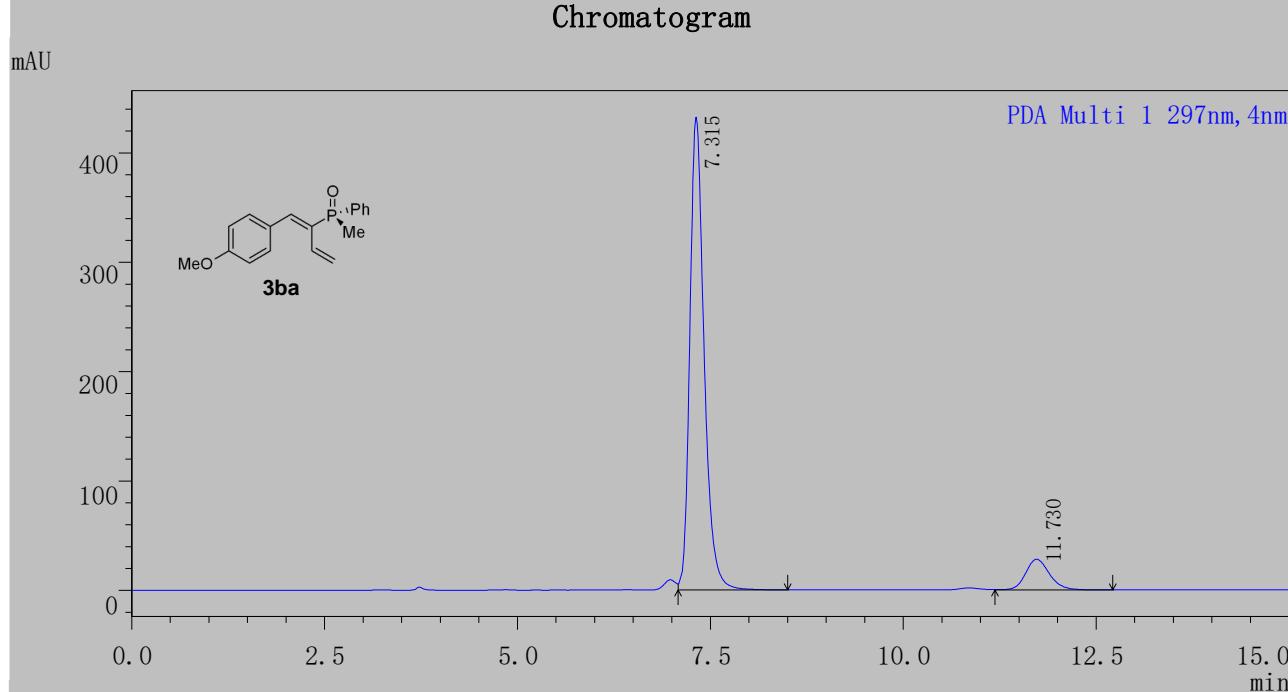






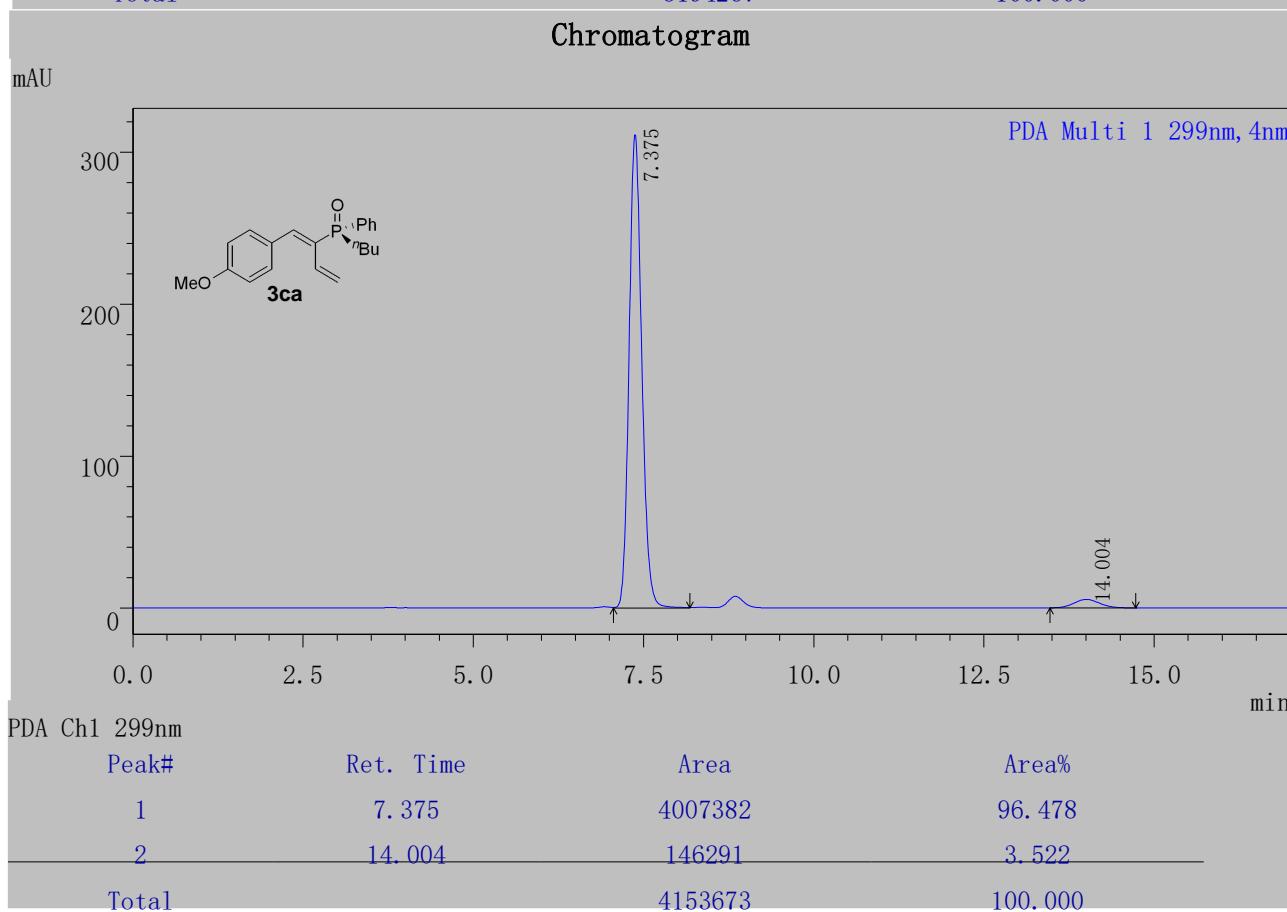
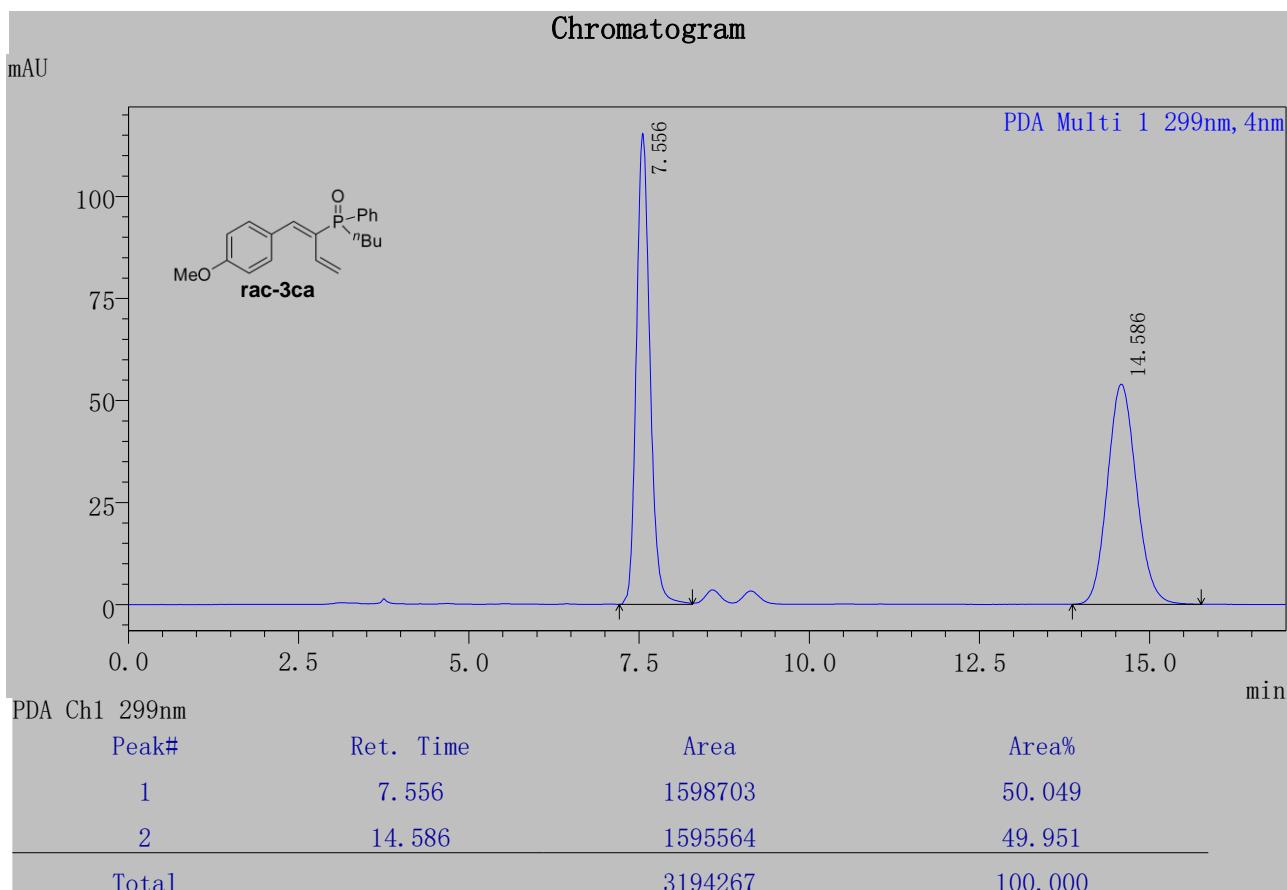
PDA Ch1 297nm

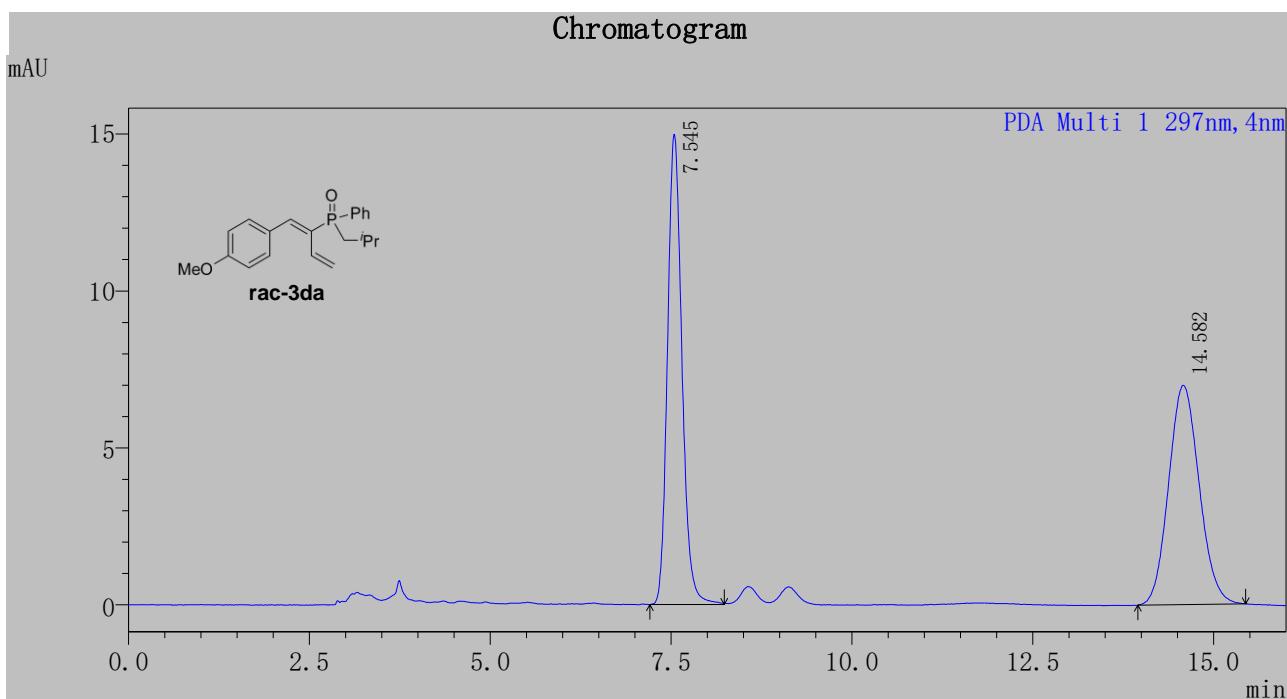
Peak#	Ret. Time	Area	Area%
1	8.263	297537	49.869
2	13.003	299102	50.131
Total		596638	100.000



PDA Ch1 297nm

Peak#	Ret. Time	Area	Area%
1	7.315	5531584	90.137
2	11.730	605299	9.863
Total		6136883	100.000



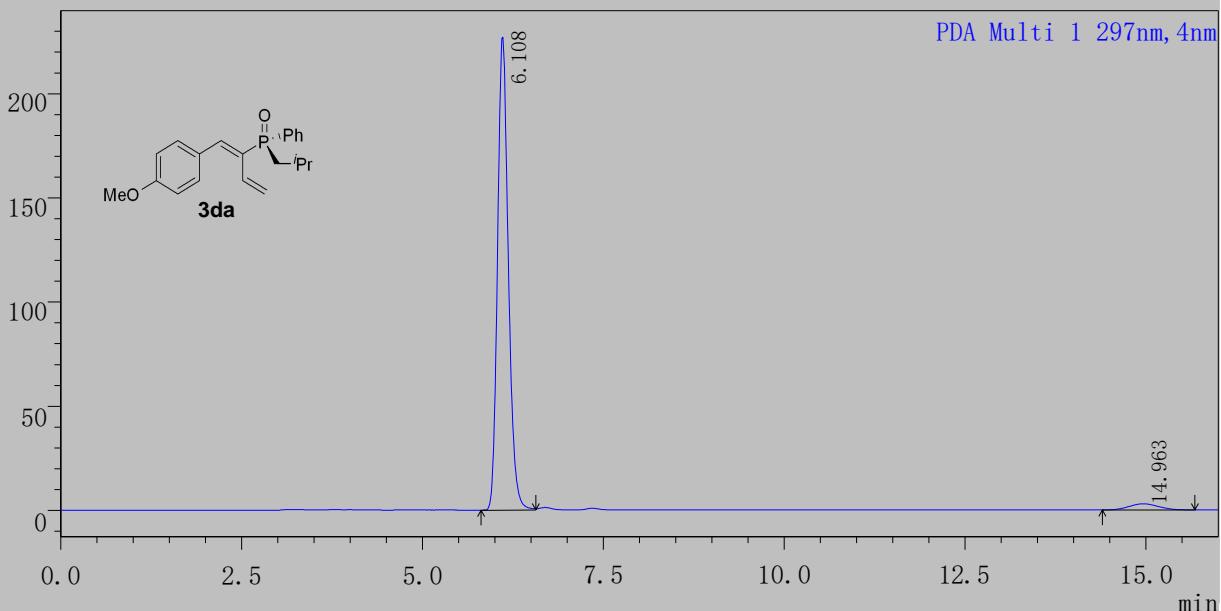


PDA Ch1 297nm

Peak#	Ret. Time	Area	Area%
1	7.545	207810	50.284
2	14.582	205463	49.716
Total		413273	100.000

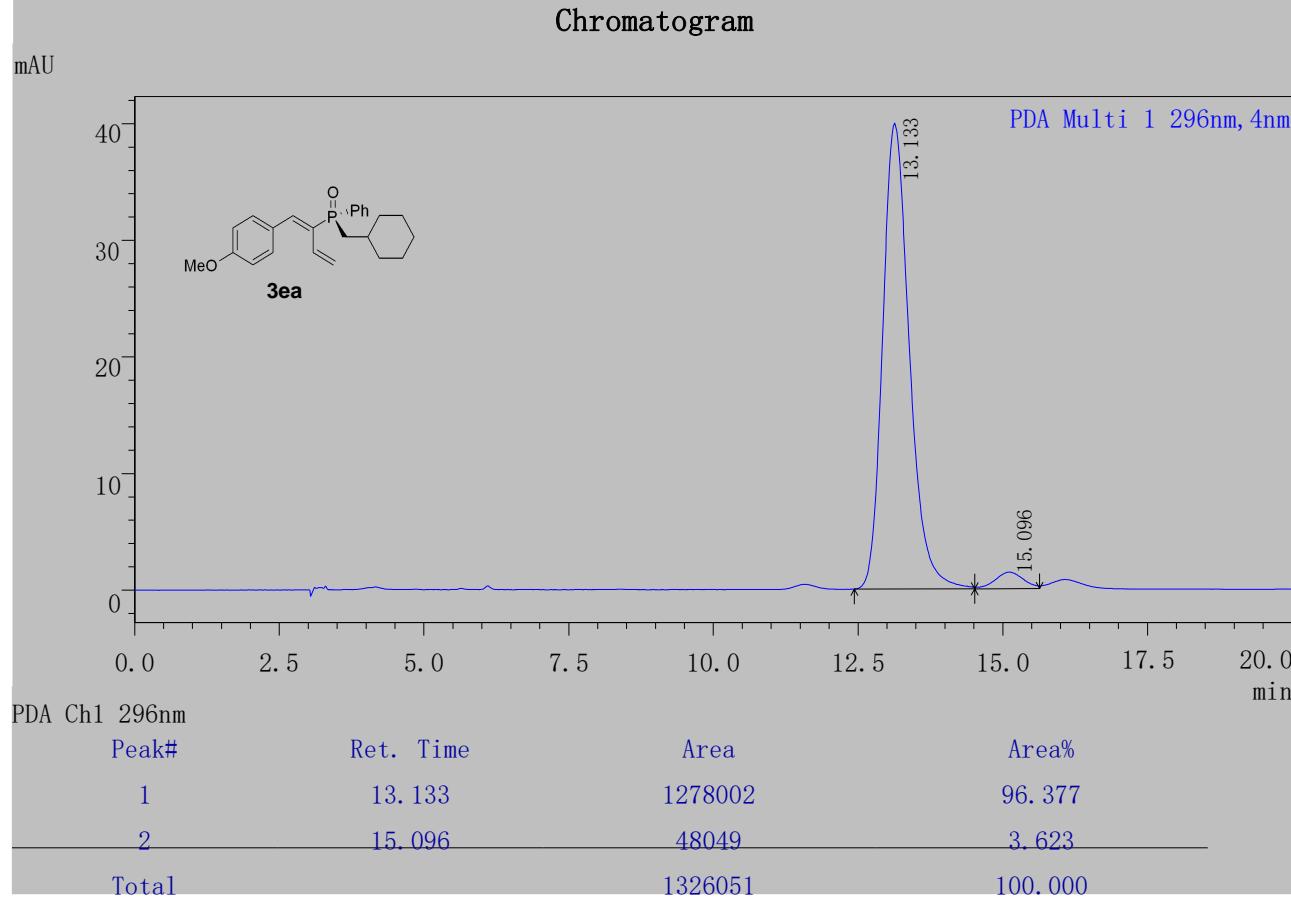
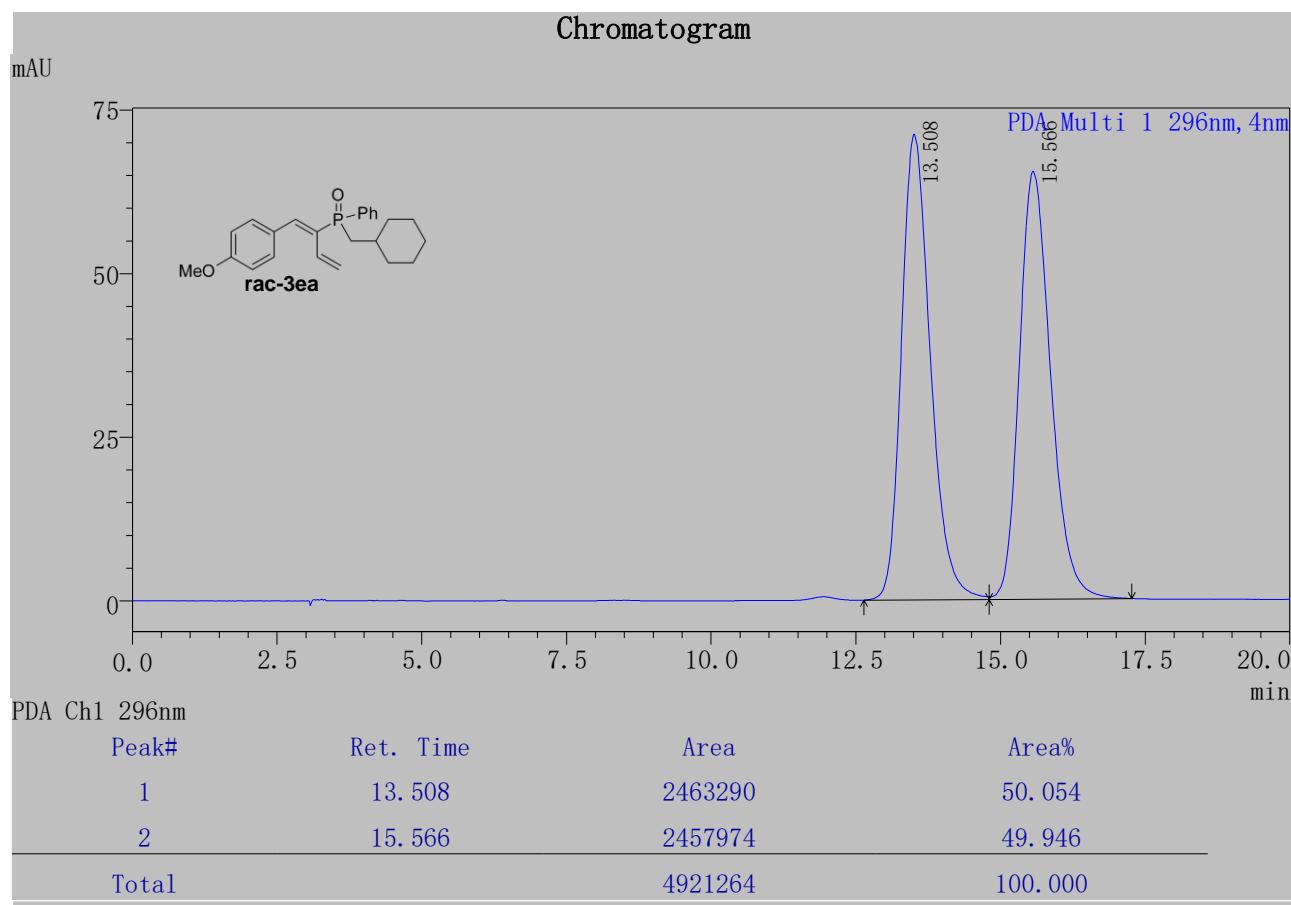
Chromatogram

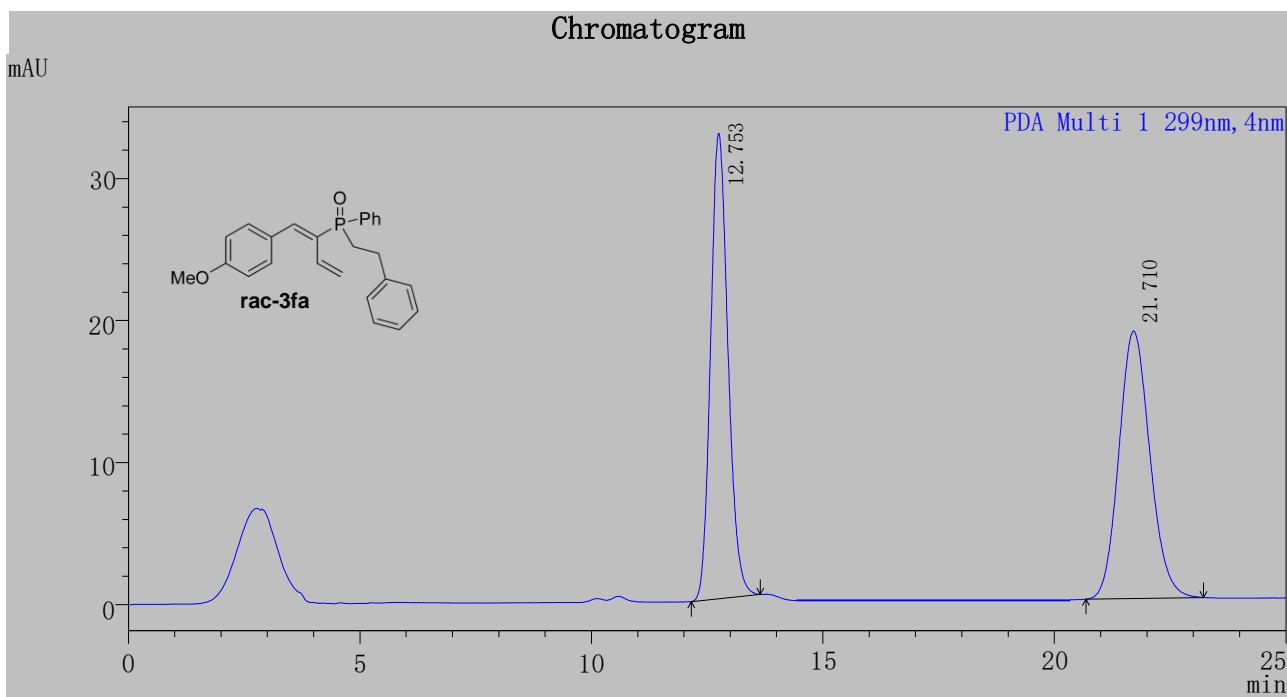
mAU



PDA Ch1 297nm

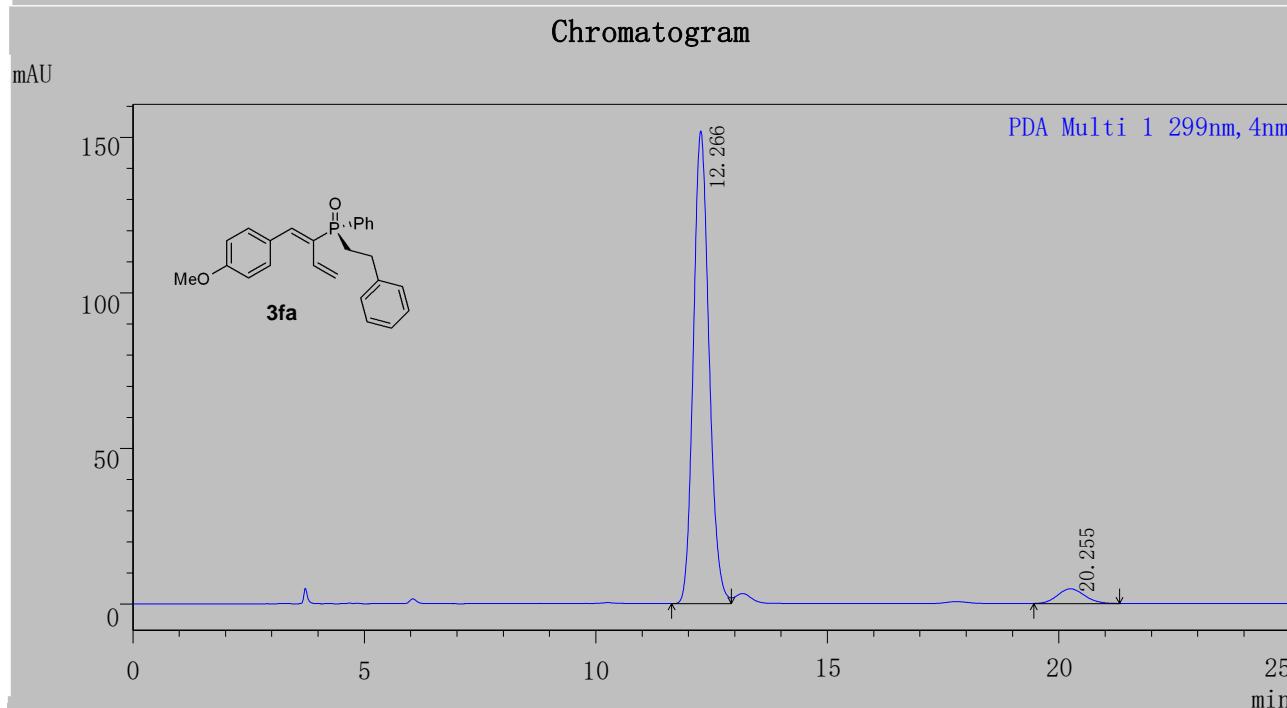
Peak#	Ret. Time	Area	Area%
1	6.108	2369362	96.545
2	14.963	84789	3.455
Total		2454151	100.000





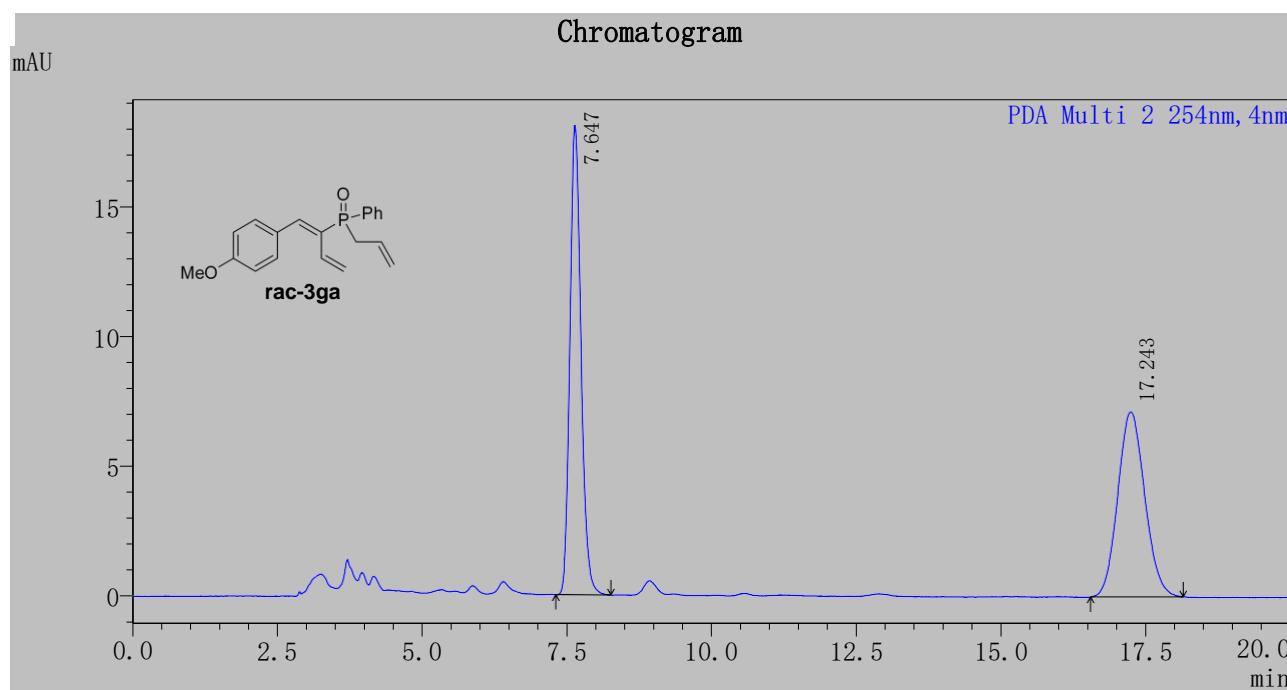
PDA Ch1 299nm

Peak#	Ret. Time	Area	Area%
1	12.753	860985	49.520
2	21.710	877677	50.480
Total		1738662	100.000

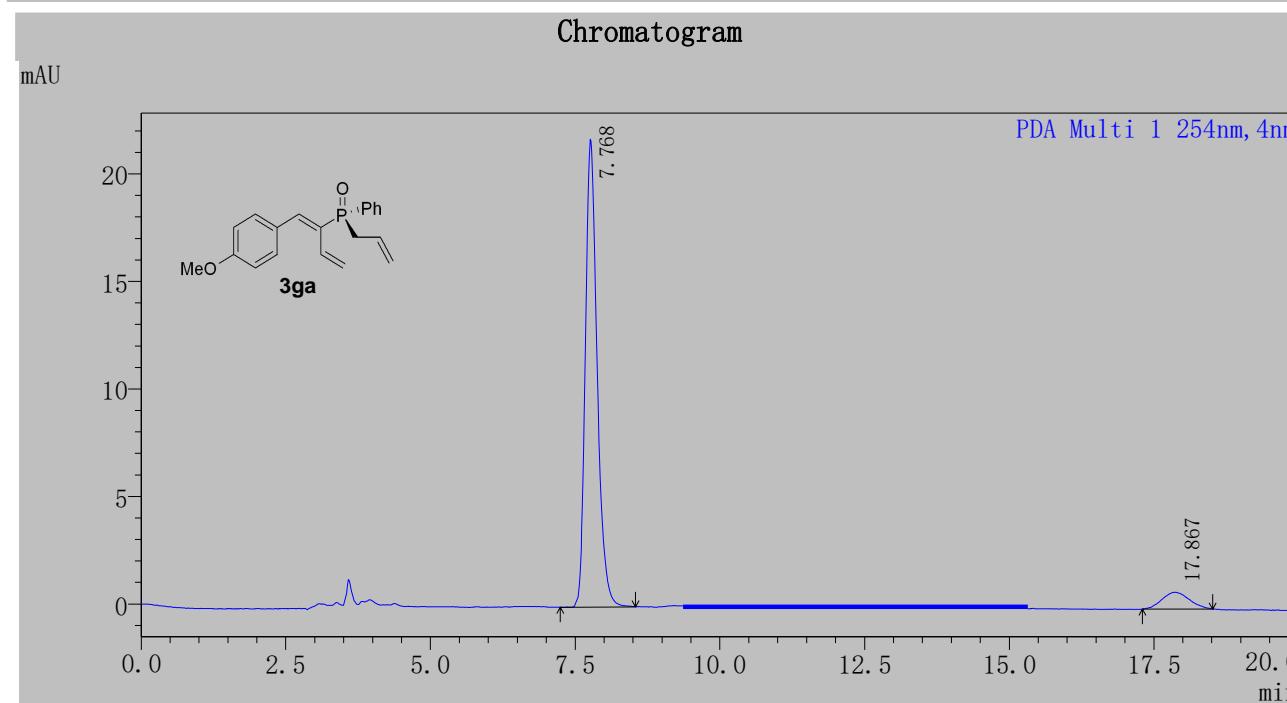


PDA Ch1 299nm

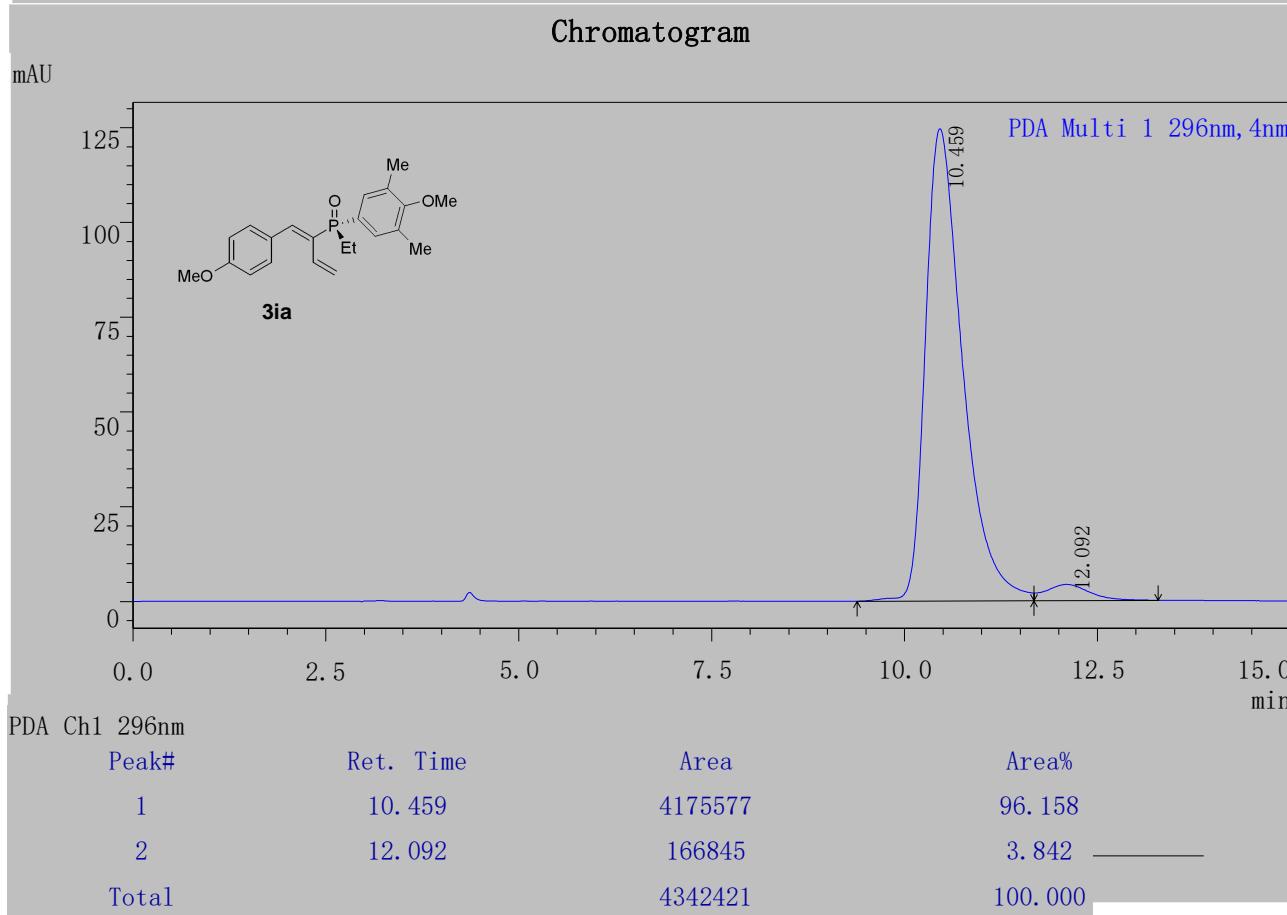
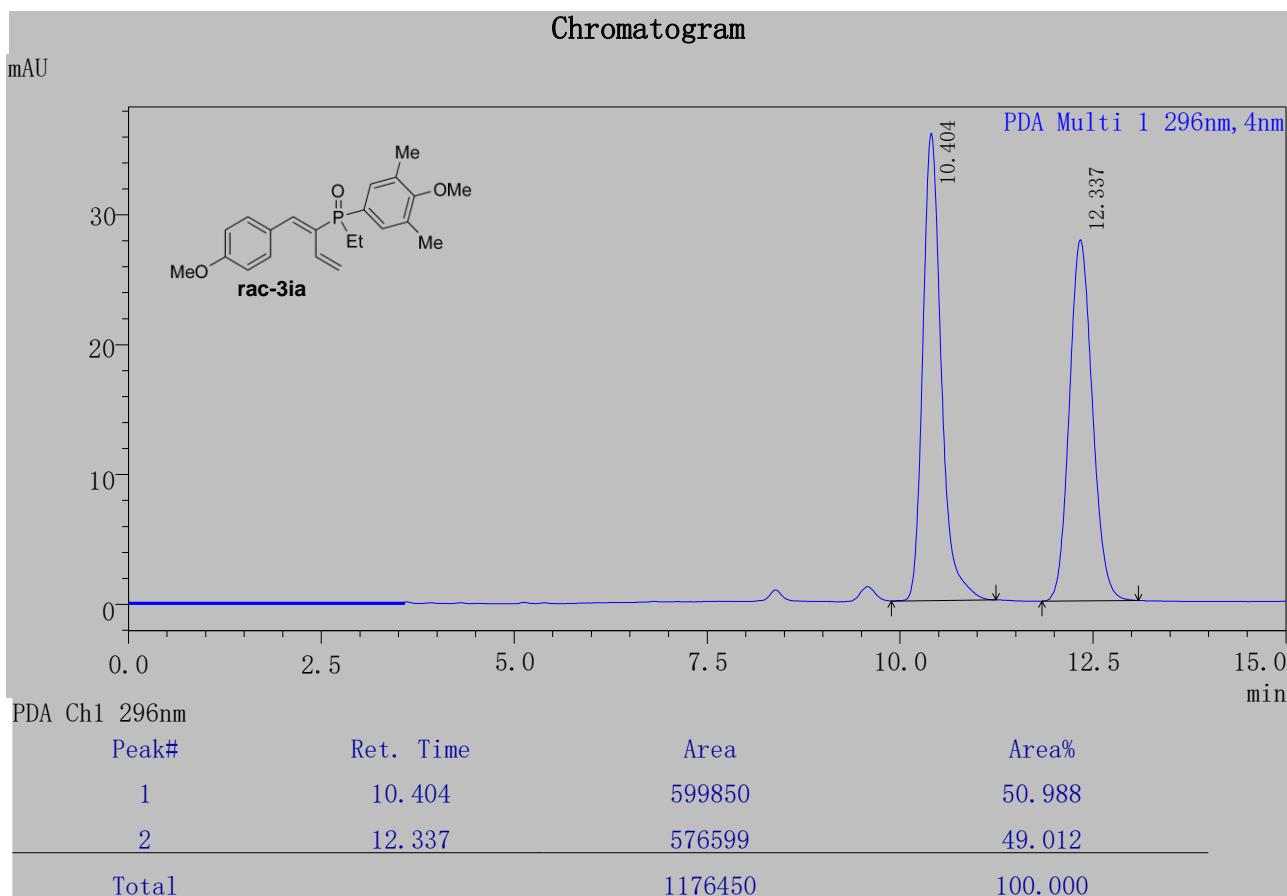
Peak#	Ret. Time	Area	Area%
1	12.266	3584795	94.930
2	20.255	191454	5.070
Total		3776249	100.000

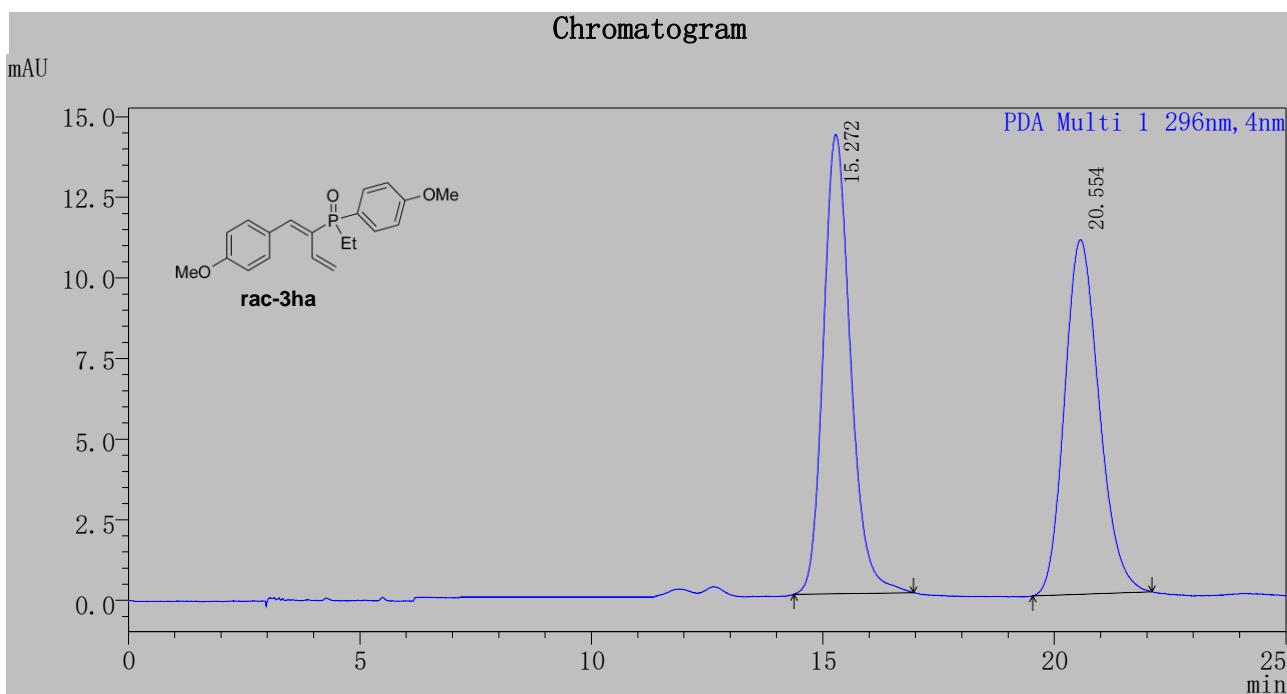


PDA Ch2 254nm			
Peak#	Ret. Time	Area	Area%
1	7.647	240978	51.084
2	17.243	230752	48.916
Total		471730	100.000



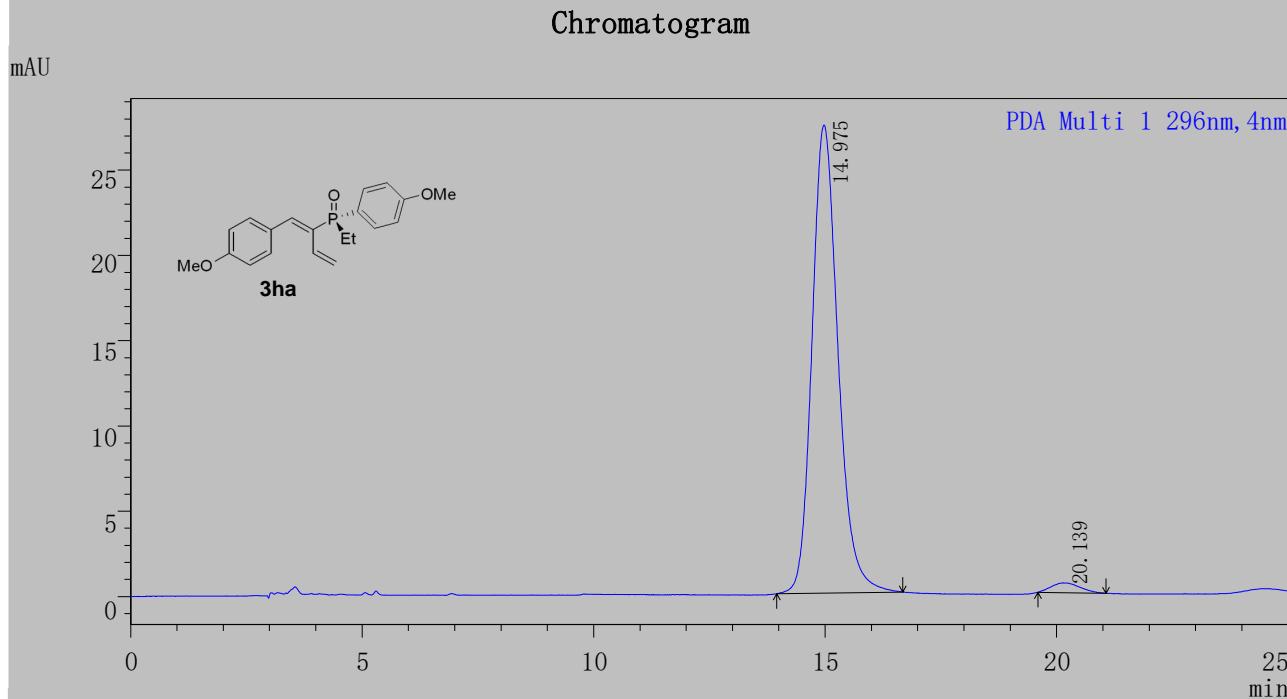
PDA Ch1 254nm			
Peak#	Ret. Time	Area	Area%
1	7.768	307909	92.384
2	17.867	25383	7.616
Total		333292	100.000





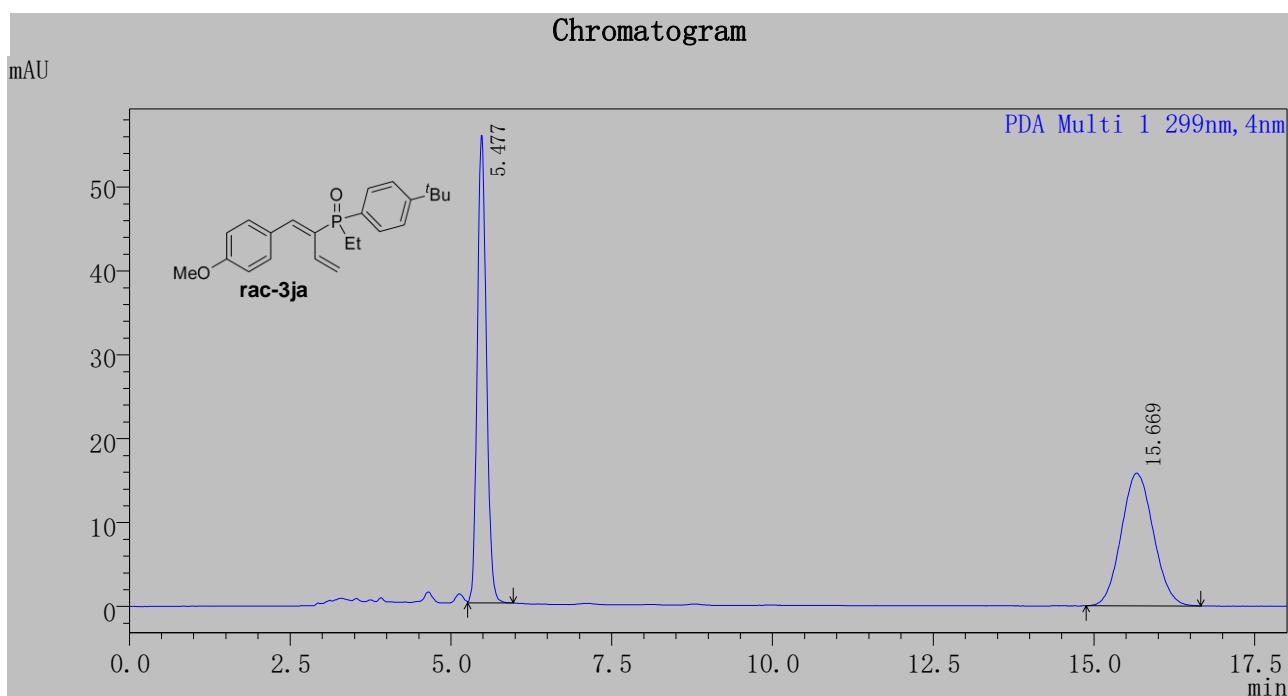
PDA Ch1 296nm

Peak#	Ret. Time	Area	Area%
1	15.272	580456	50.446
2	20.554	570184	49.554
Total		1150640	100.000



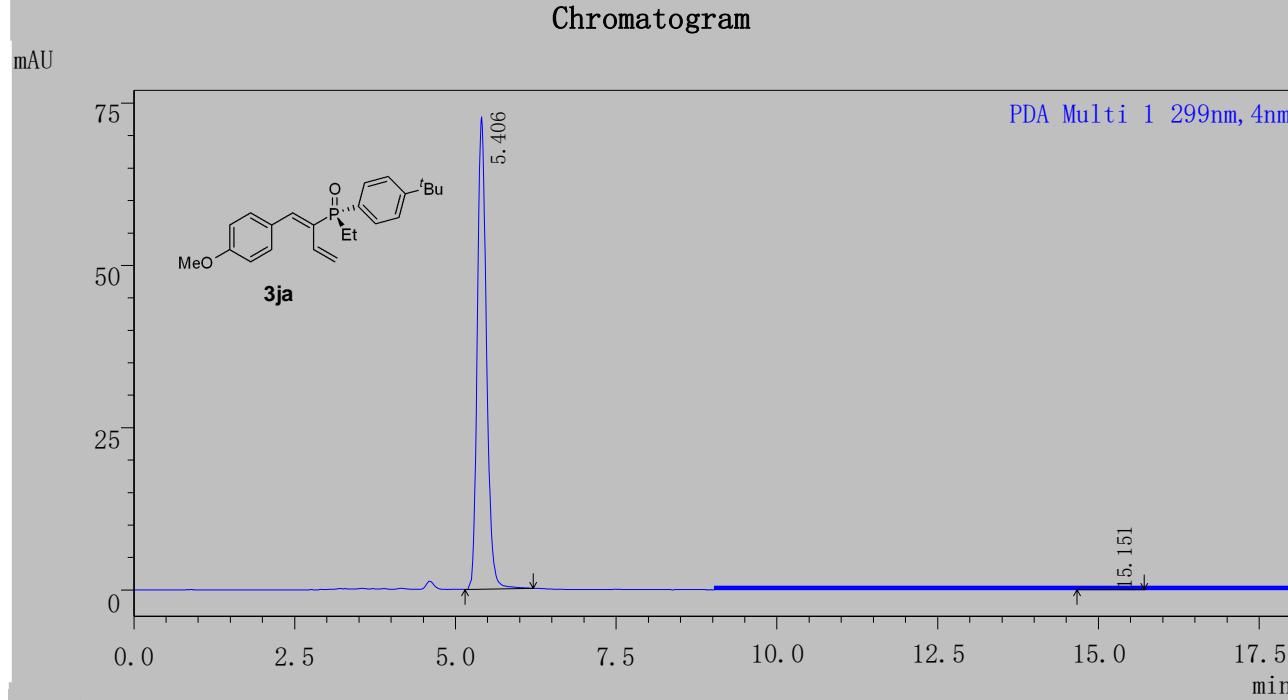
PDA Ch1 296nm

Peak#	Ret. Time	Area	Area%
1	14.975	1071506	97.719
2	20.139	25007	2.281
Total		1096513	100.000



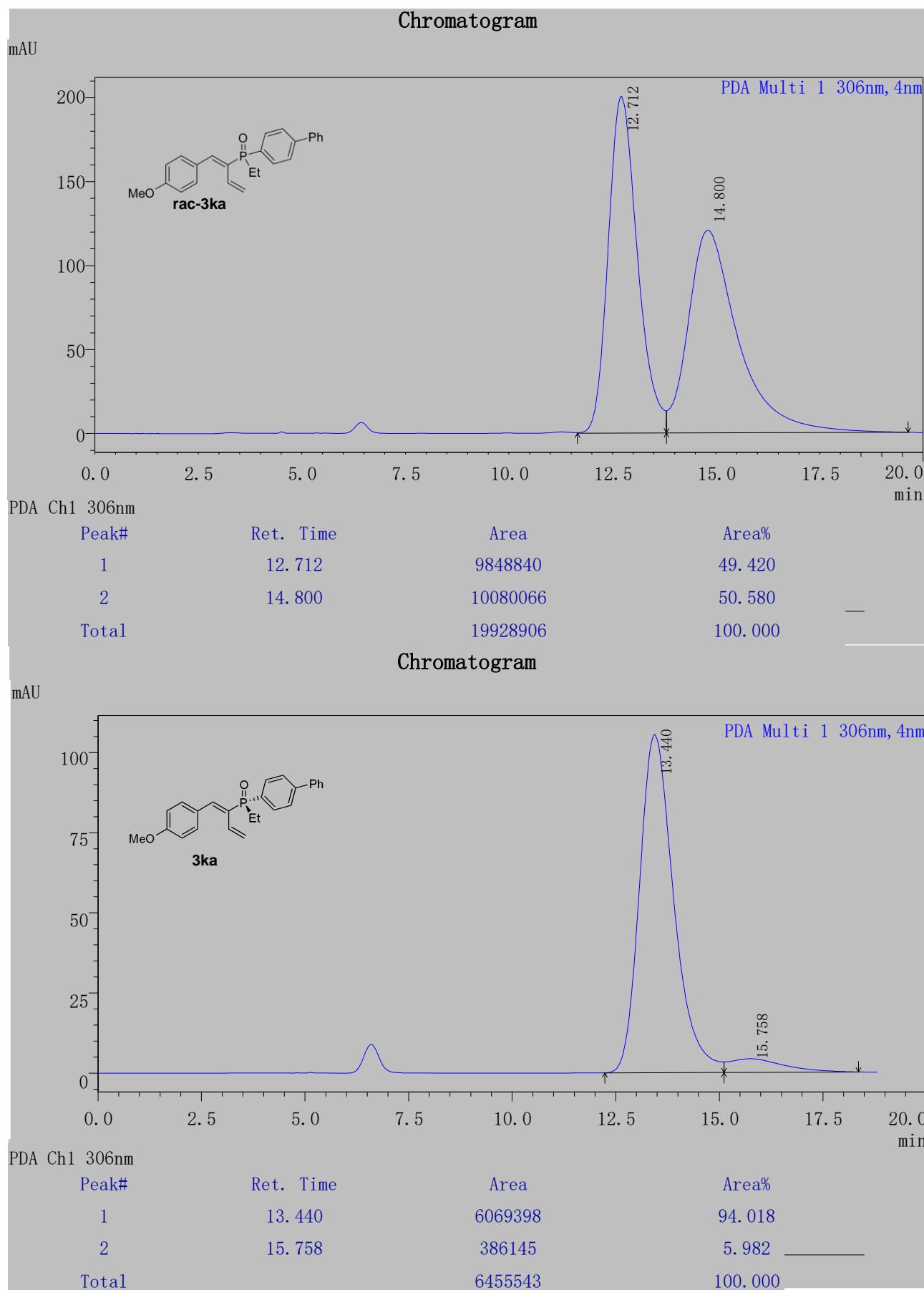
PDA Ch1 299nm

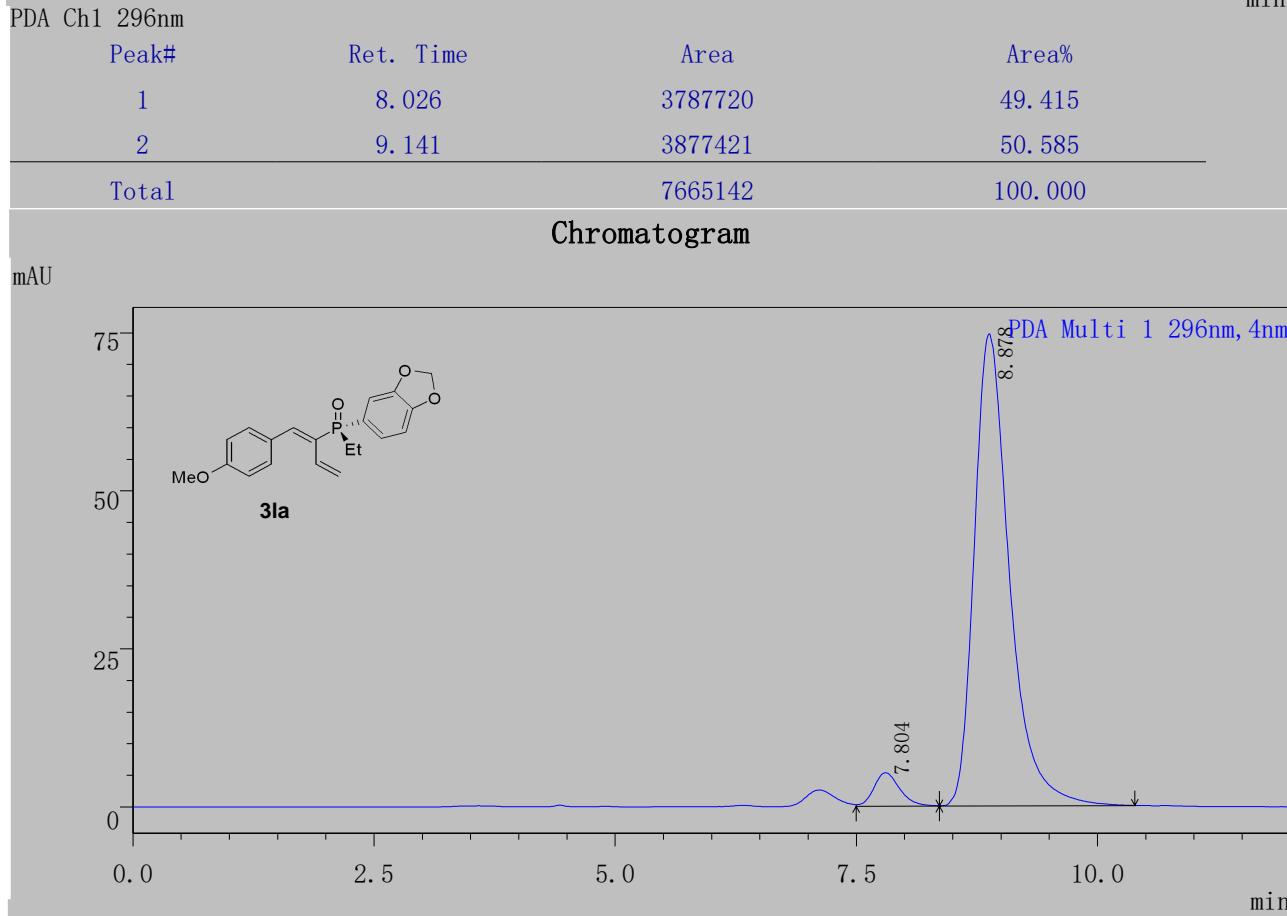
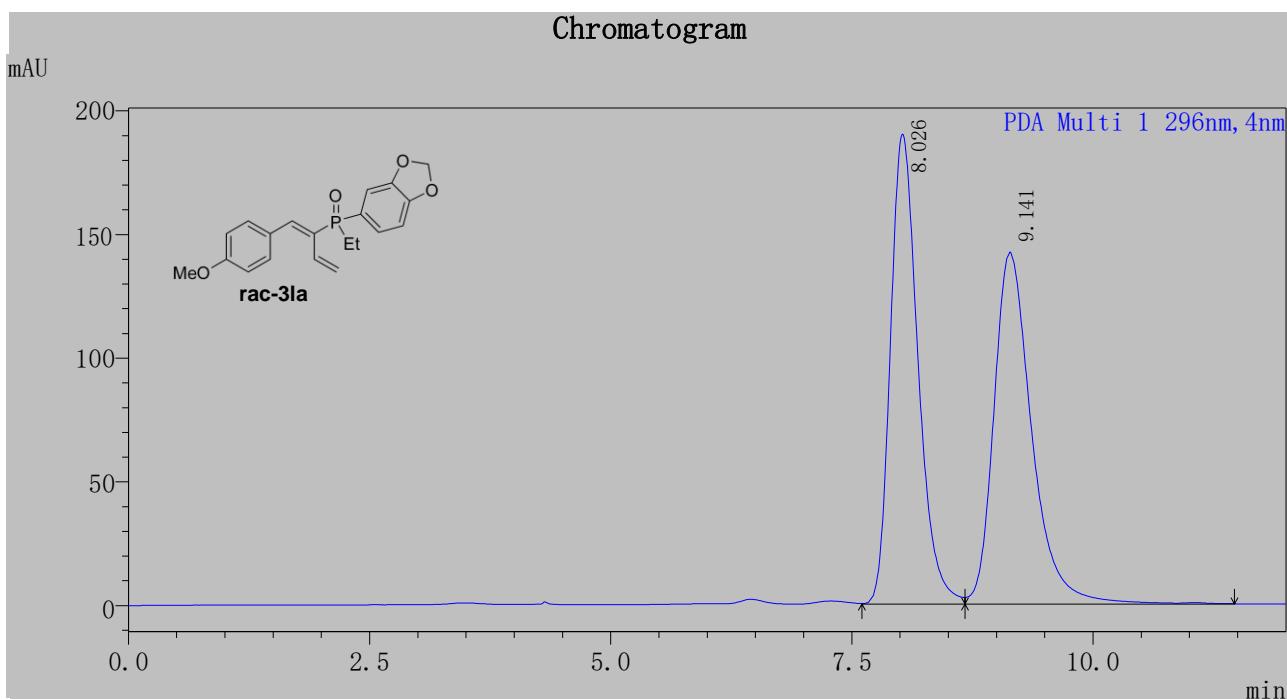
Peak#	Ret. Time	Area	Area%
1	5.477	550109	50.005
2	15.669	550004	49.995
Total		1100113	100.000

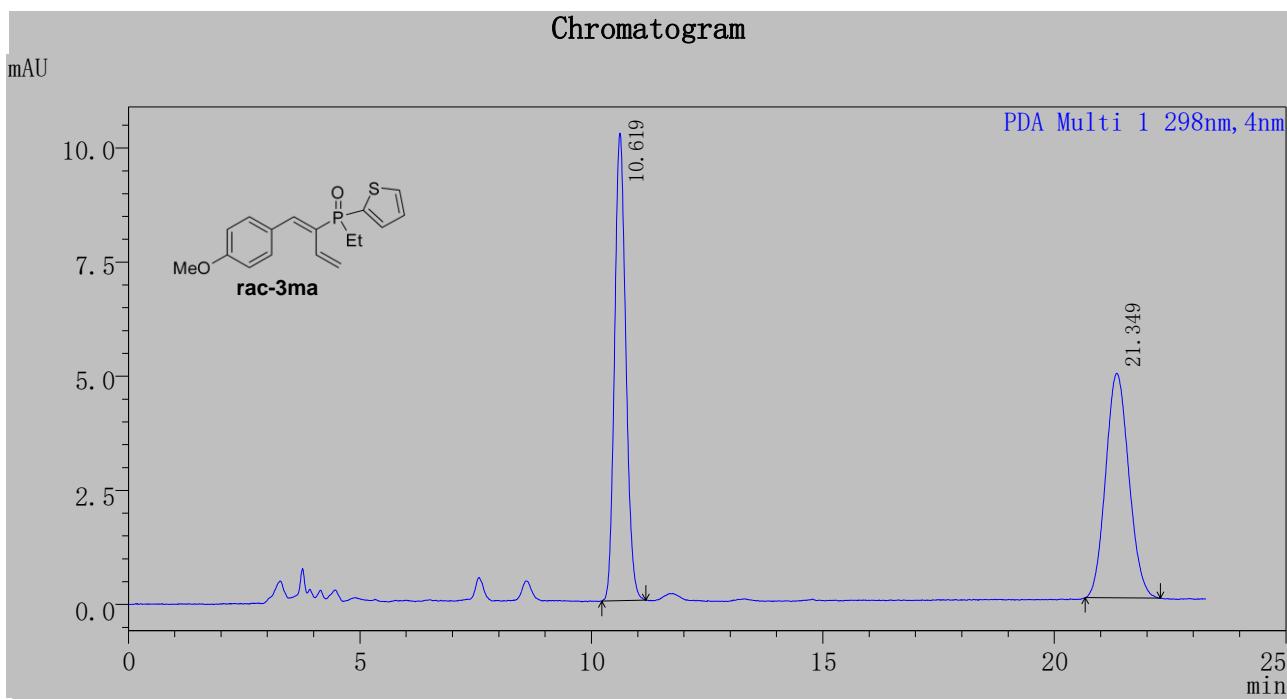


PDA Ch1 299nm

Peak#	Ret. Time	Area	Area%
1	5.406	724363	97.726
2	15.151	16853	2.274
Total		741216	100.000

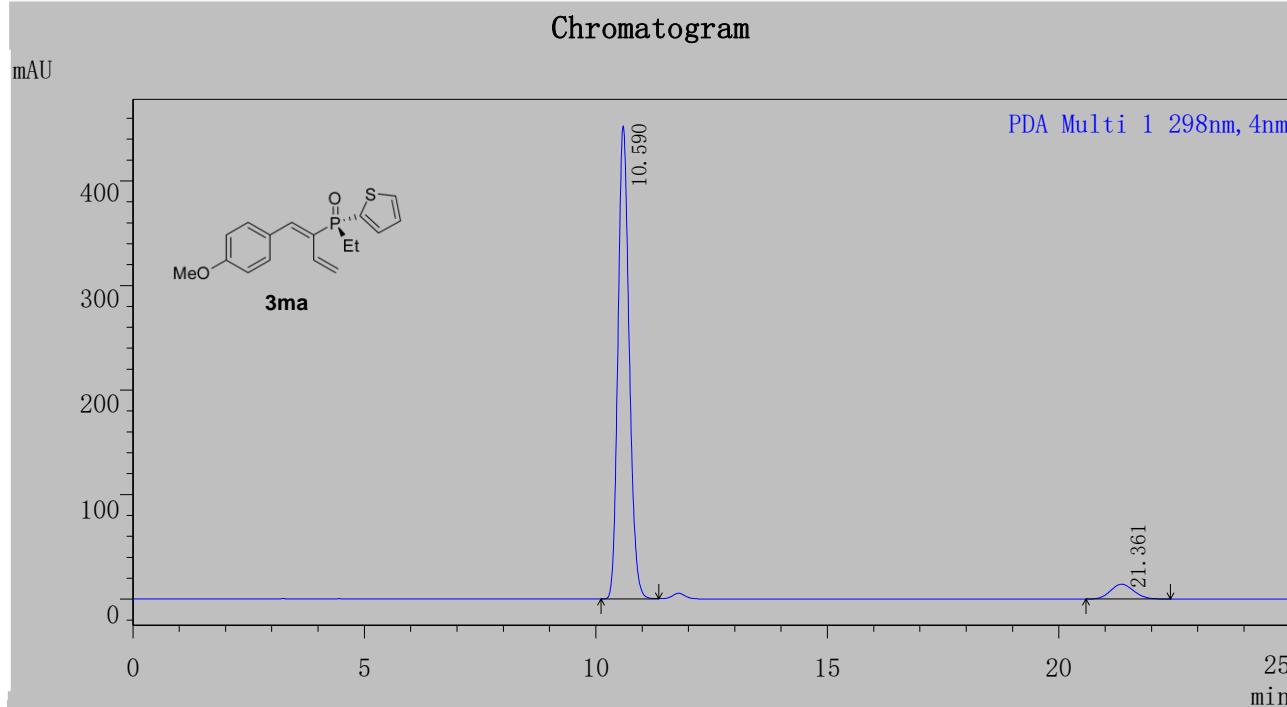






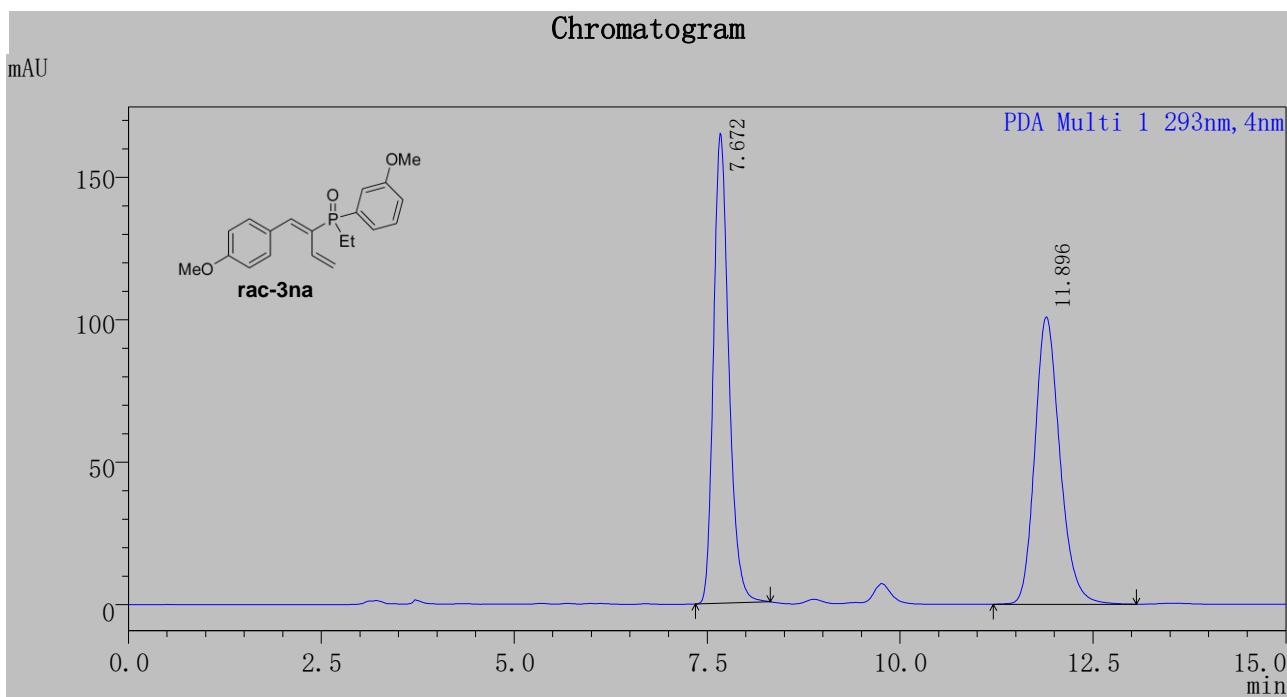
PDA Ch1 298nm

Peak#	Ret. Time	Area	Area%
1	10.619	173723	50.286
2	21.349	171745	49.714
Total		345468	100.000



PDA Ch1 298nm

Peak#	Ret. Time	Area	Area%
1	10.590	7637215	93.824
2	21.361	502705	6.176
Total		8139920	100.000

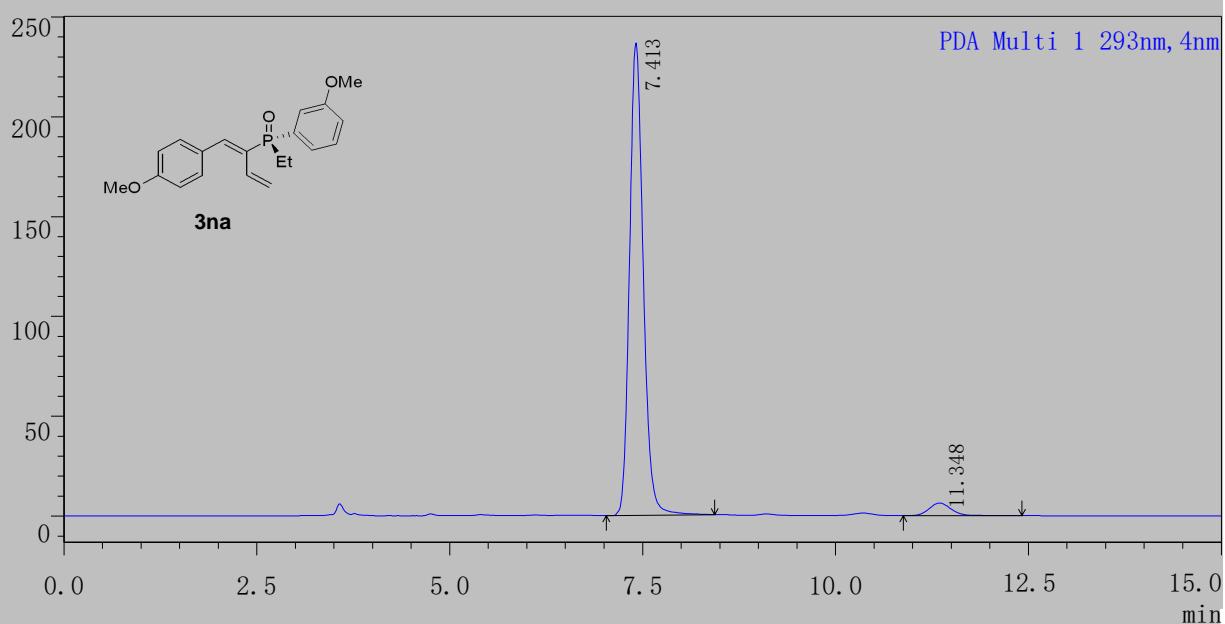


PDA Ch1 293nm

Peak#	Ret. Time	Area	Area%
1	7.672	2272441	49.914
2	11.896	2280287	50.086
Total		4552728	100.000

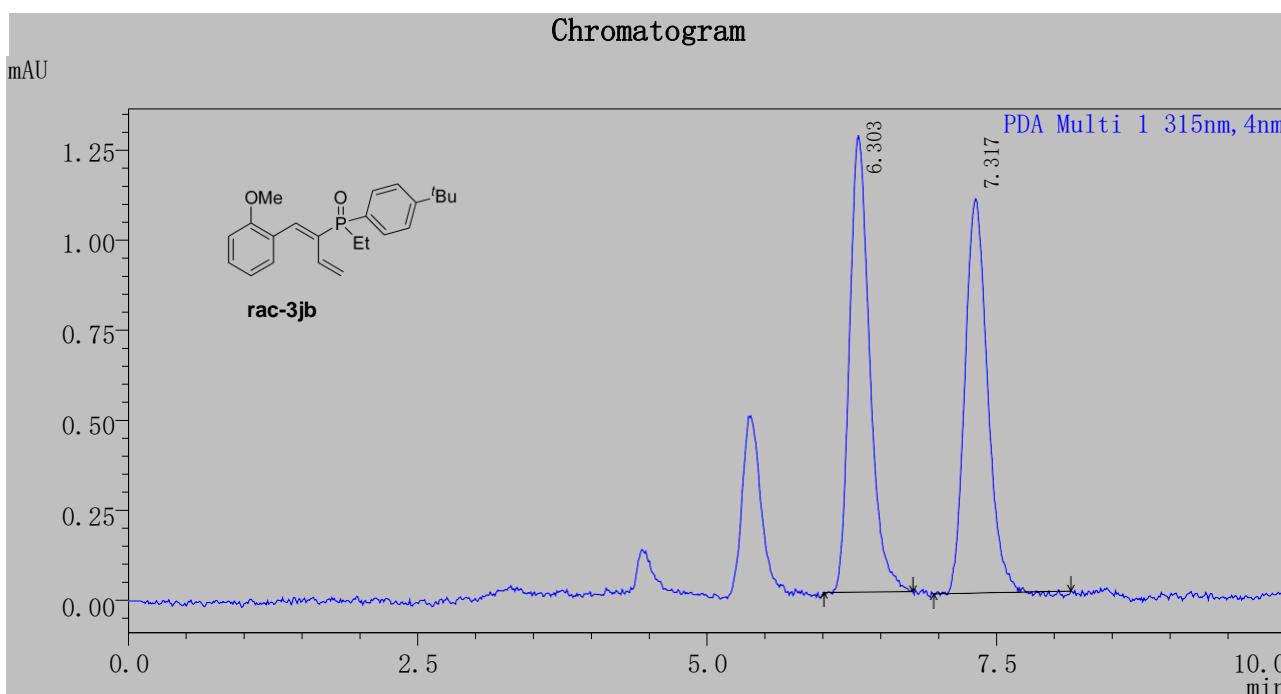
Chromatogram

mAU



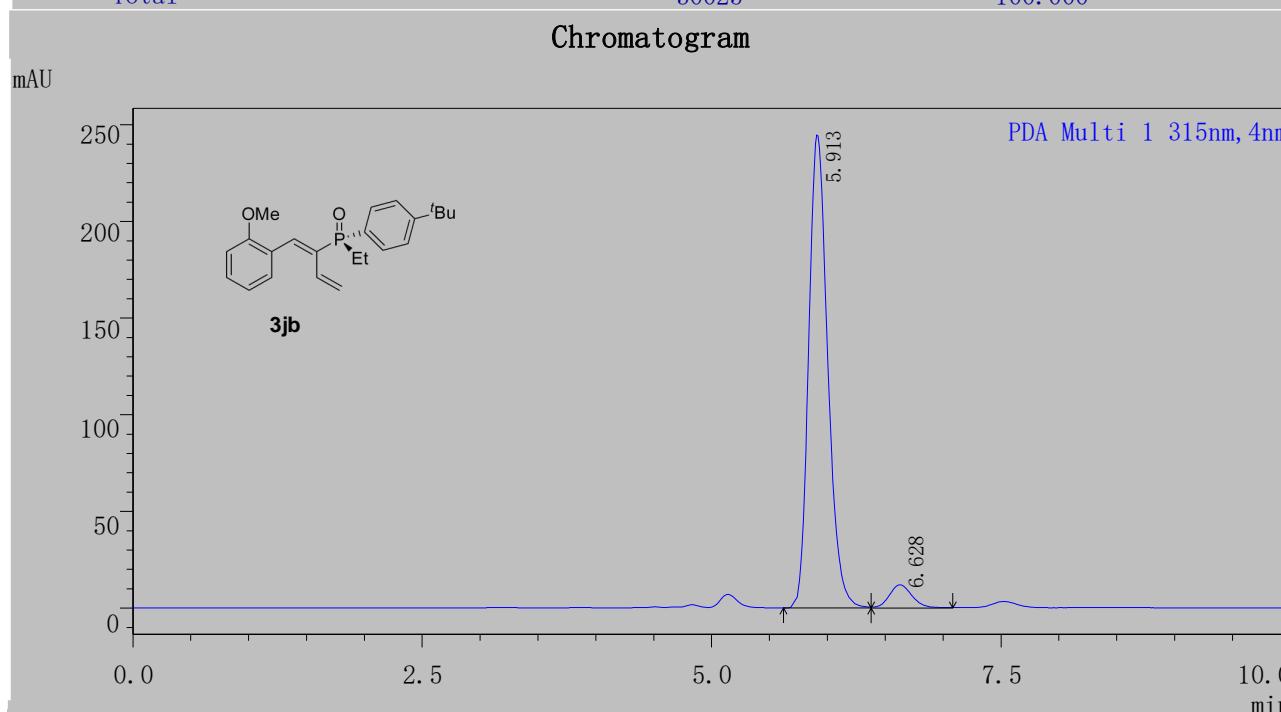
PDA Ch1 293nm

Peak#	Ret. Time	Area	Area%
1	7.413	2915667	95.901
2	11.348	124633	4.099
Total		3040300	100.000



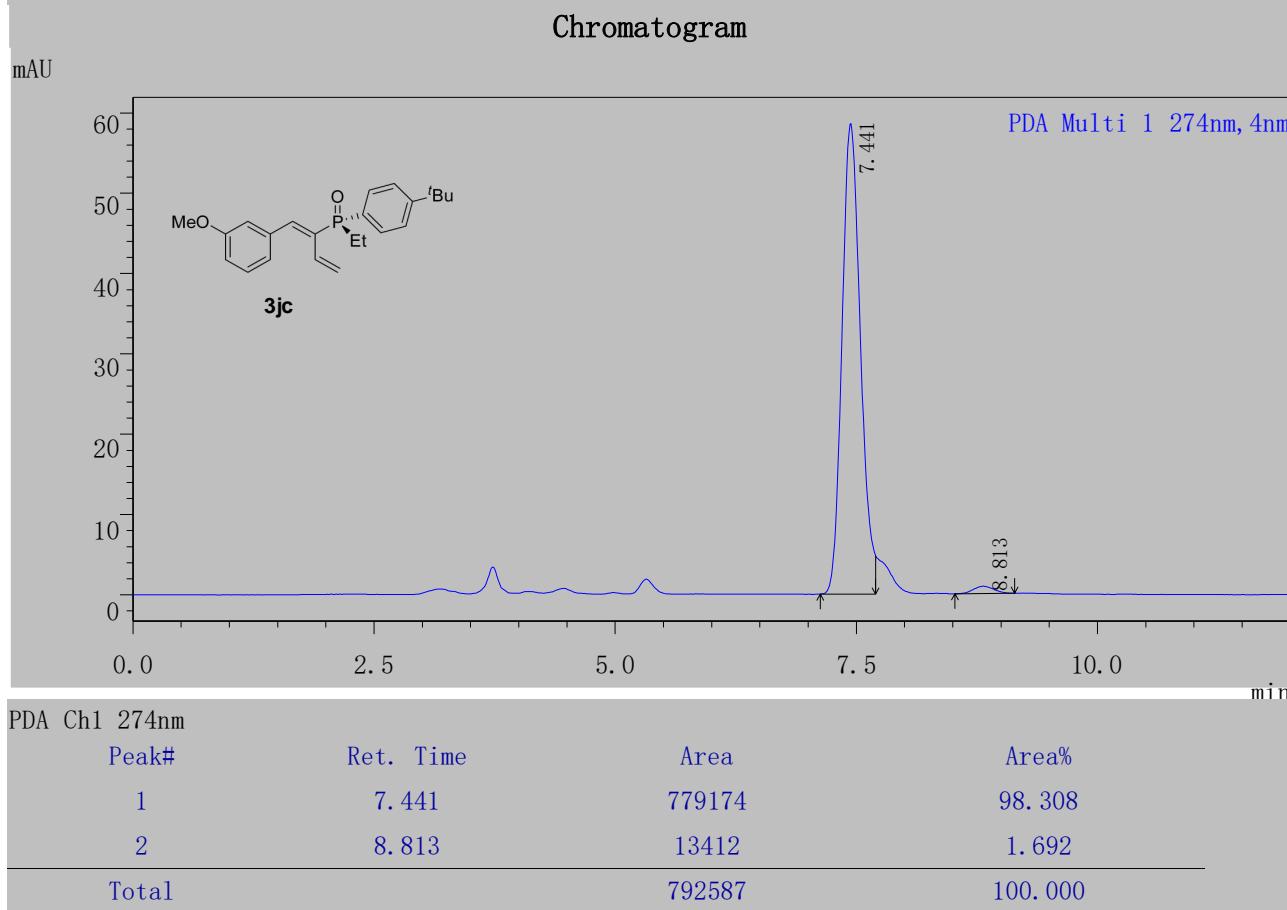
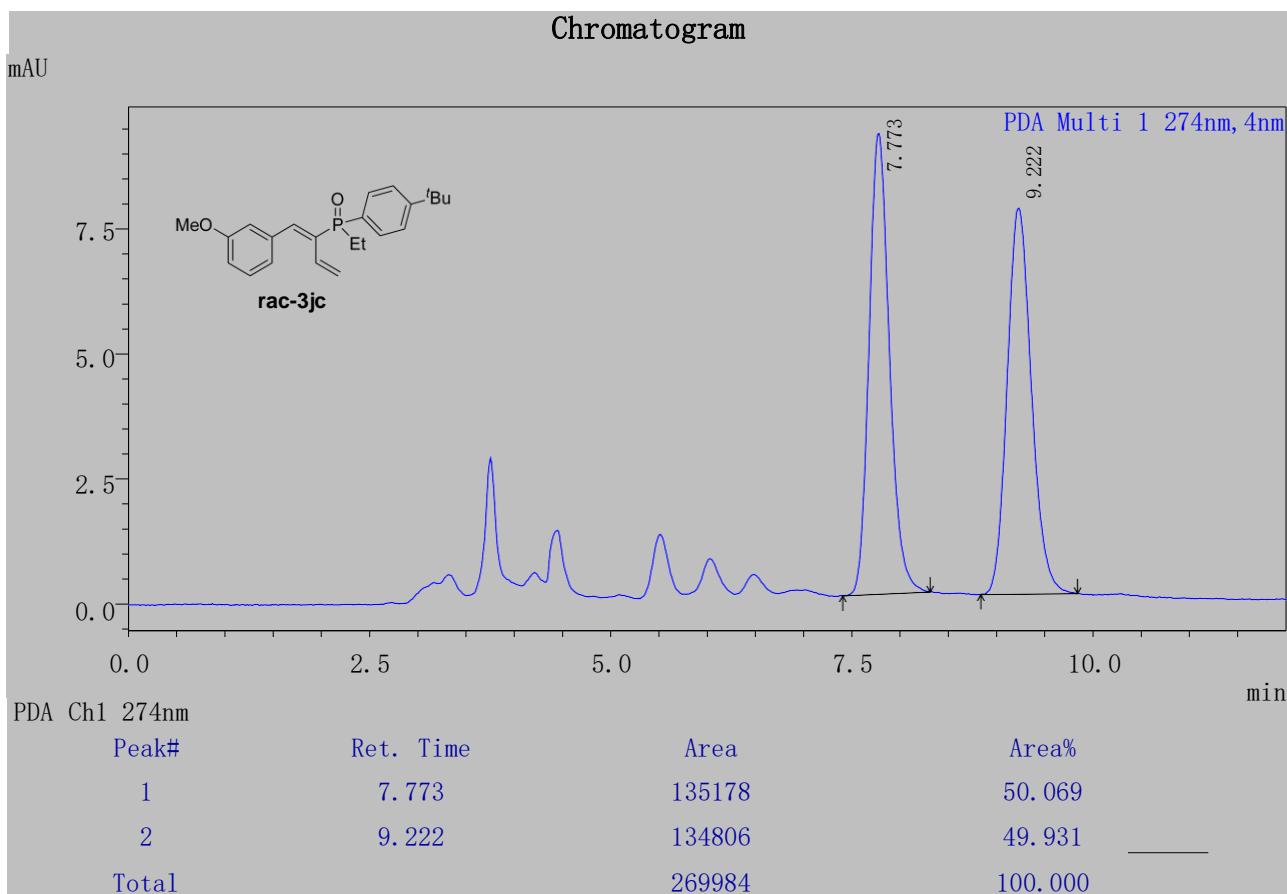
PDA Ch1 315nm

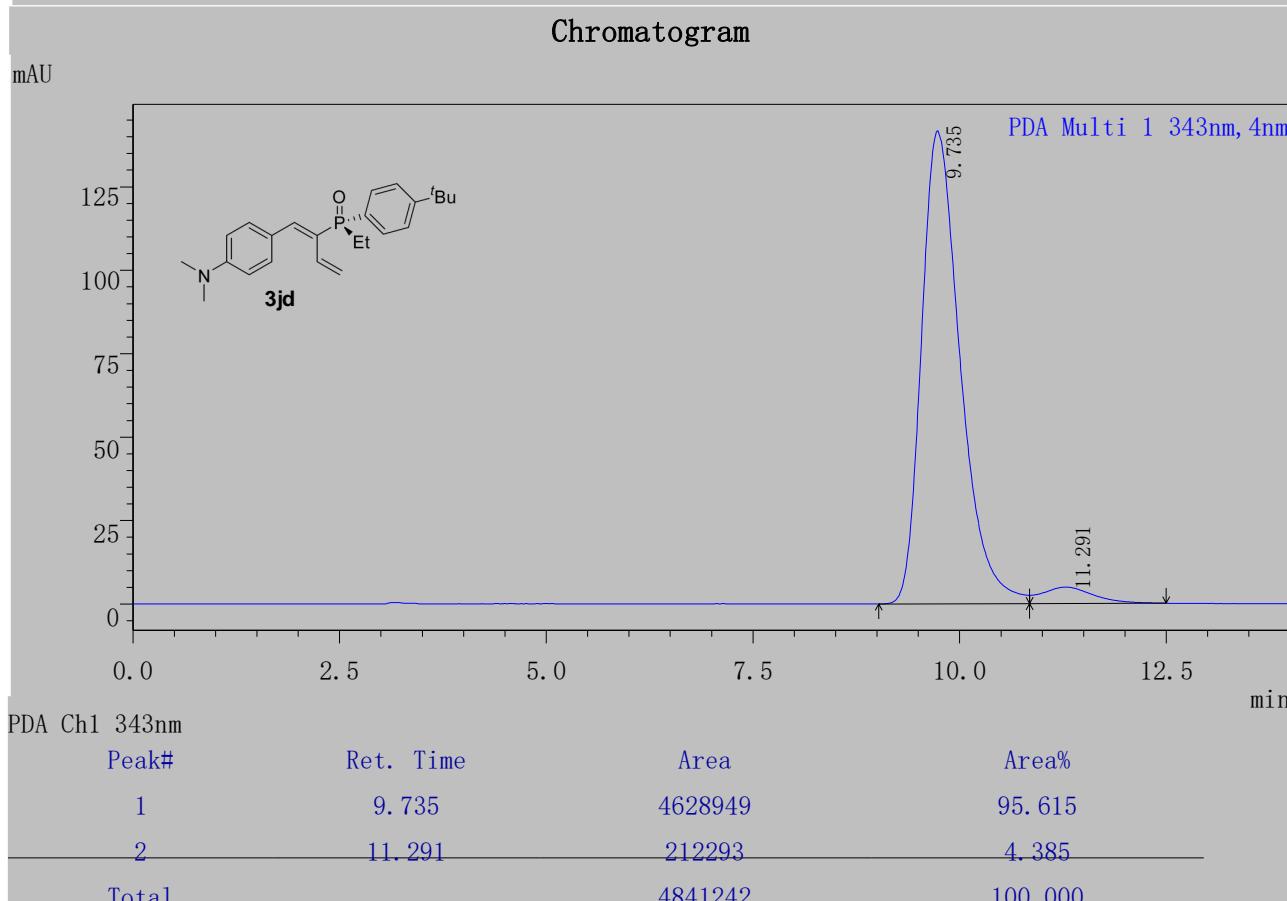
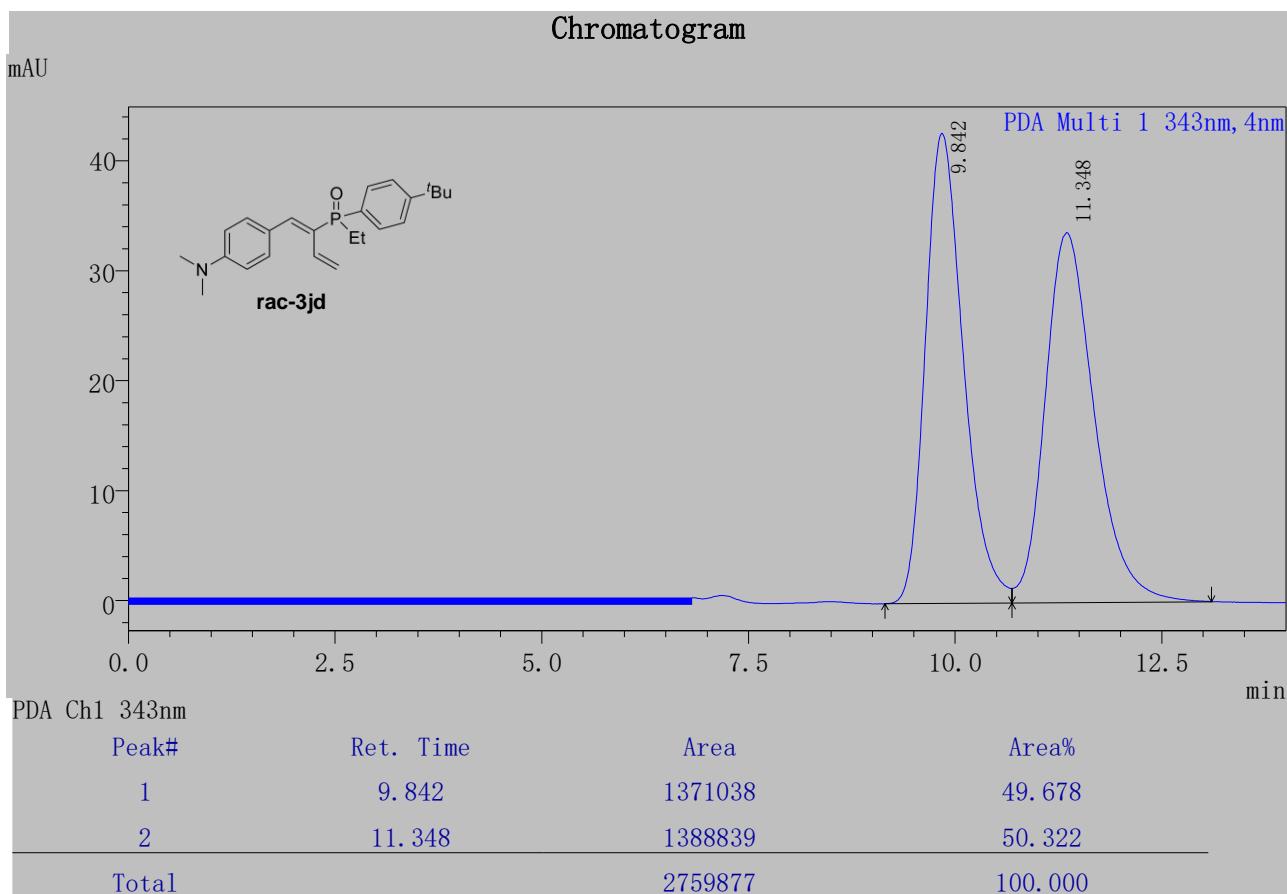
Peak#	Ret. Time	Area	Area%
1	6.303	15364	51.170
2	7.317	14661	48.830
Total		30025	100.000

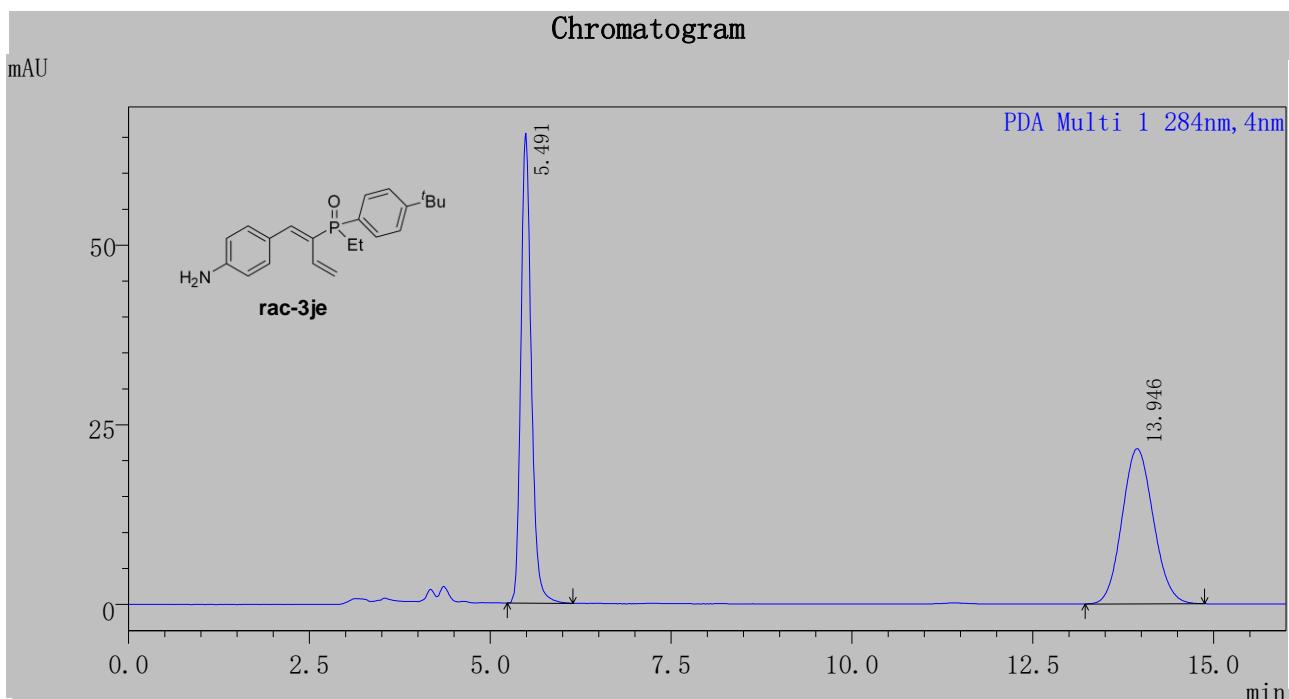


PDA Ch1 315nm

Peak#	Ret. Time	Area	Area%
1	5.913	2790944	94.540
2	6.628	161173	5.460
Total		2952117	100.000





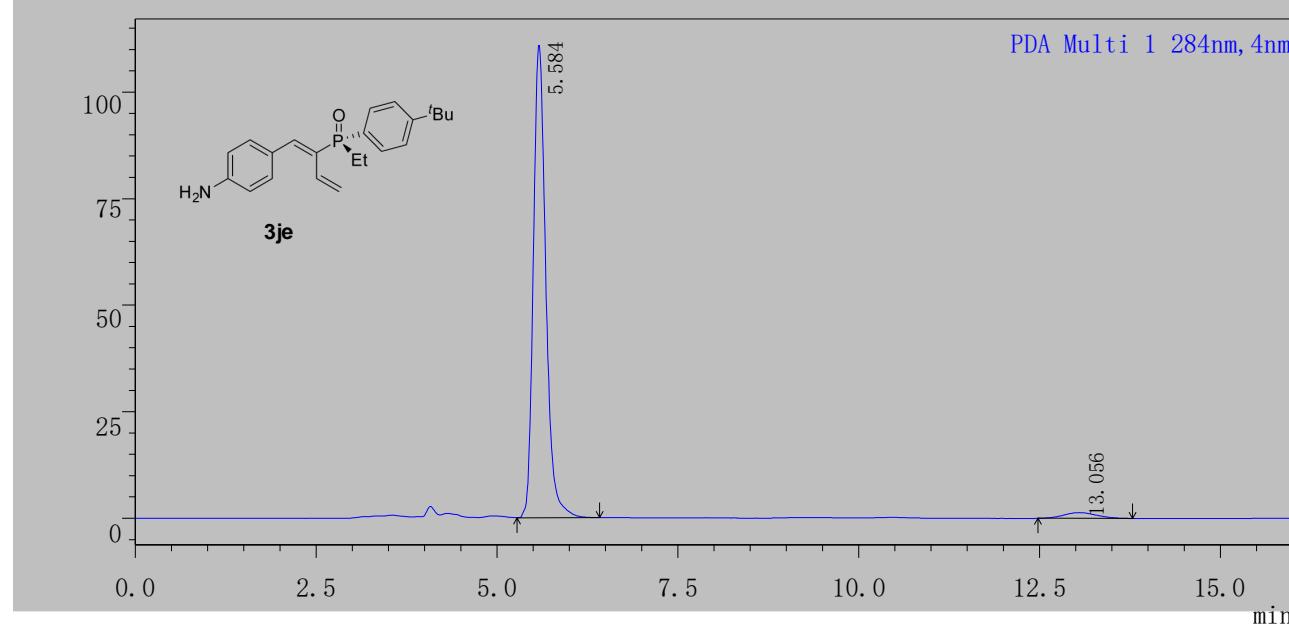


PDA Ch1 284nm

Peak#	Ret. Time	Area	Area%
1	5.491	653735	50.122
2	13.946	650553	49.878
Total		1304288	100.000

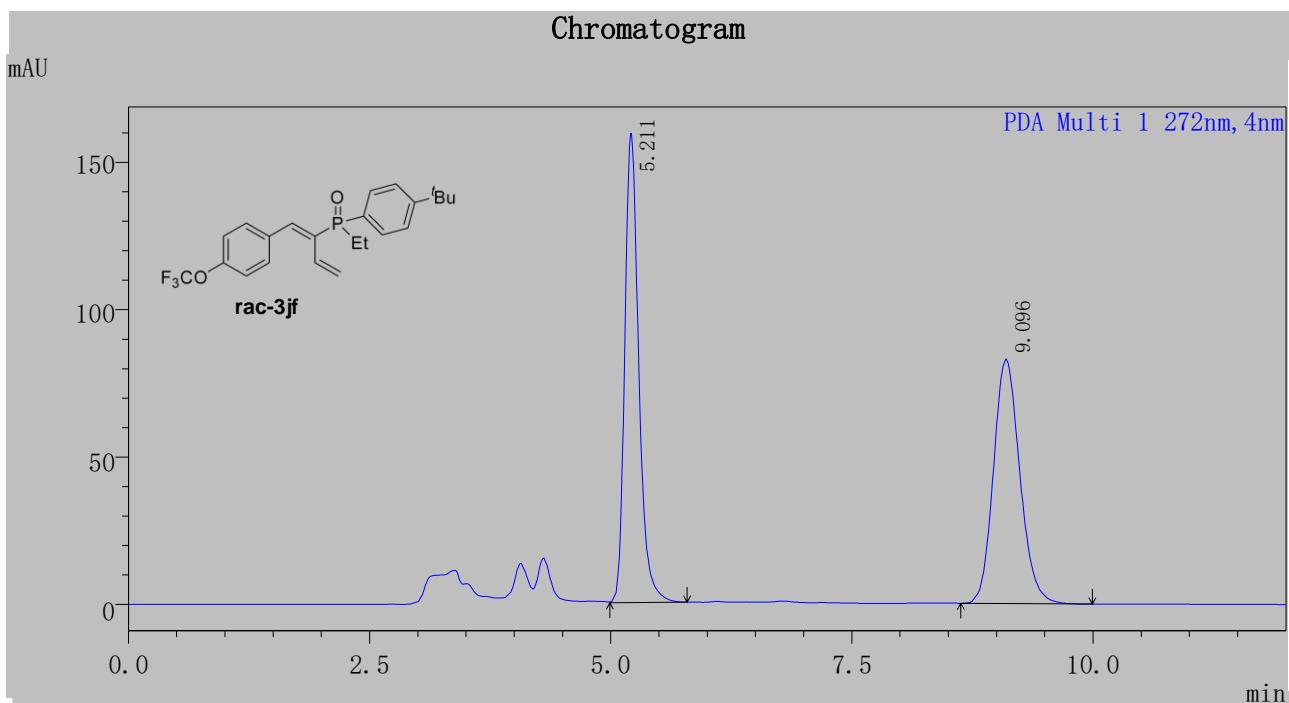
Chromatogram

mAU

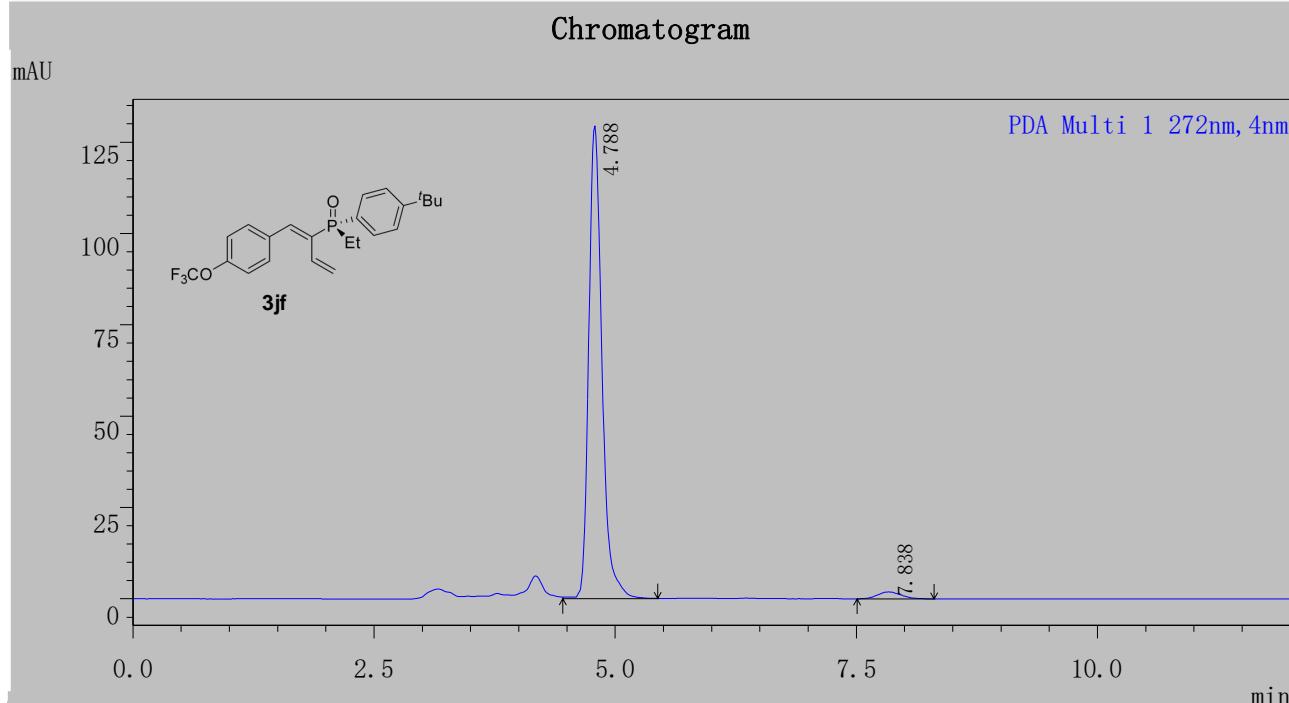


PDA Ch1 284nm

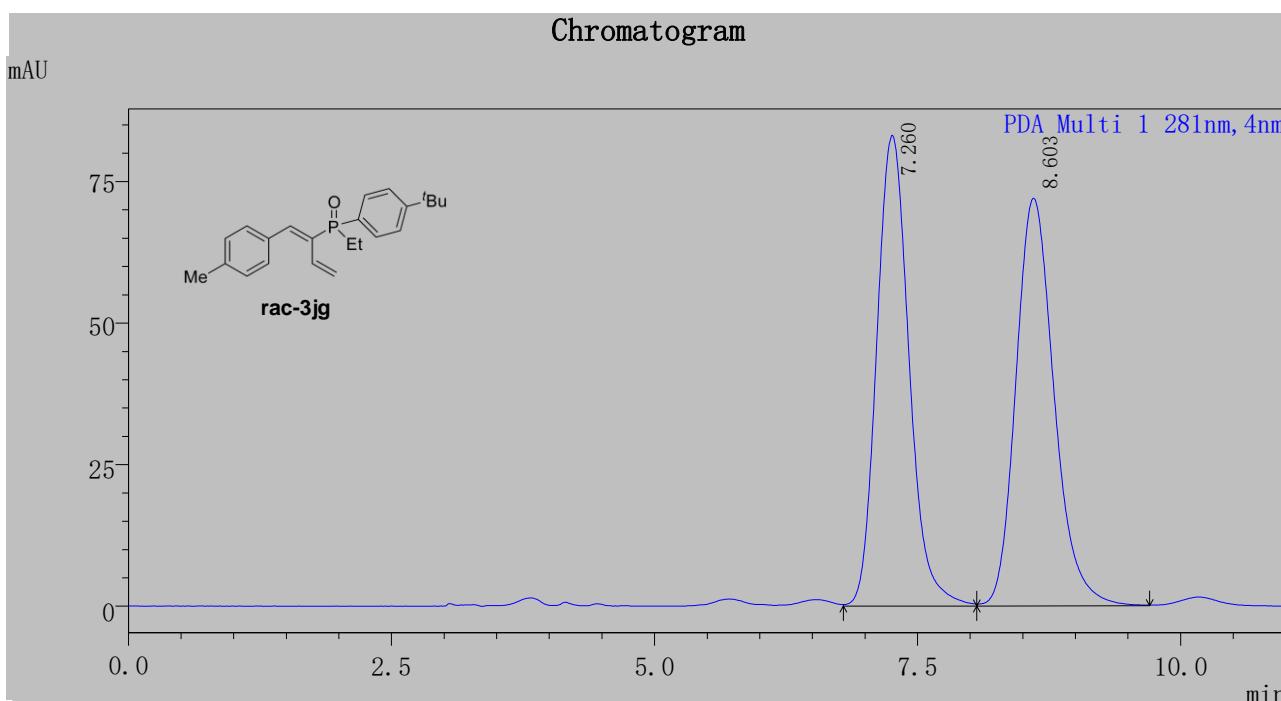
Peak#	Ret. Time	Area	Area%
1	5.584	1329652	96.864
2	13.056	43054	3.136
Total		1372706	100.000



Peak#	Ret. Time	Area	Area%
1	5.211	1603874	50.400
2	9.096	1578396	49.600
Total		3182269	100.000

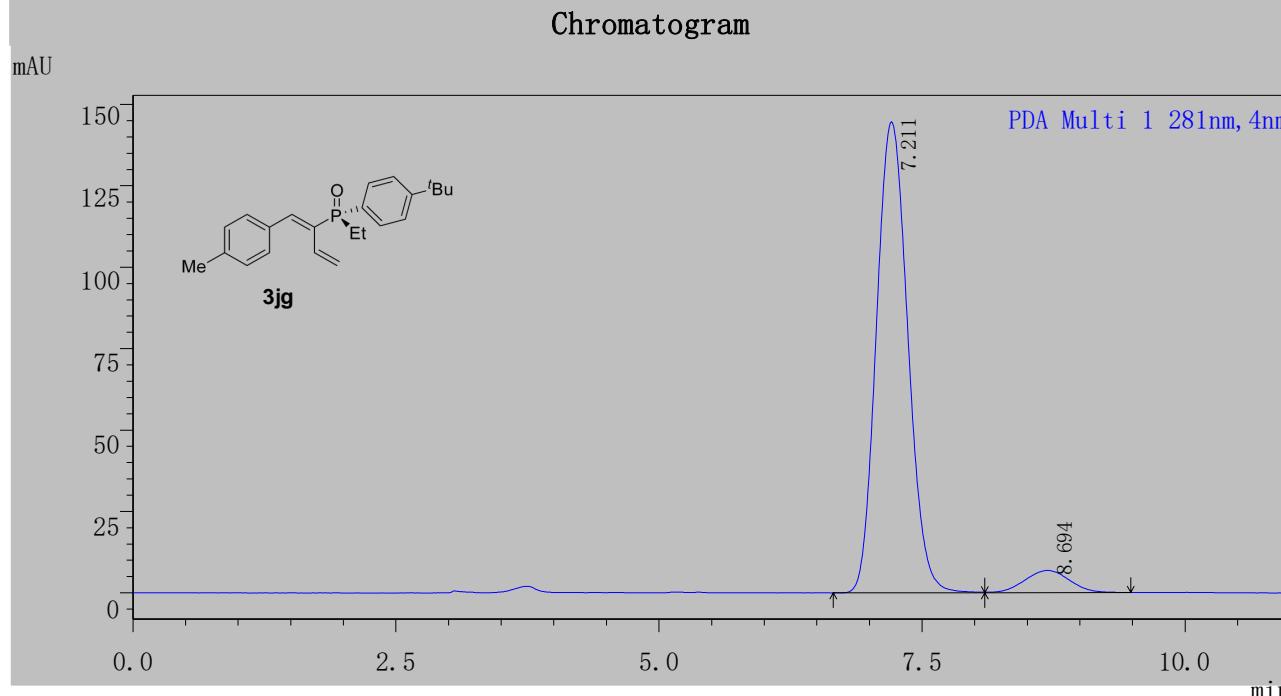


Peak#	Ret. Time	Area	Area%
1	4.788	1232286	97.422
2	7.838	32603	2.578
Total		1264889	100.000



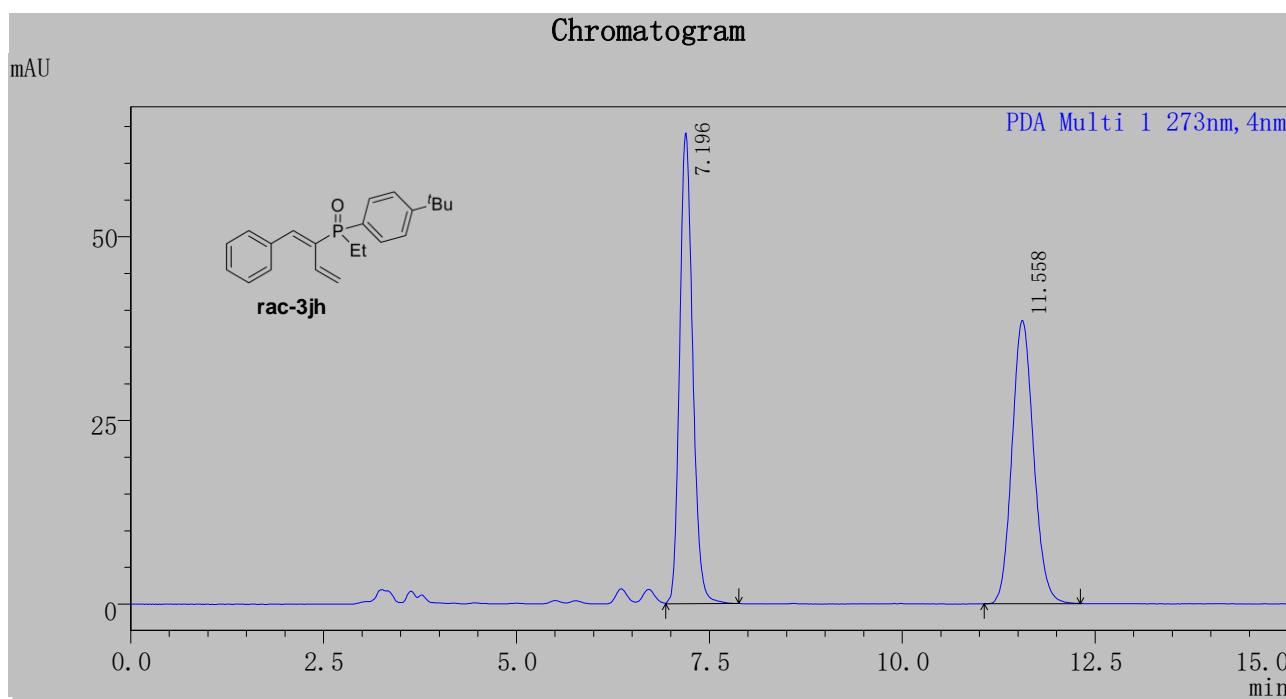
PDA Ch1 281nm

Peak#	Ret. Time	Area	Area%
1	7.260	1781023	49.499
2	8.603	1817051	50.501
Total		3598074	100.000



PDA Ch1 281nm

Peak#	Ret. Time	Area	Area%
1	7.211	3004033	93.709
2	8.694	201679	6.291
Total		3205713	100.000

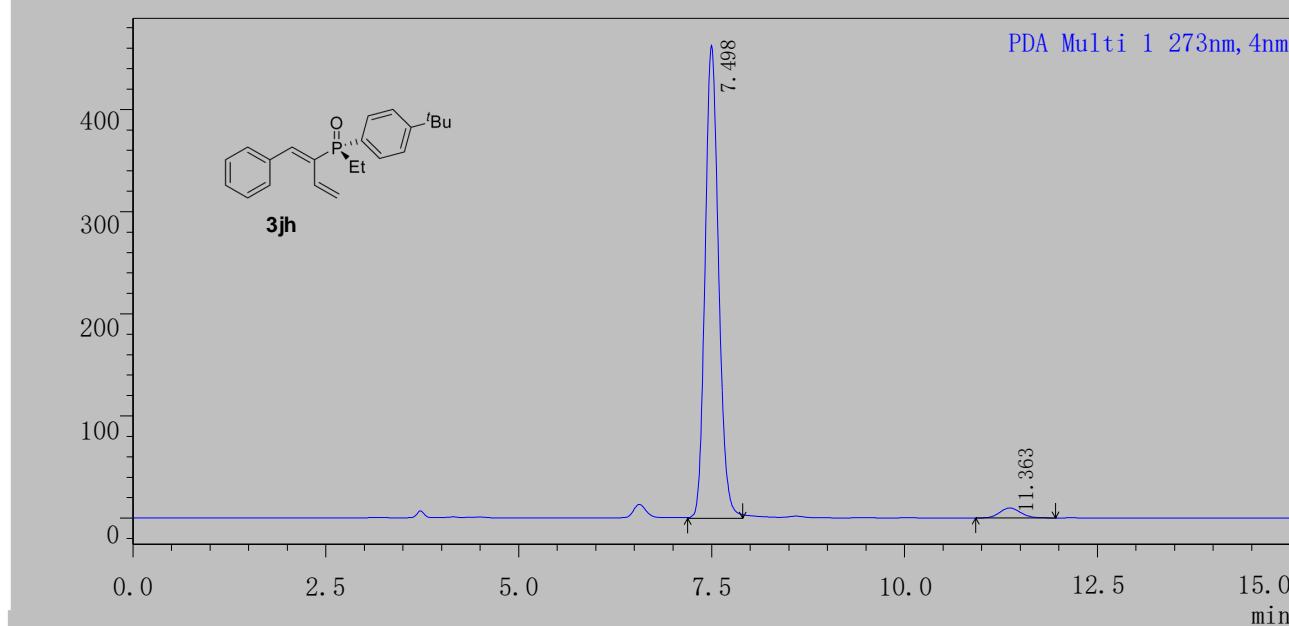


PDA Ch1 273nm

Peak#	Ret. Time	Area	Area%
1	7.196	751270	50.030
2	11.558	750364	49.970
Total	1501633		100.000

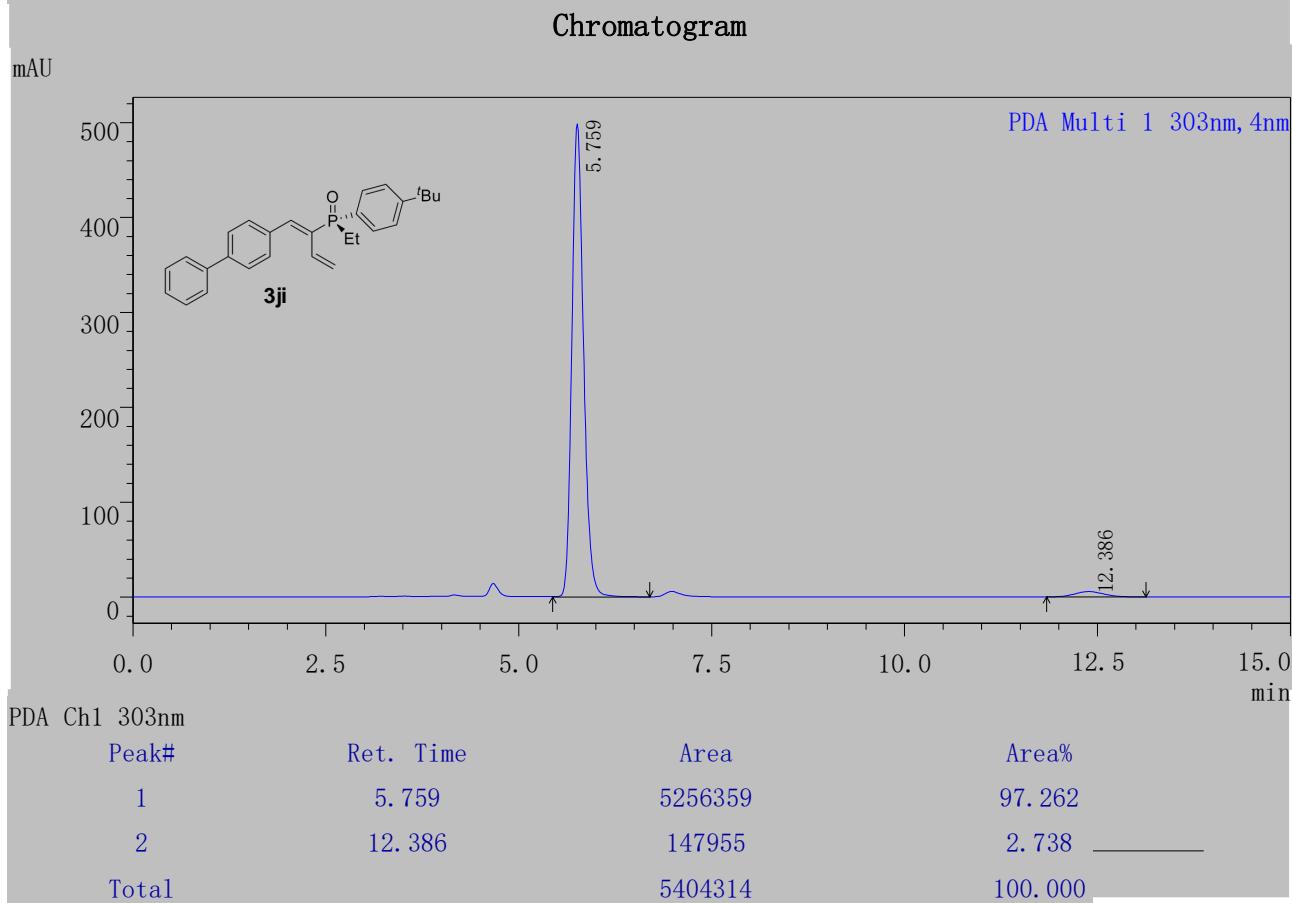
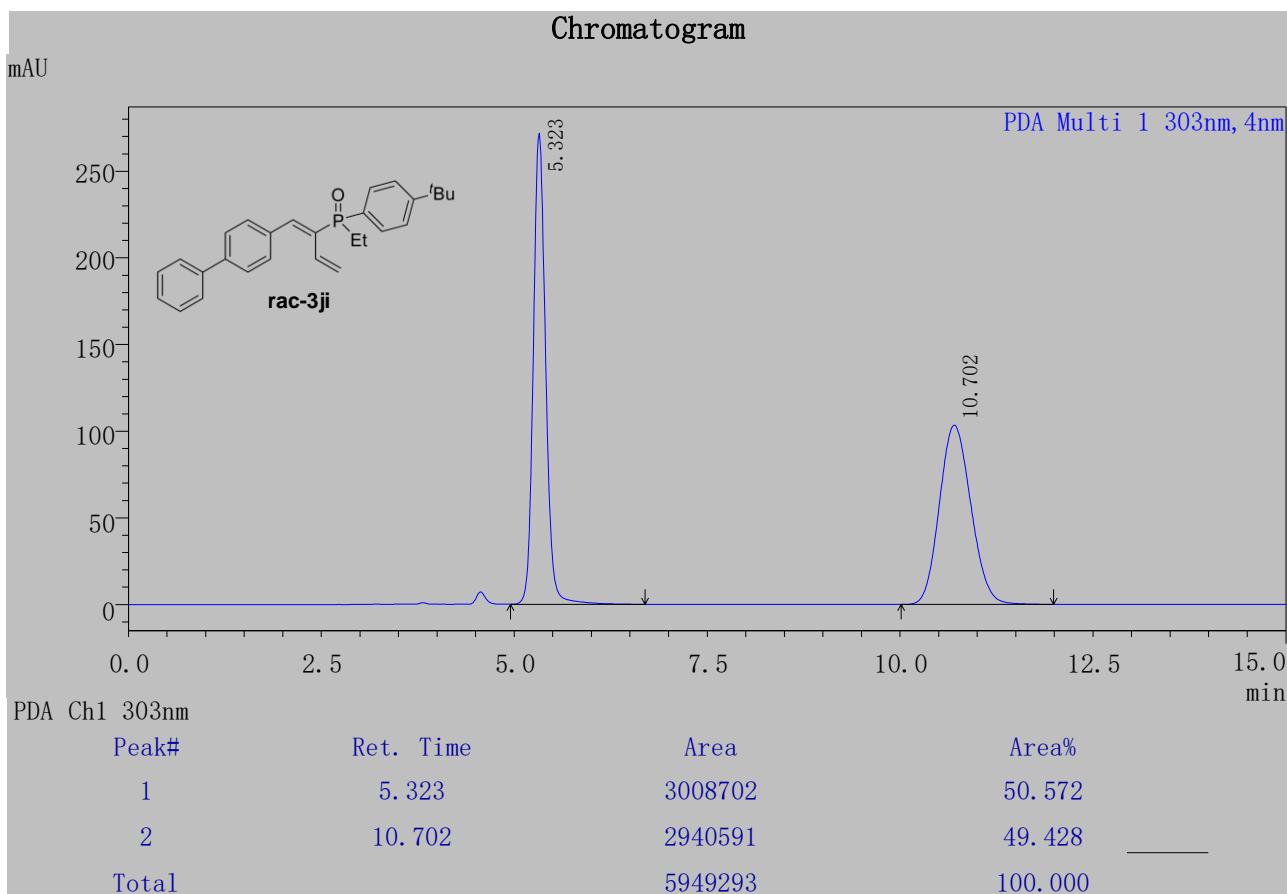
Chromatogram

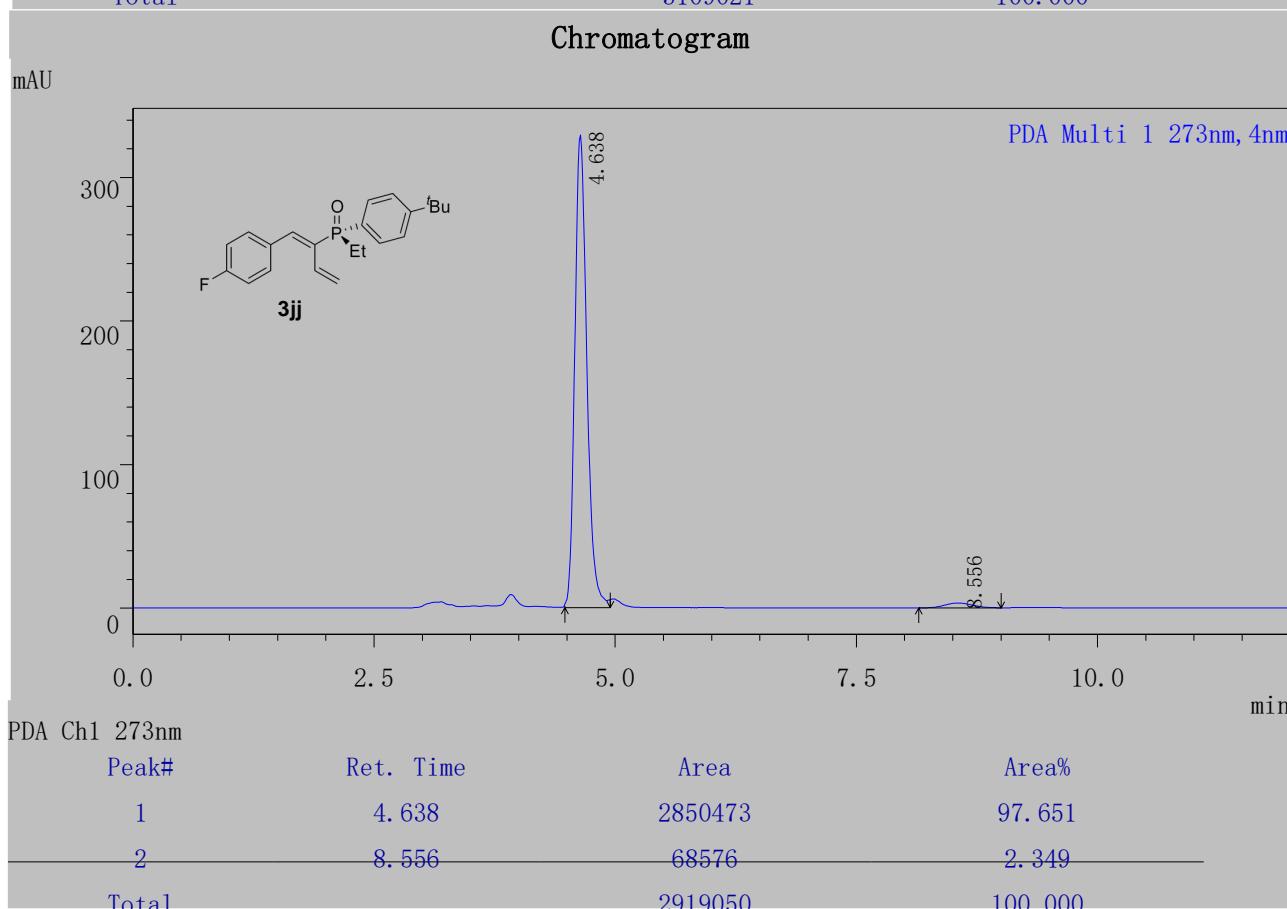
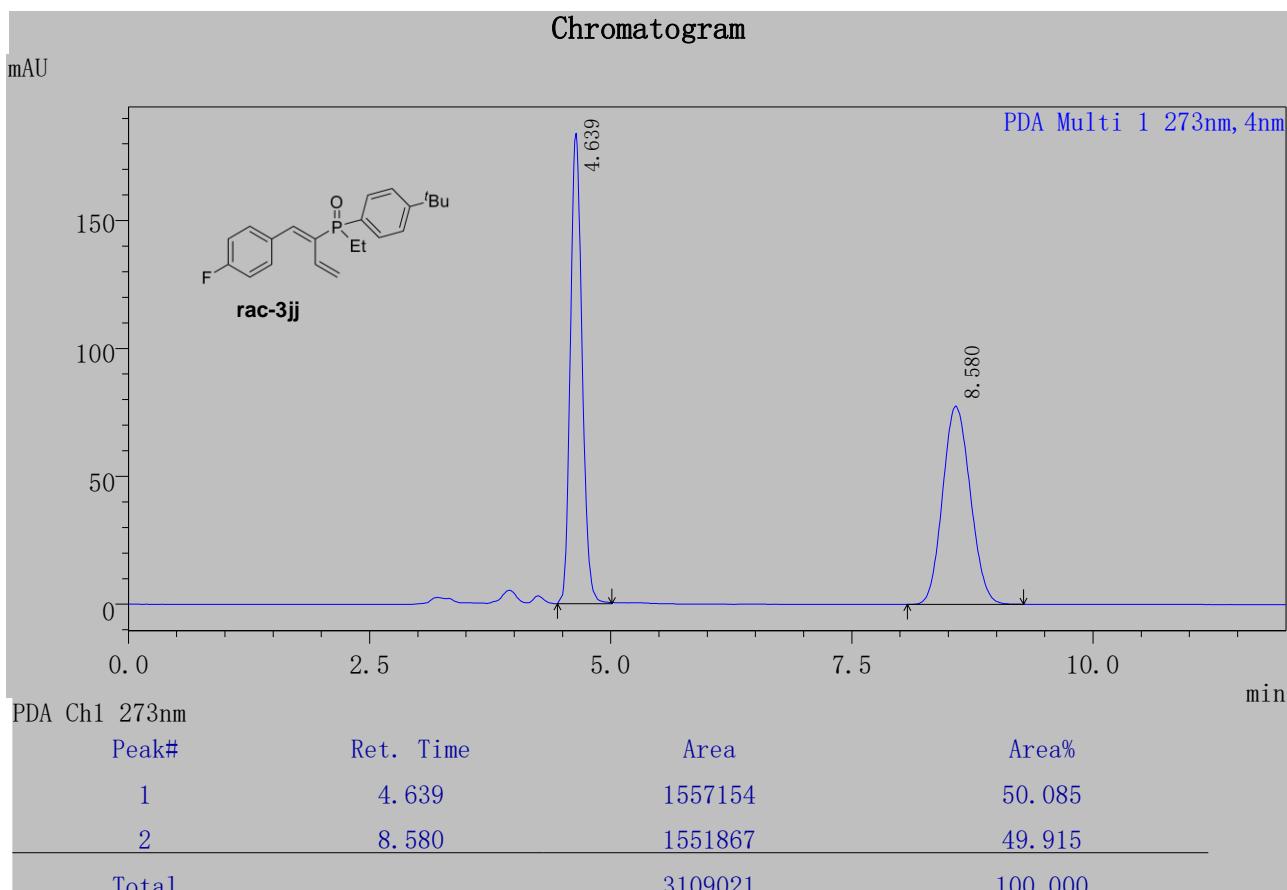
mAU

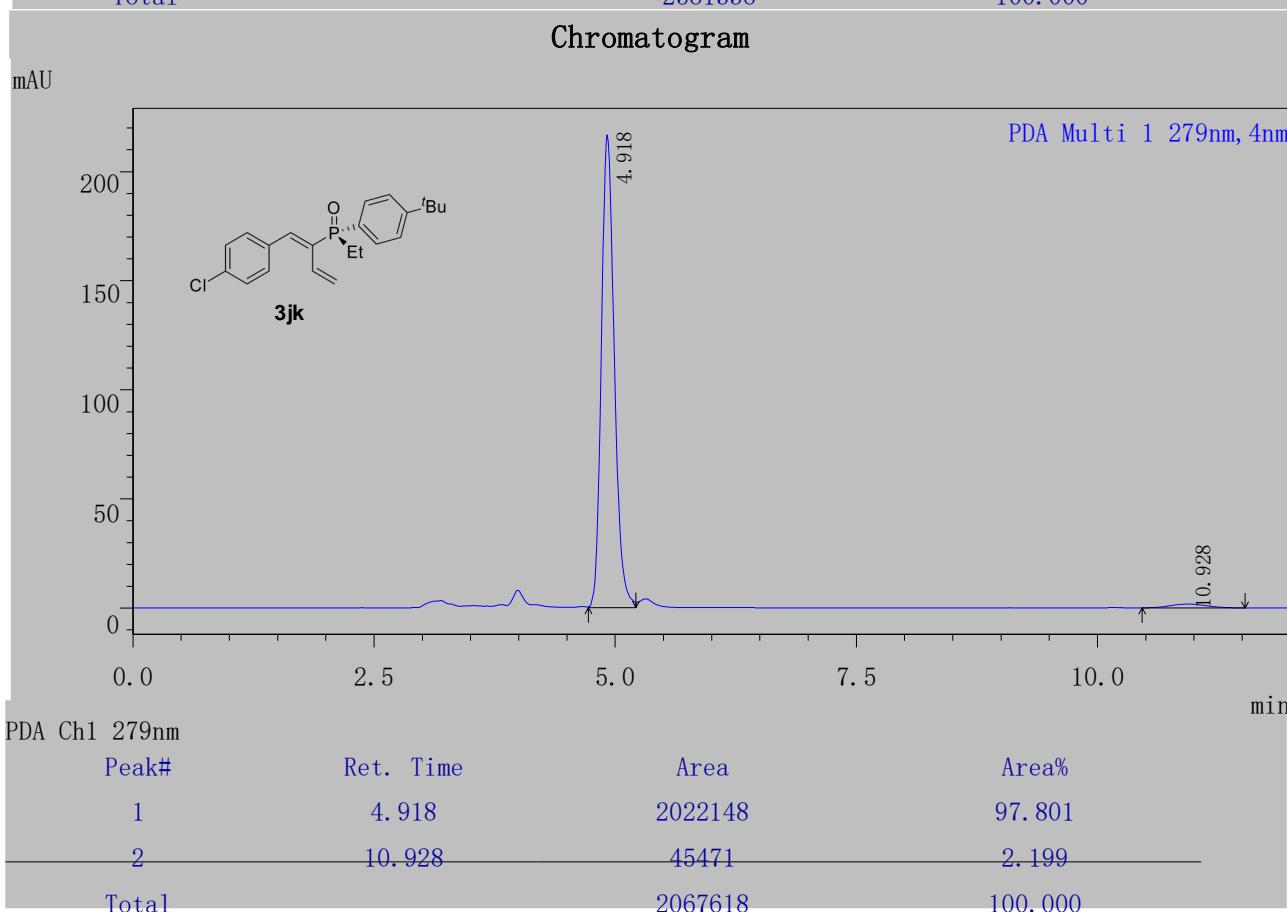
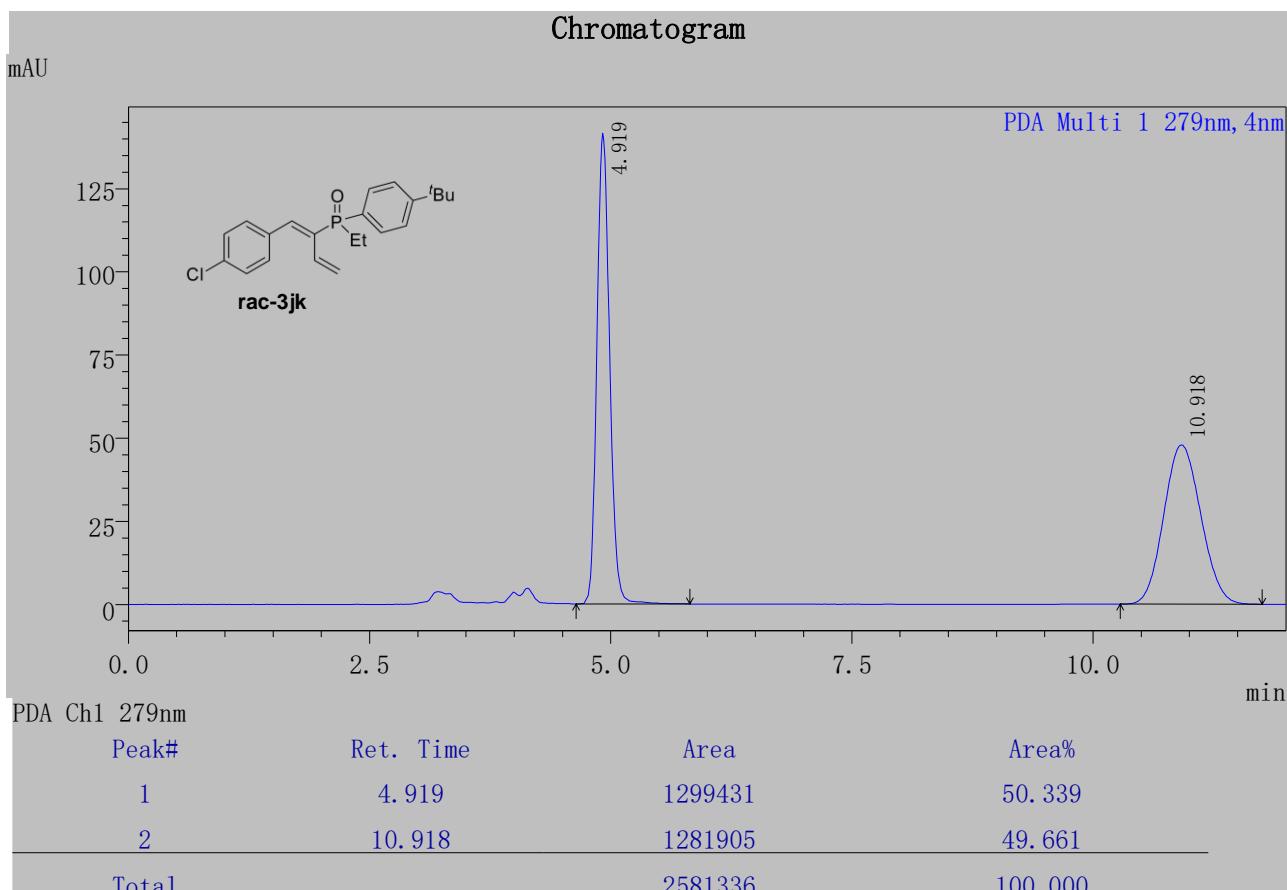


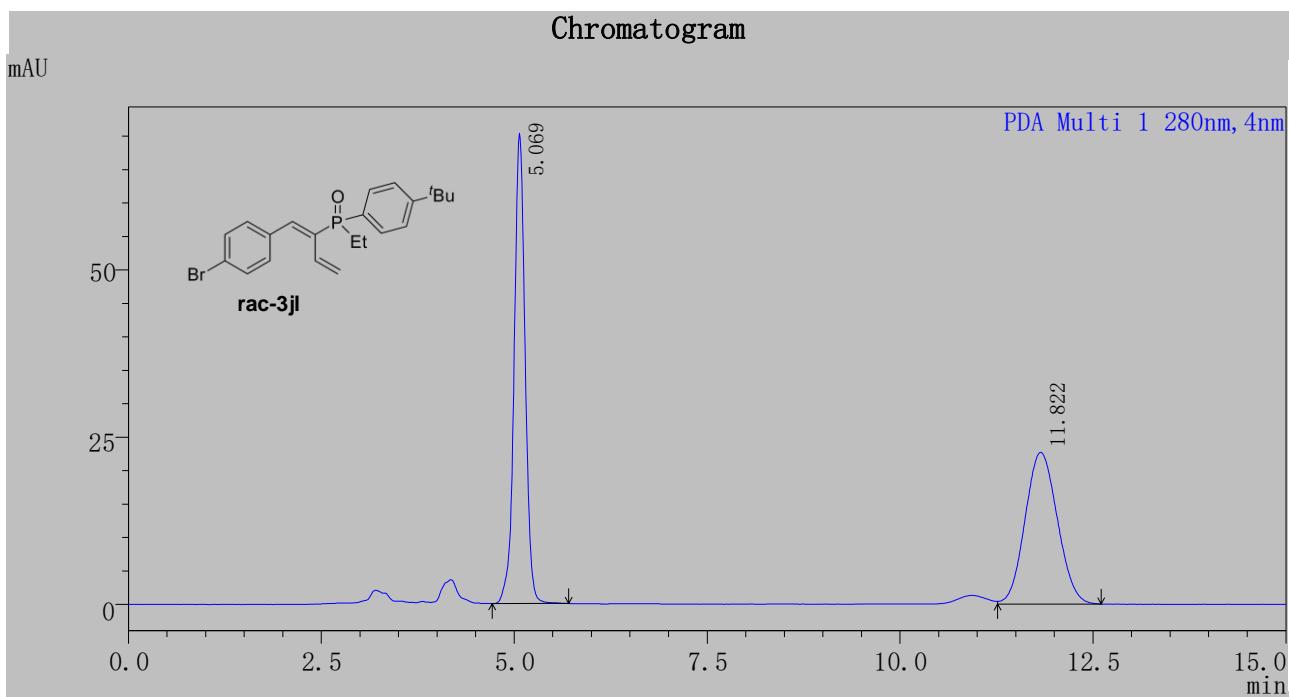
PDA Ch1 273nm

Peak#	Ret. Time	Area	Area%
1	7.498	5646809	96.805
2	11.363	186380	3.195
Total	5833189		100.000

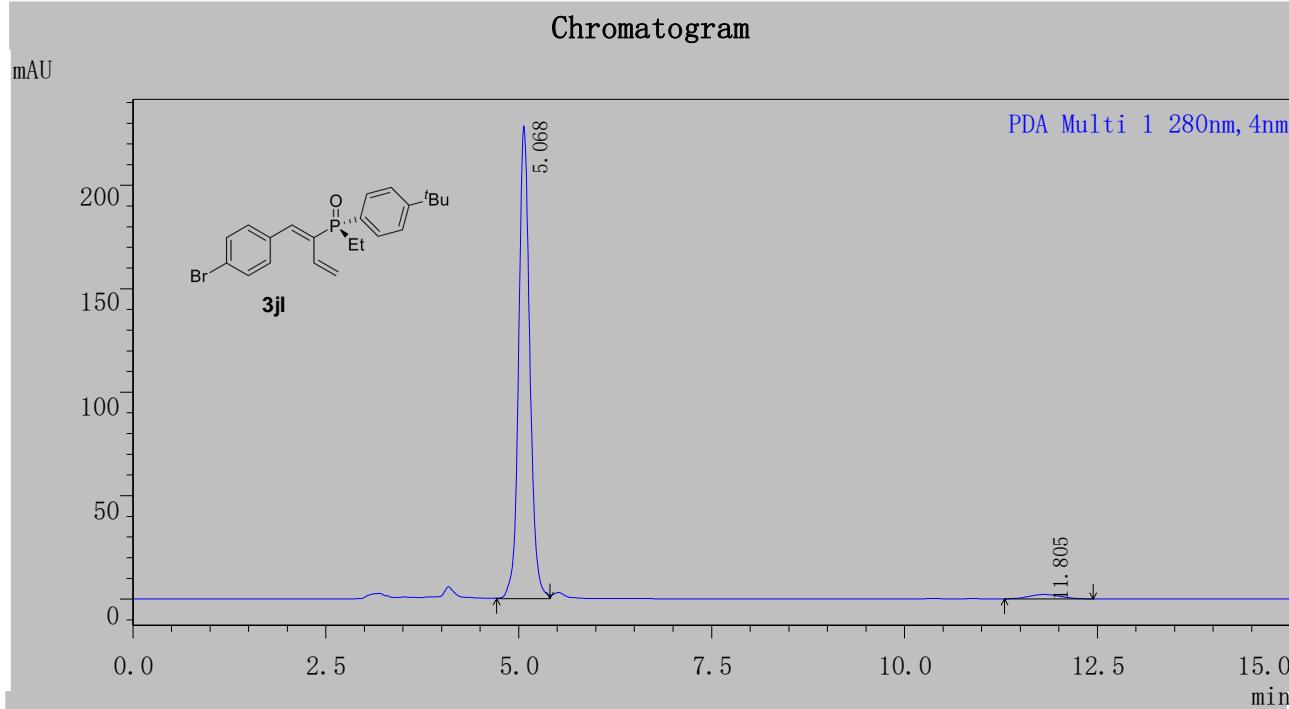




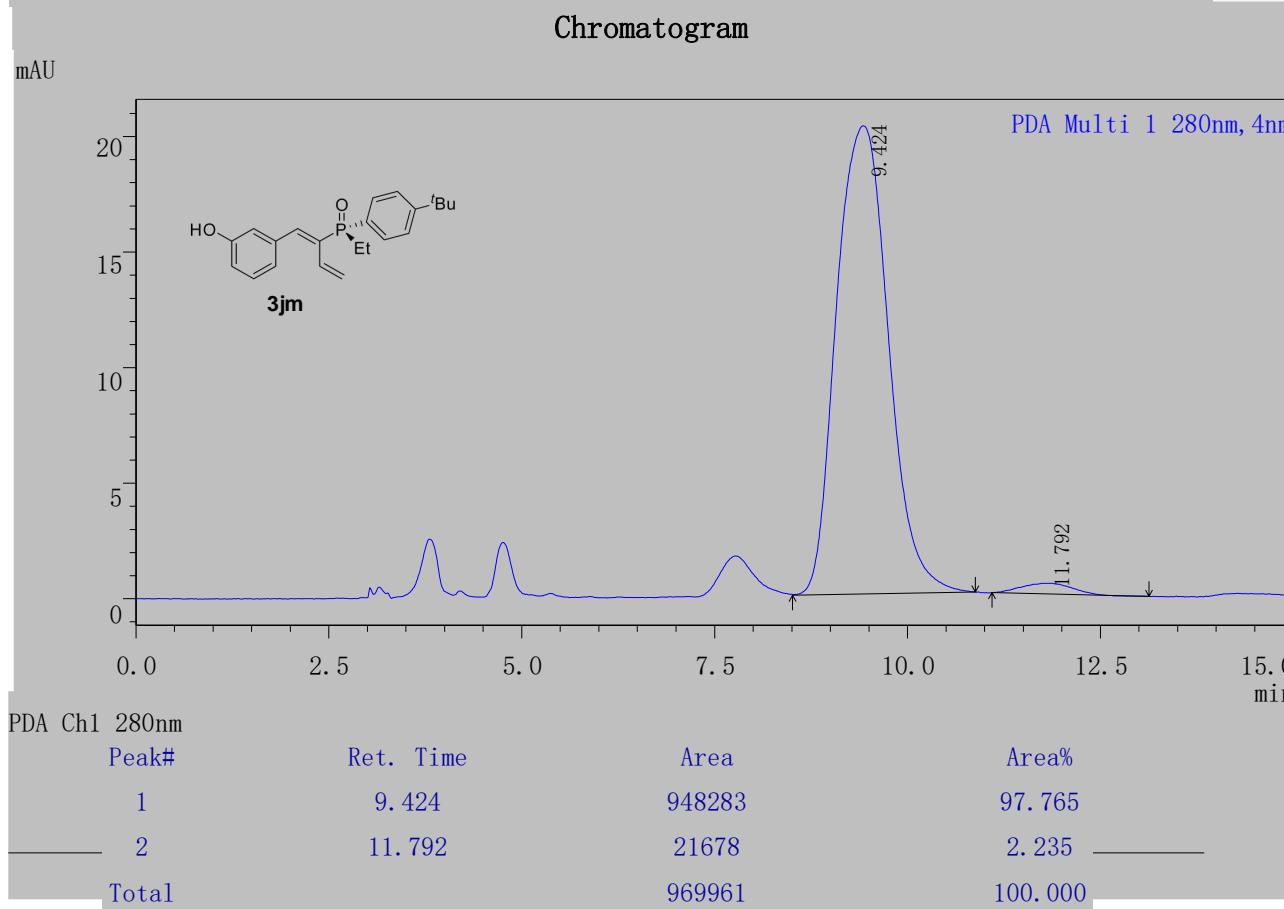
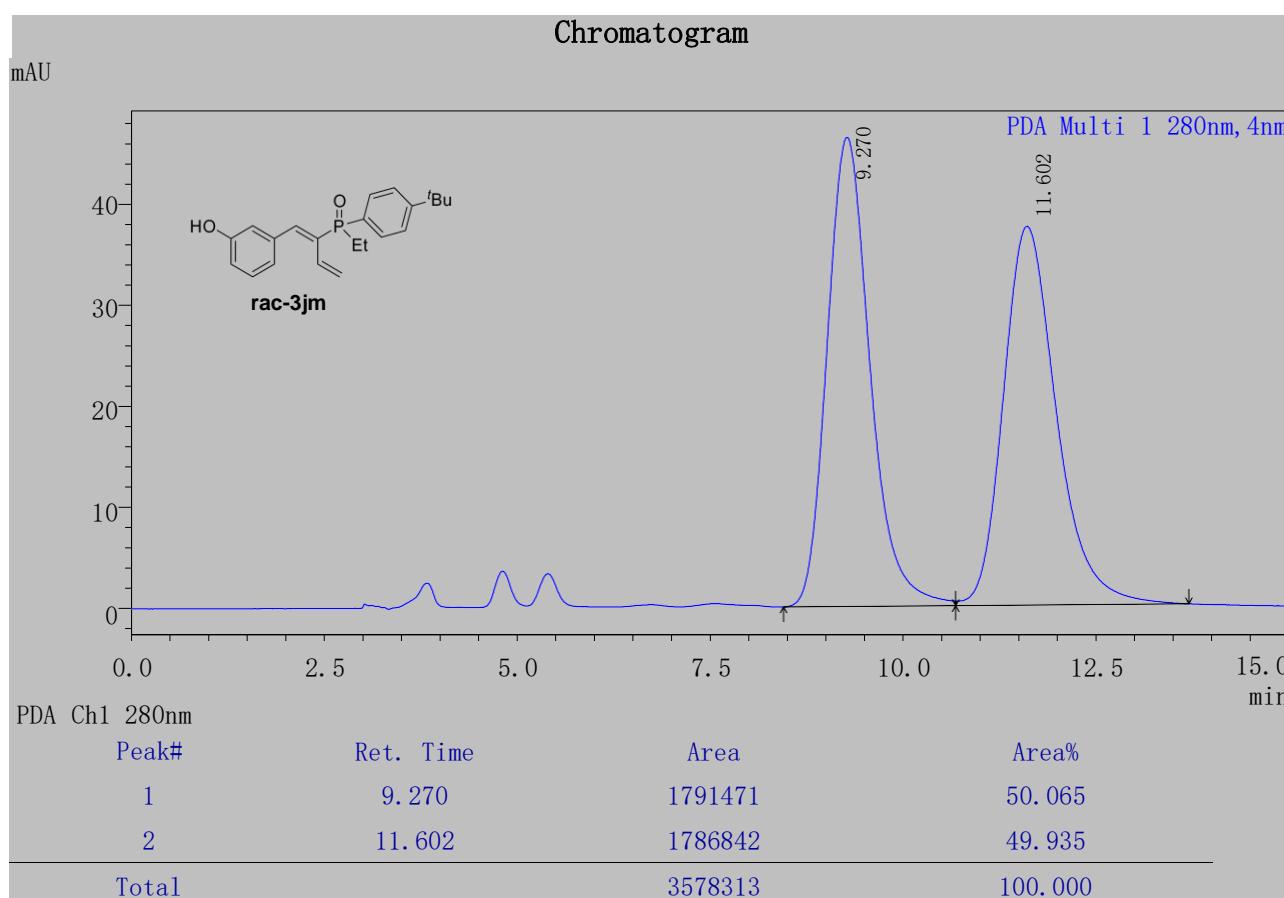


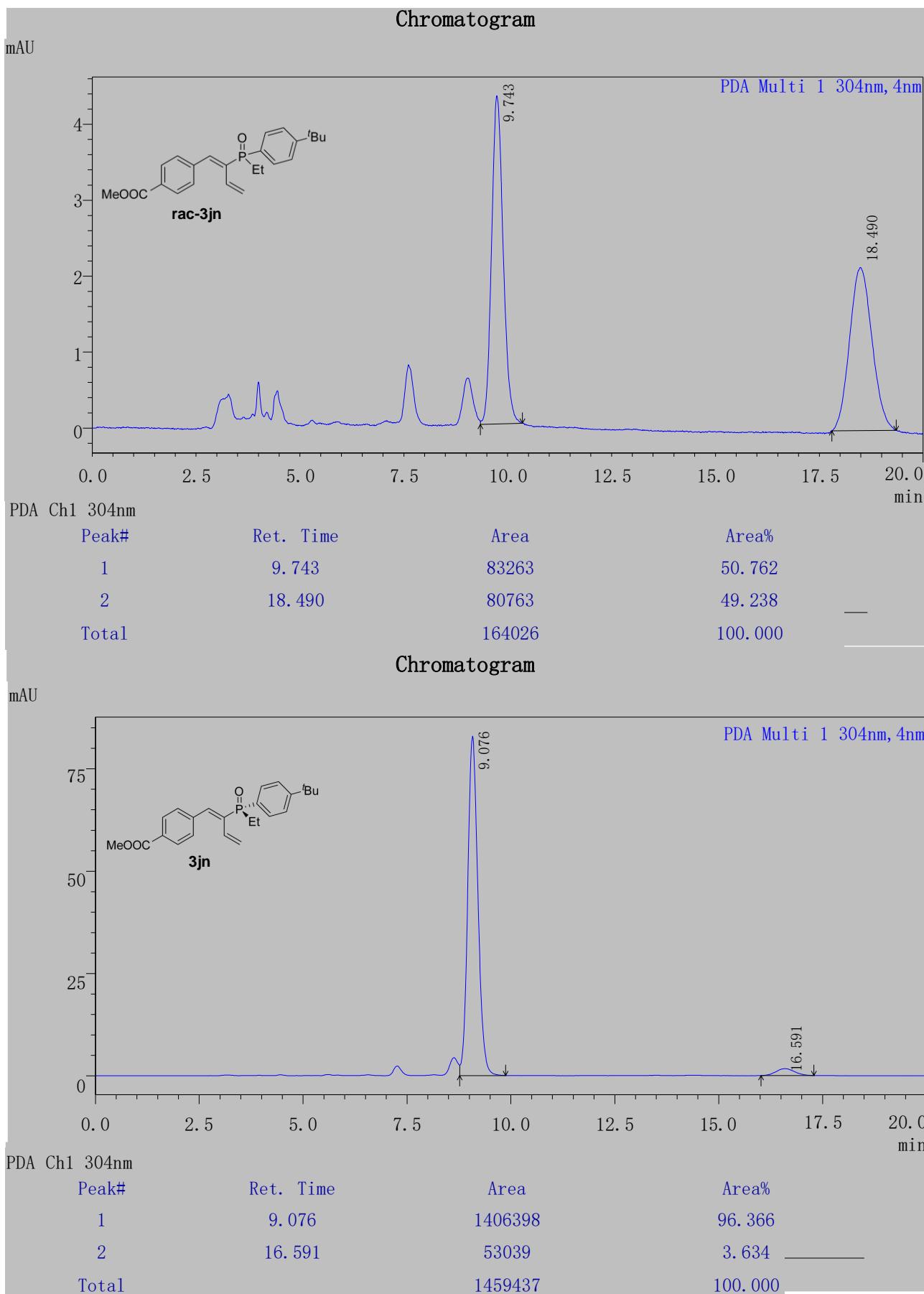


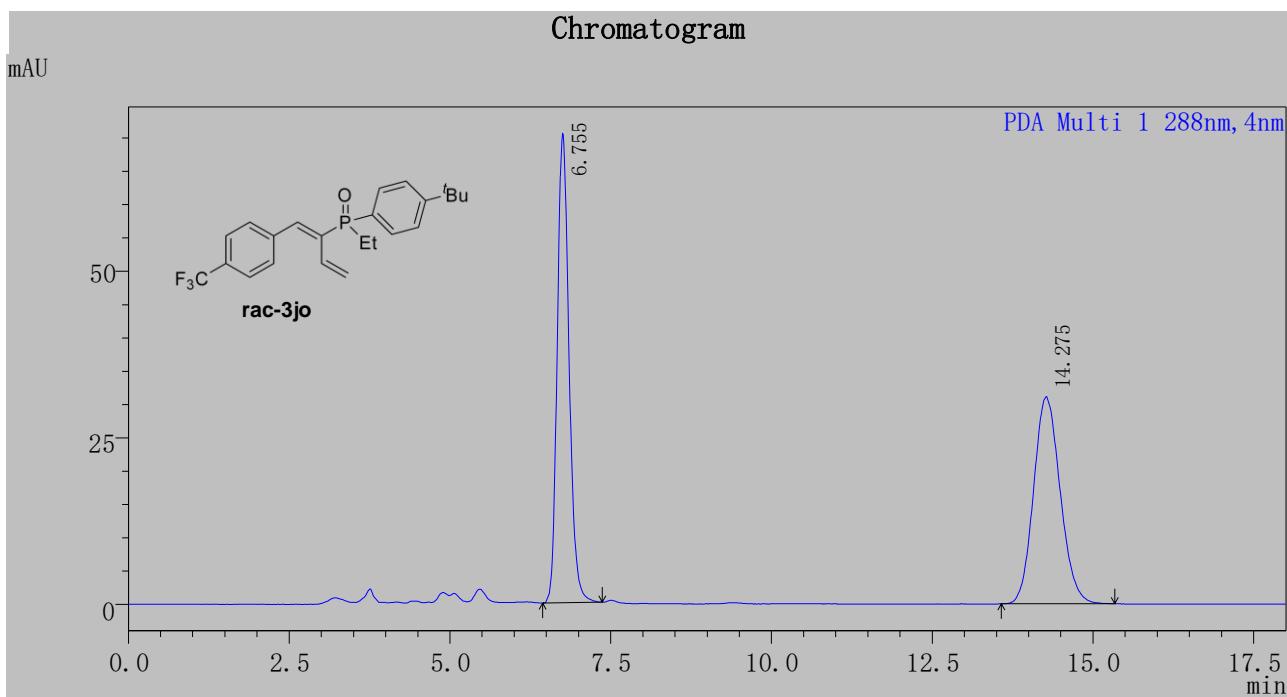
Peak#	Ret. Time	Area	Area%
1	5.069	698973	51.485
2	11.822	658647	48.515
Total	1357620		100.000



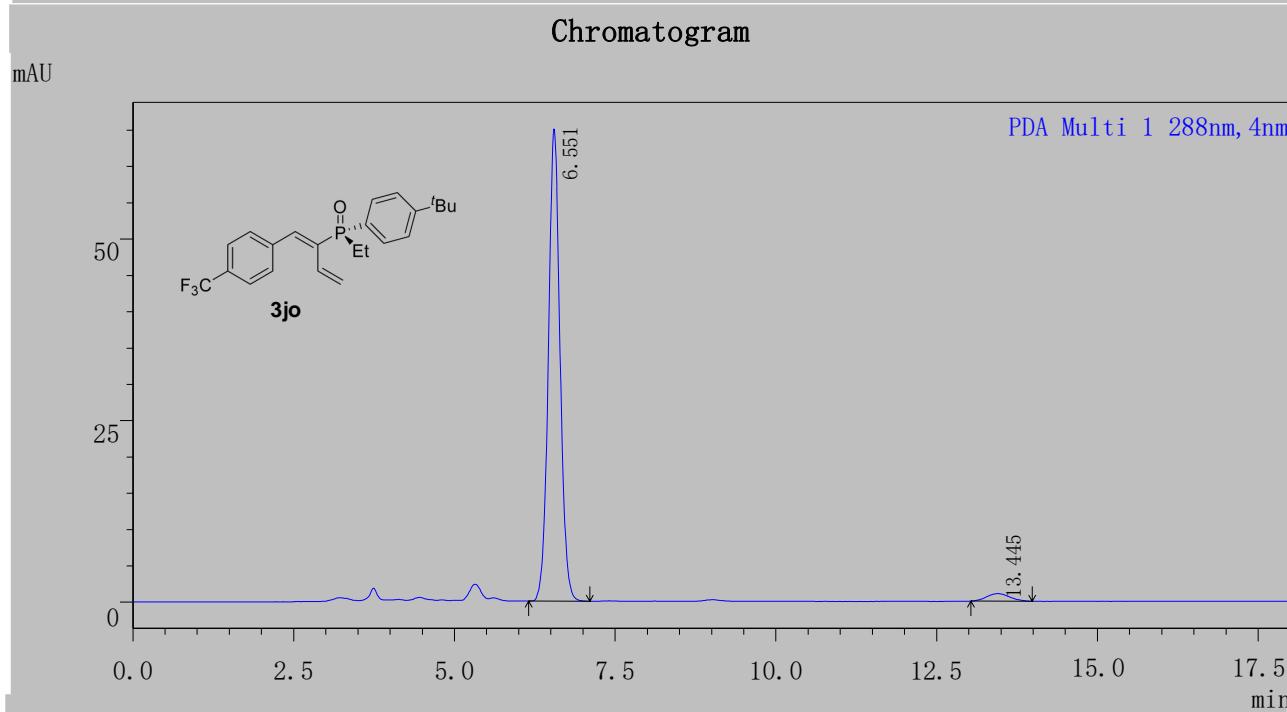
Peak#	Ret. Time	Area	Area%
1	5.068	2300025	97.432
2	11.805	60613	2.568
Total	2360638		100.000



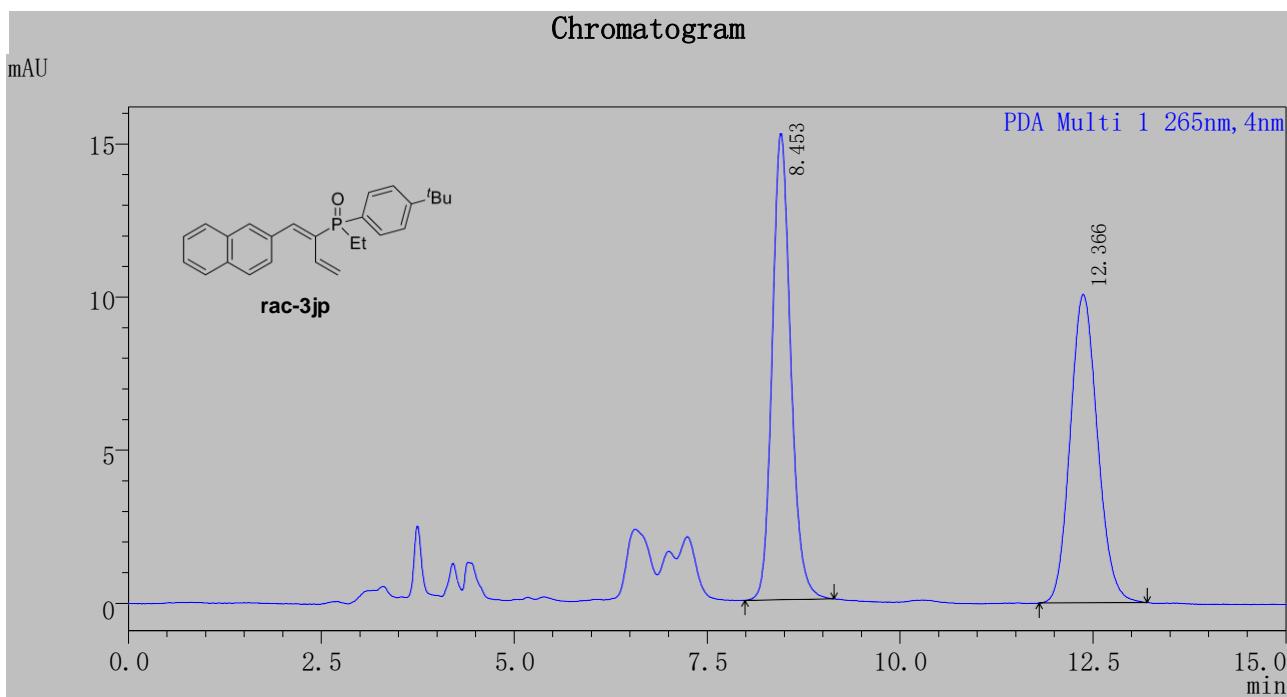




Peak#	Ret. Time	Area	Area%
1	6.755	893376	49.926
2	14.275	896017	50.074
Total	1789393		100.000

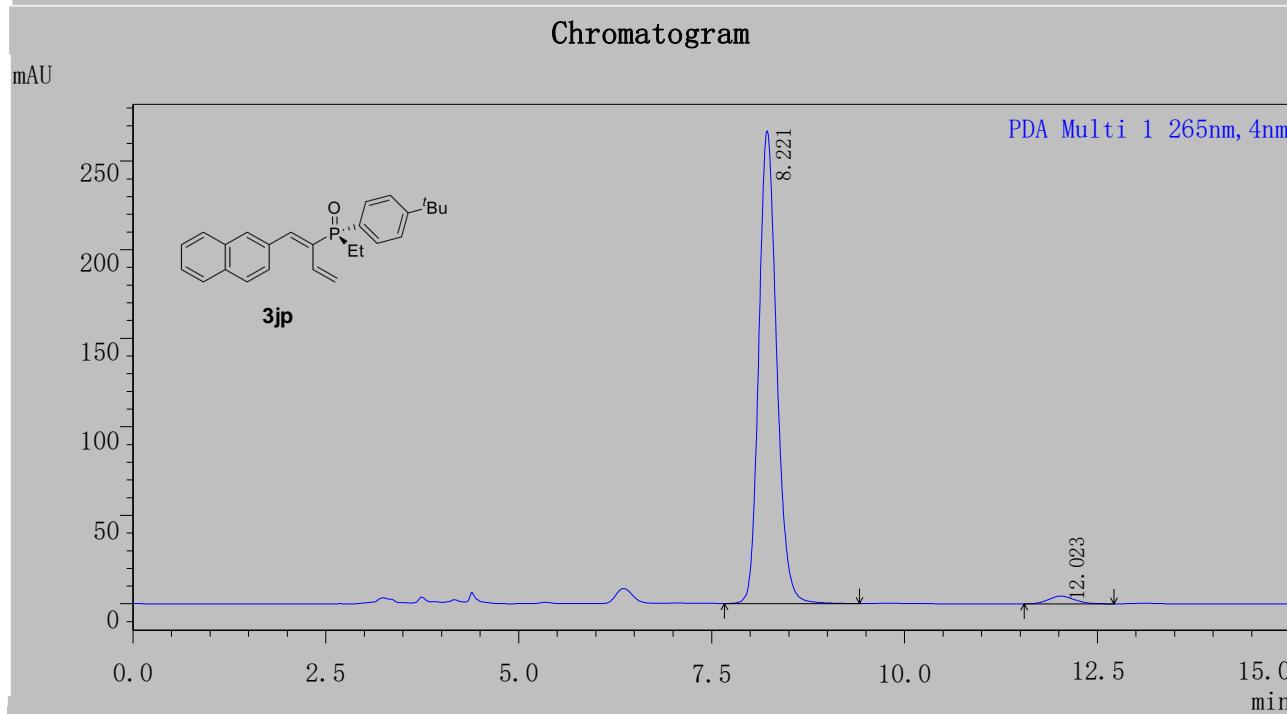


Peak#	Ret. Time	Area	Area%
1	6.551	824915	96.994
2	13.445	25570	3.006
Total	850484		100.000



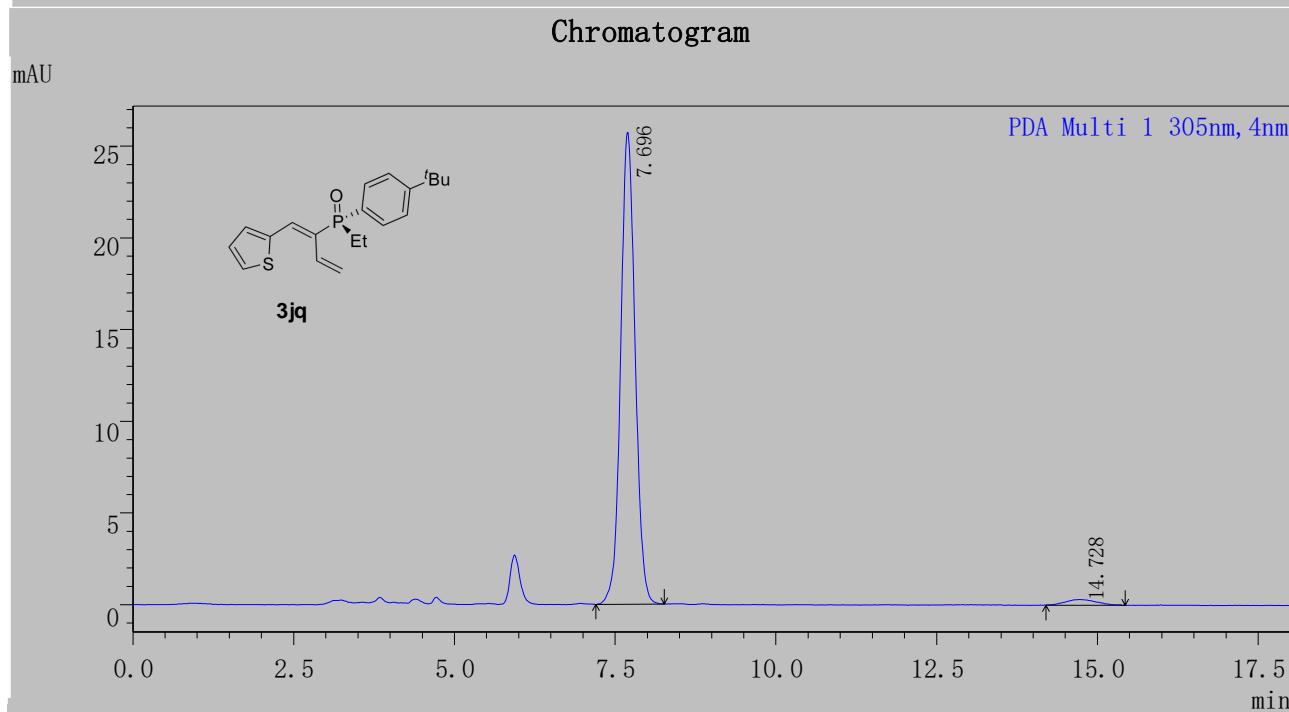
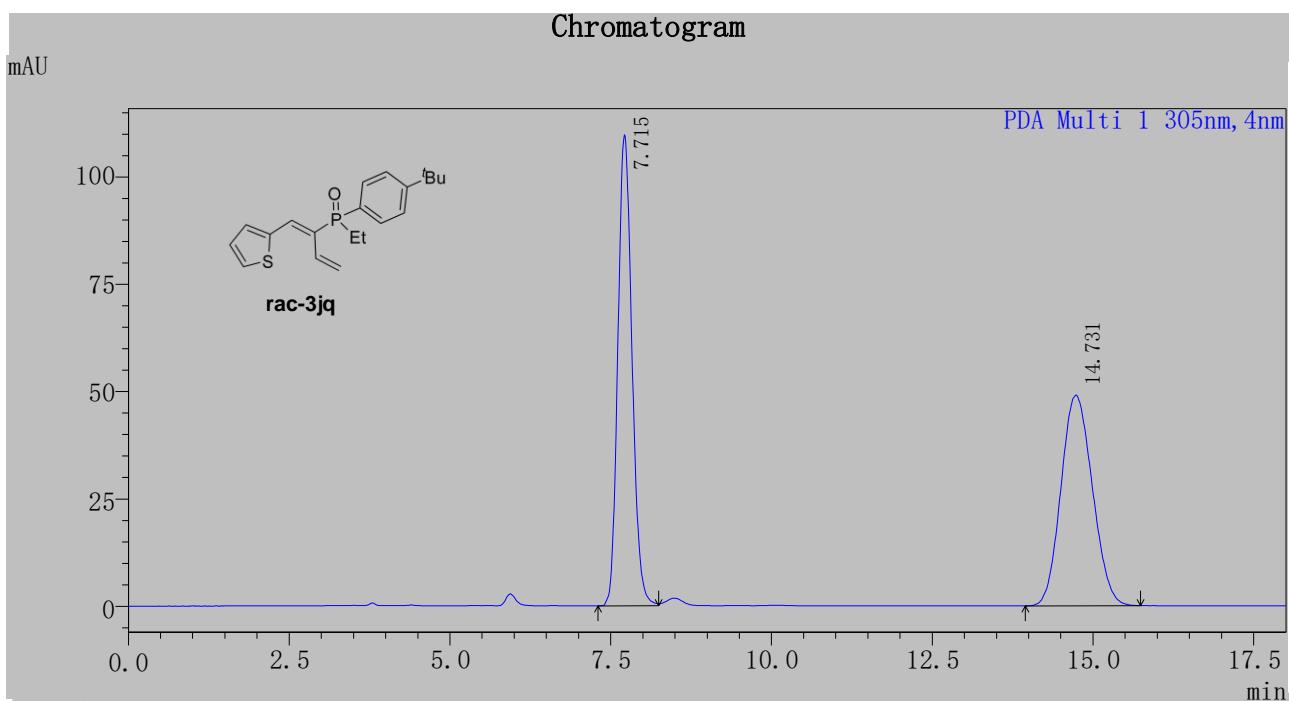
PDA Ch1 265nm

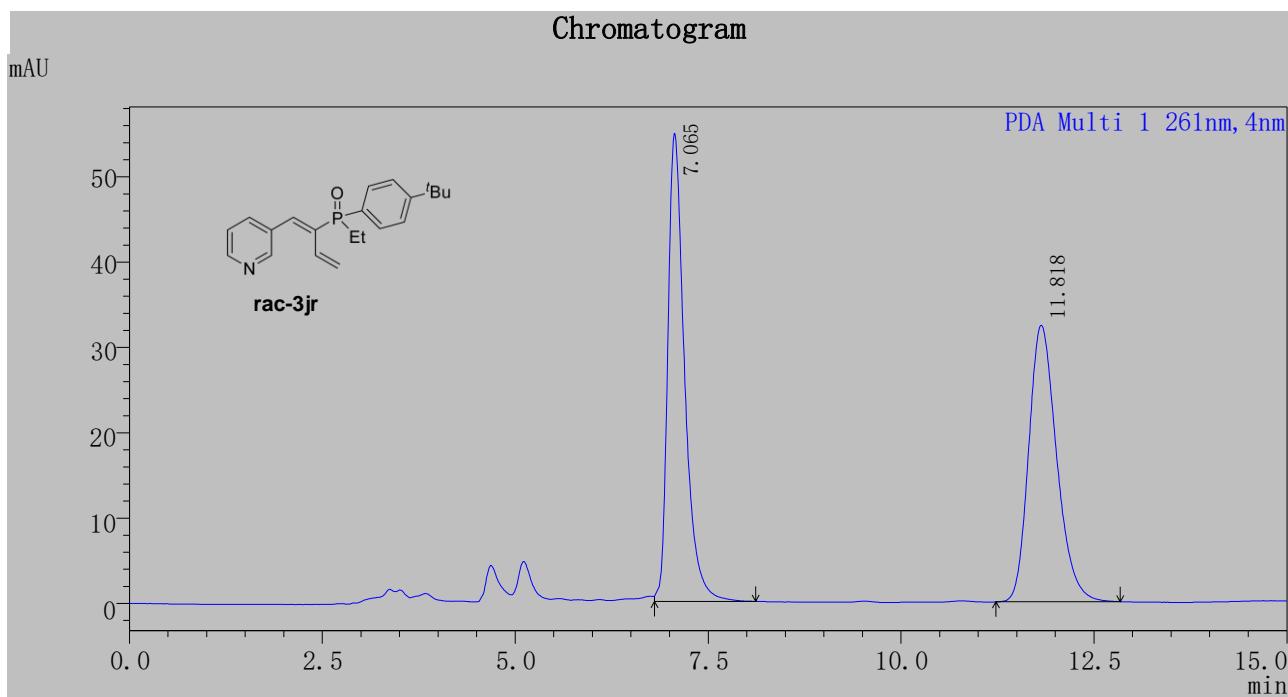
Peak#	Ret. Time	Area	Area%
1	8.453	253919	50.627
2	12.366	247634	49.373
Total		501553	100.000



PDA Ch1 265nm

Peak#	Ret. Time	Area	Area%
1	8.221	4298086	97.676
2	12.023	102258	2.324
Total		4400344	100.000



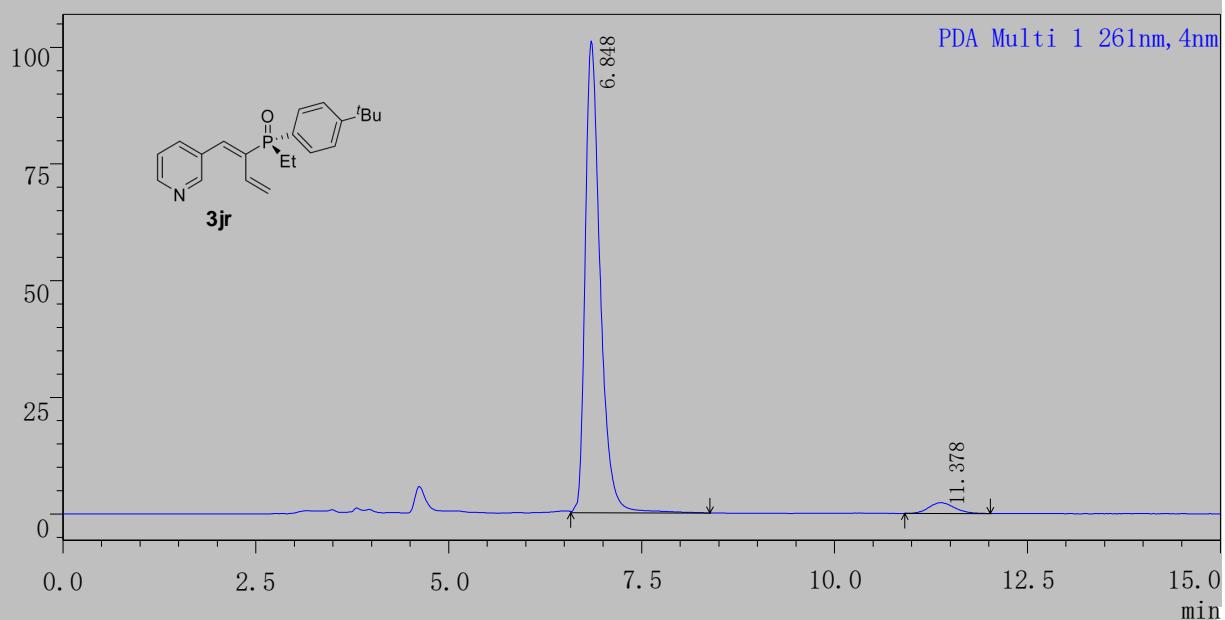


PDA Ch1 261nm

Peak#	Ret. Time	Area	Area%
1	7.065	828156	50.294
2	11.818	818471	49.706
Total	1646626		100.000

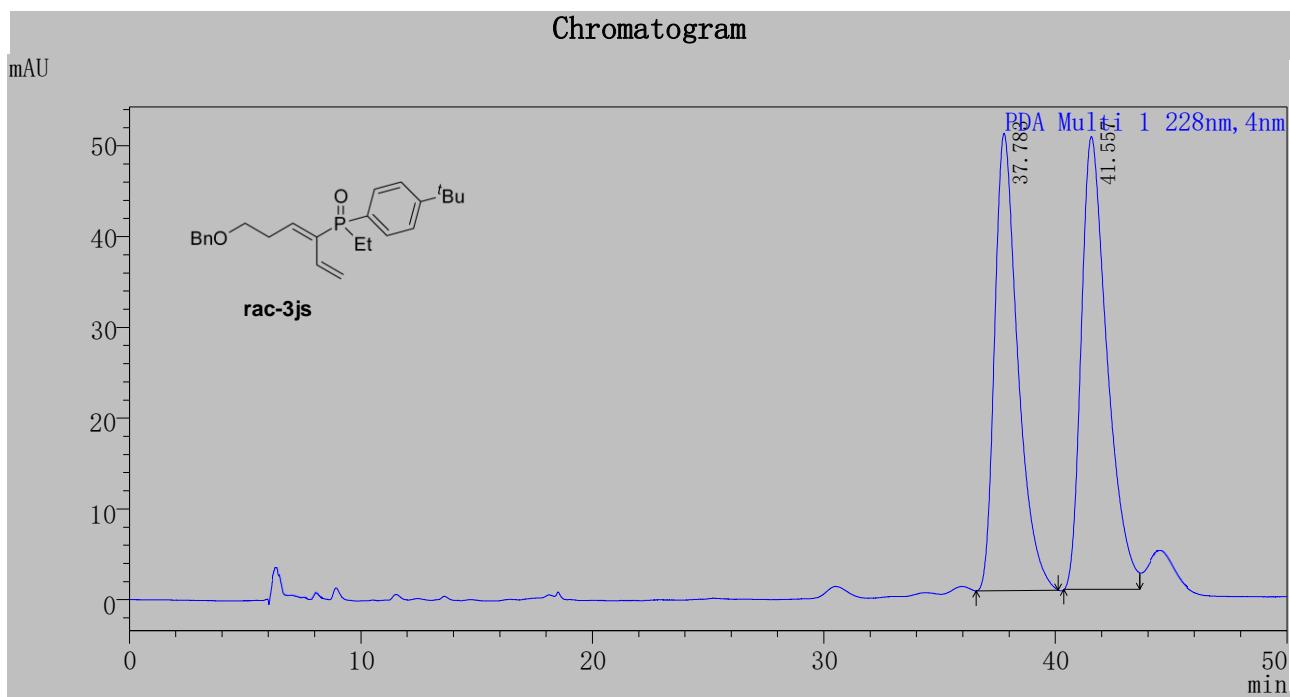
Chromatogram

mAU

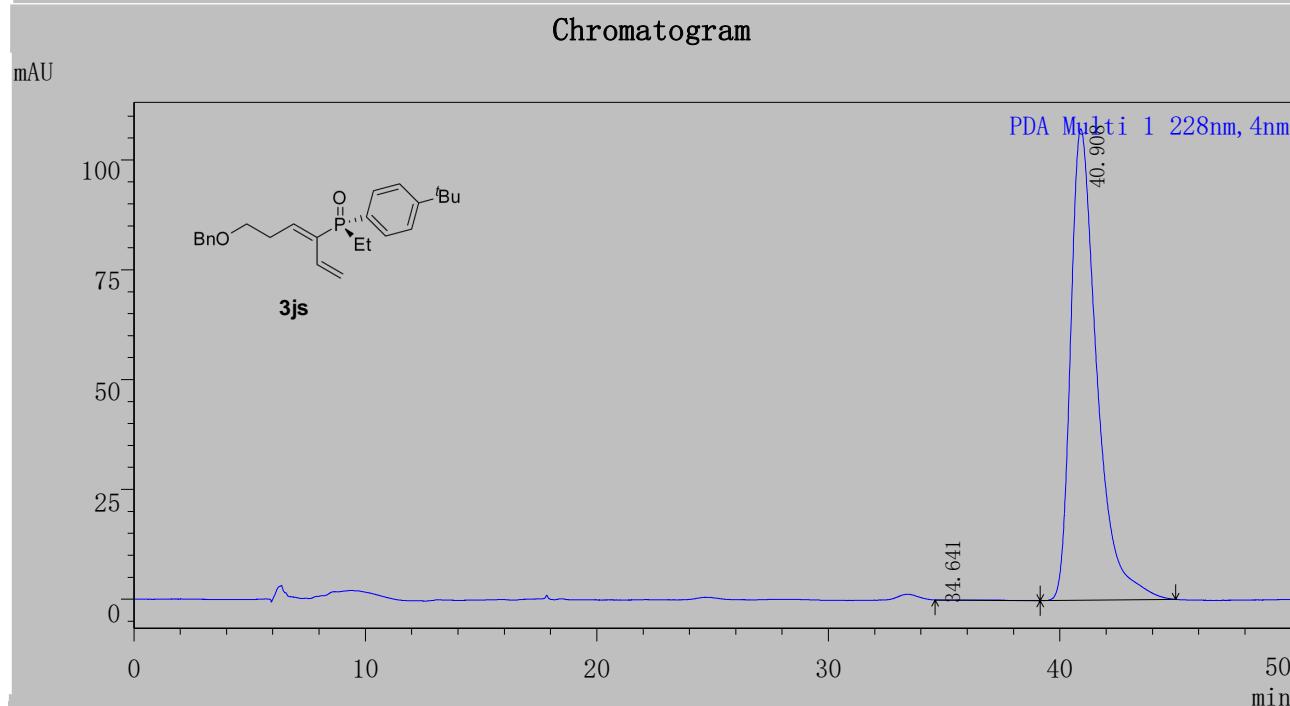


PDA Ch1 261nm

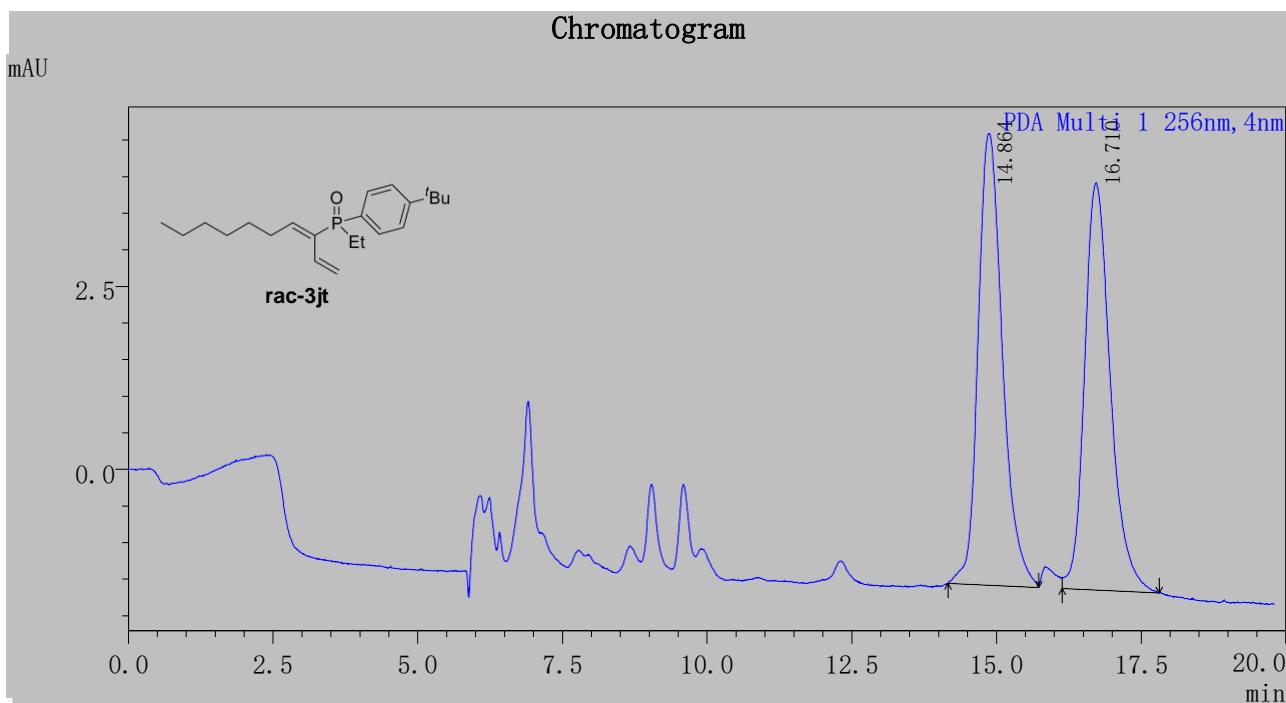
Peak#	Ret. Time	Area	Area%
1	6.848	1364398	96.212
2	11.378	53723	3.788
Total	1418120		100.000



PDA Ch1 228nm	Peak#	Ret. Time	Area	Area%
	1	37.783	3528024	47.607
	2	41.557	3882683	52.393
	Total		7410707	100.000



PDA Ch1 228nm	Peak#	Ret. Time	Area	Area%
	1	34.641	2222	0.026
	2	40.908	8465432	99.974
	Total		8467654	100.000

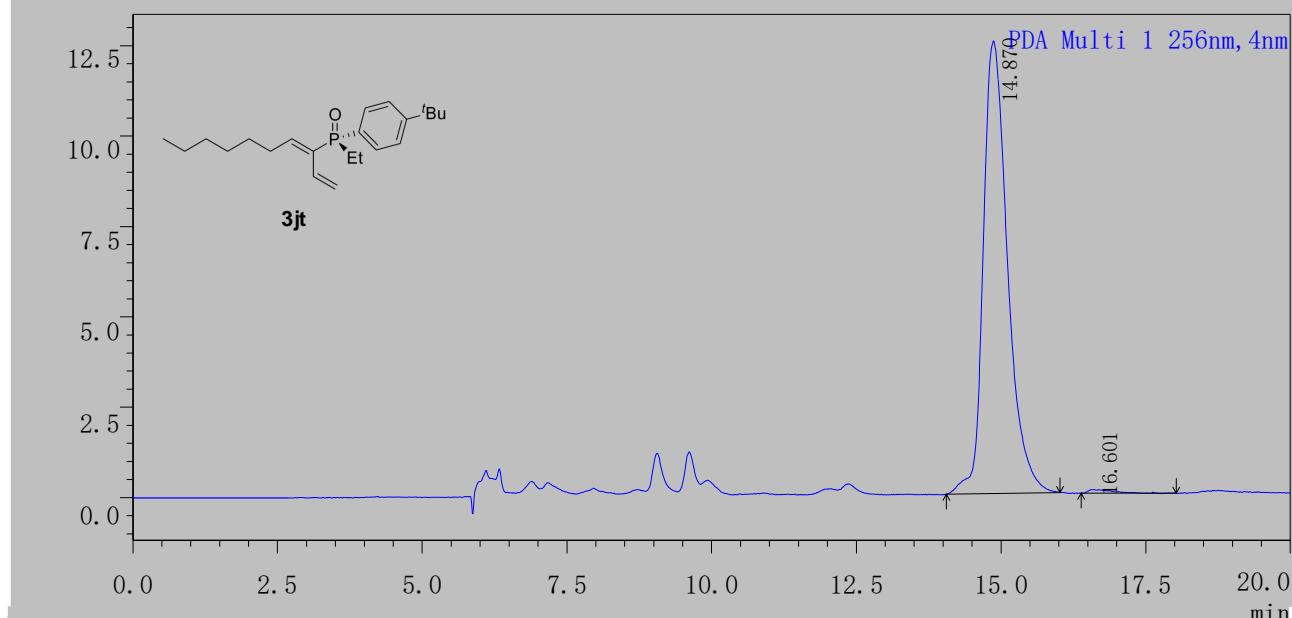


PDA Ch1 256nm

Peak#	Ret. Time	Area	Area%
1	14.864	180485	51.096
2	16.710	172742	48.904
Total		353226	100.000

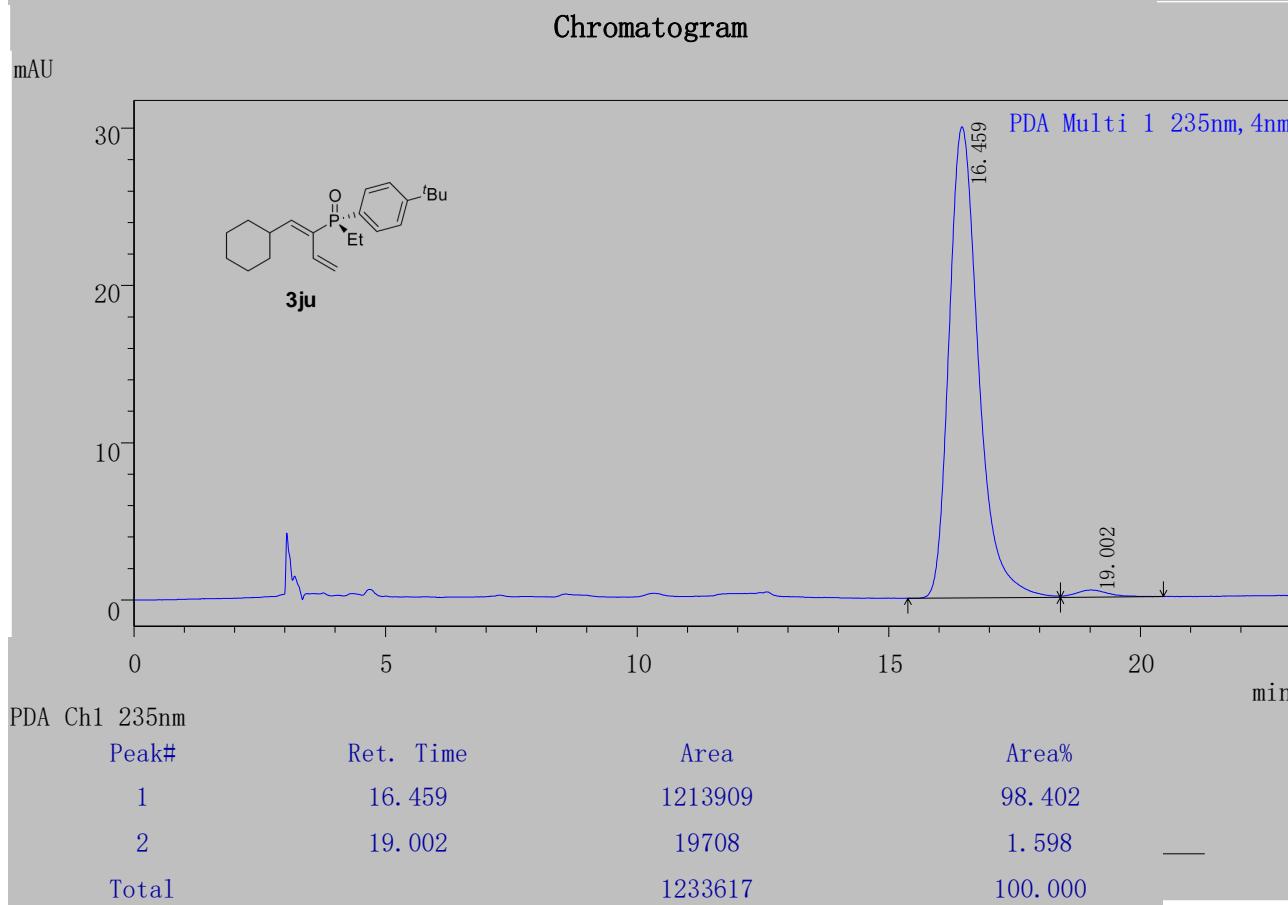
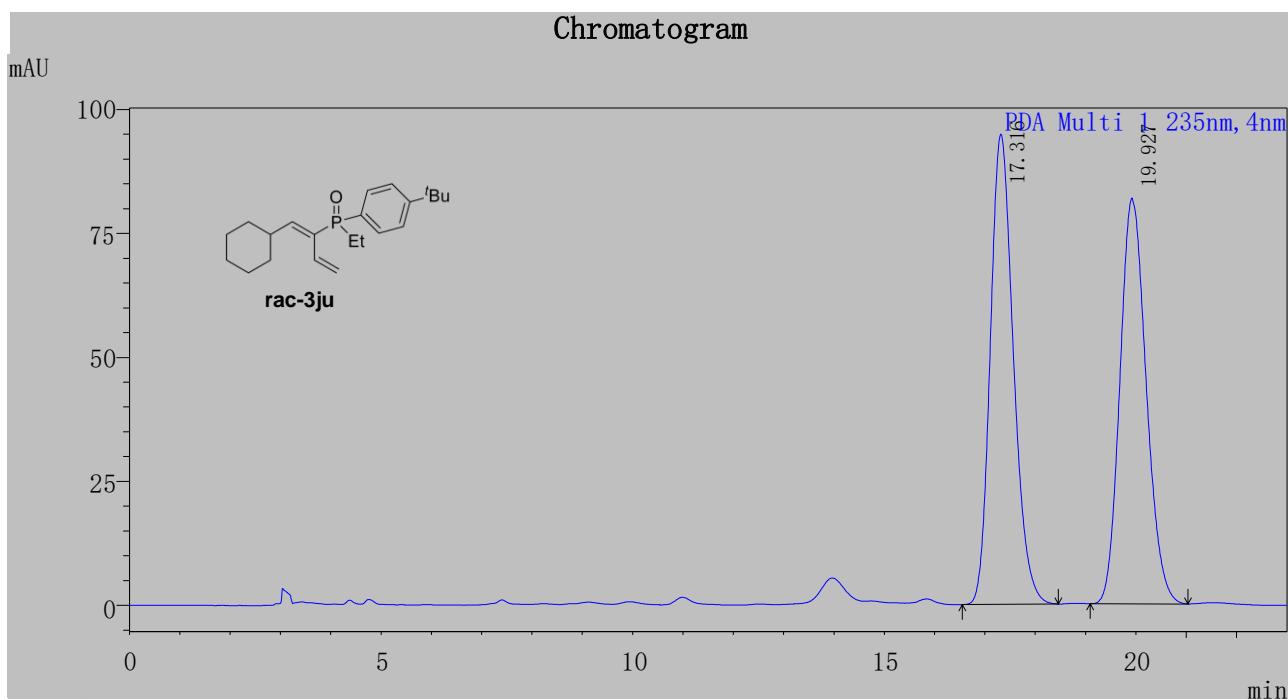
Chromatogram

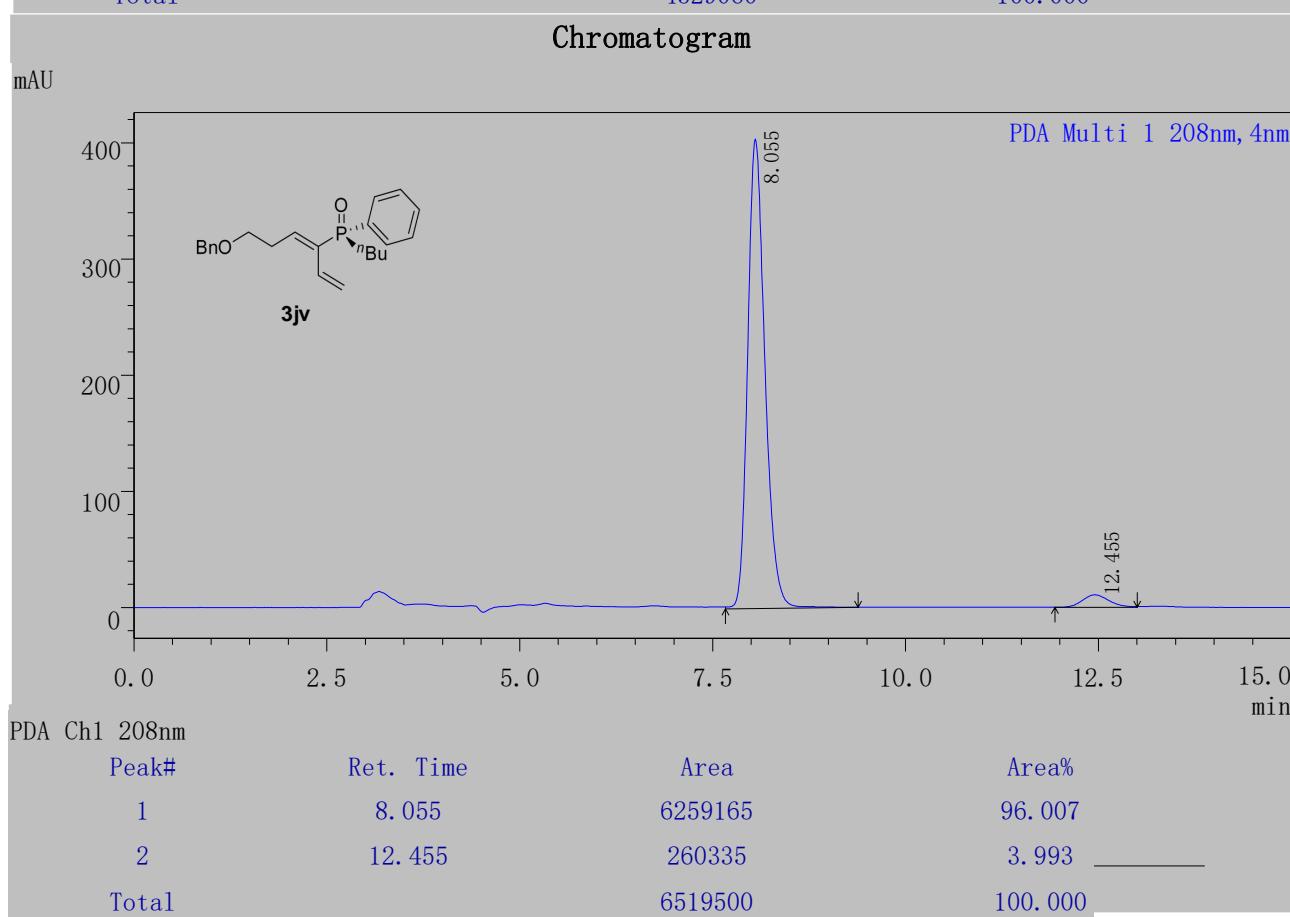
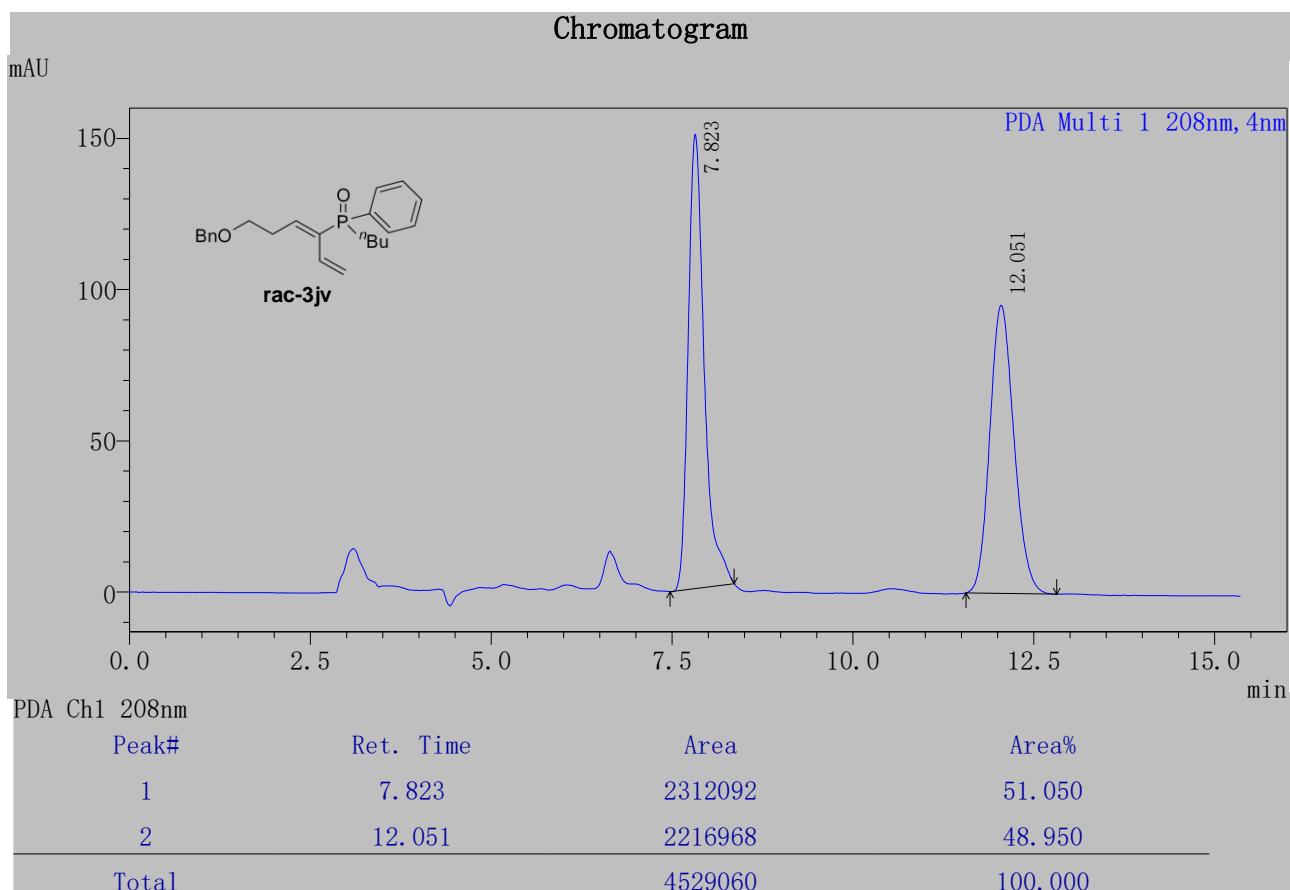
mAU

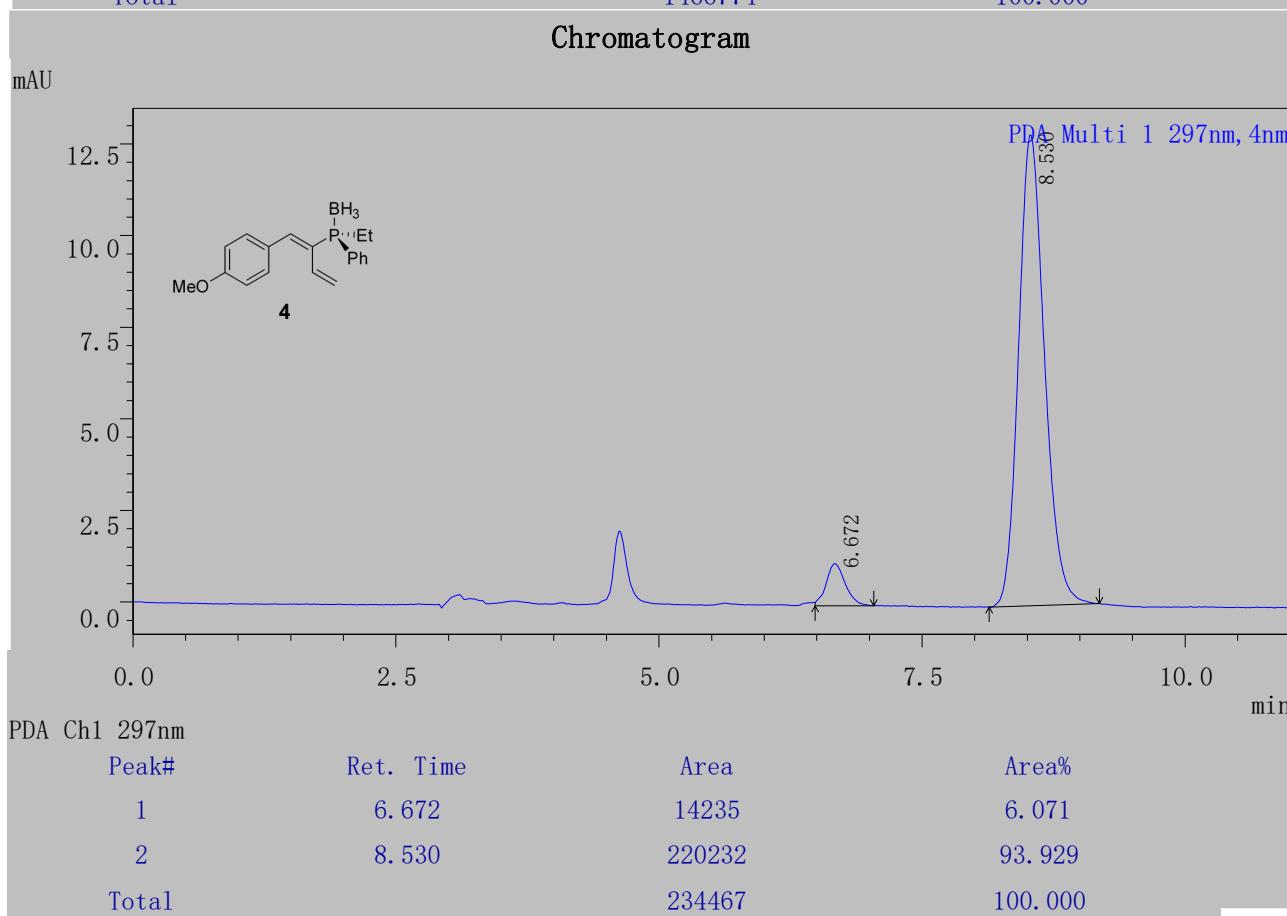
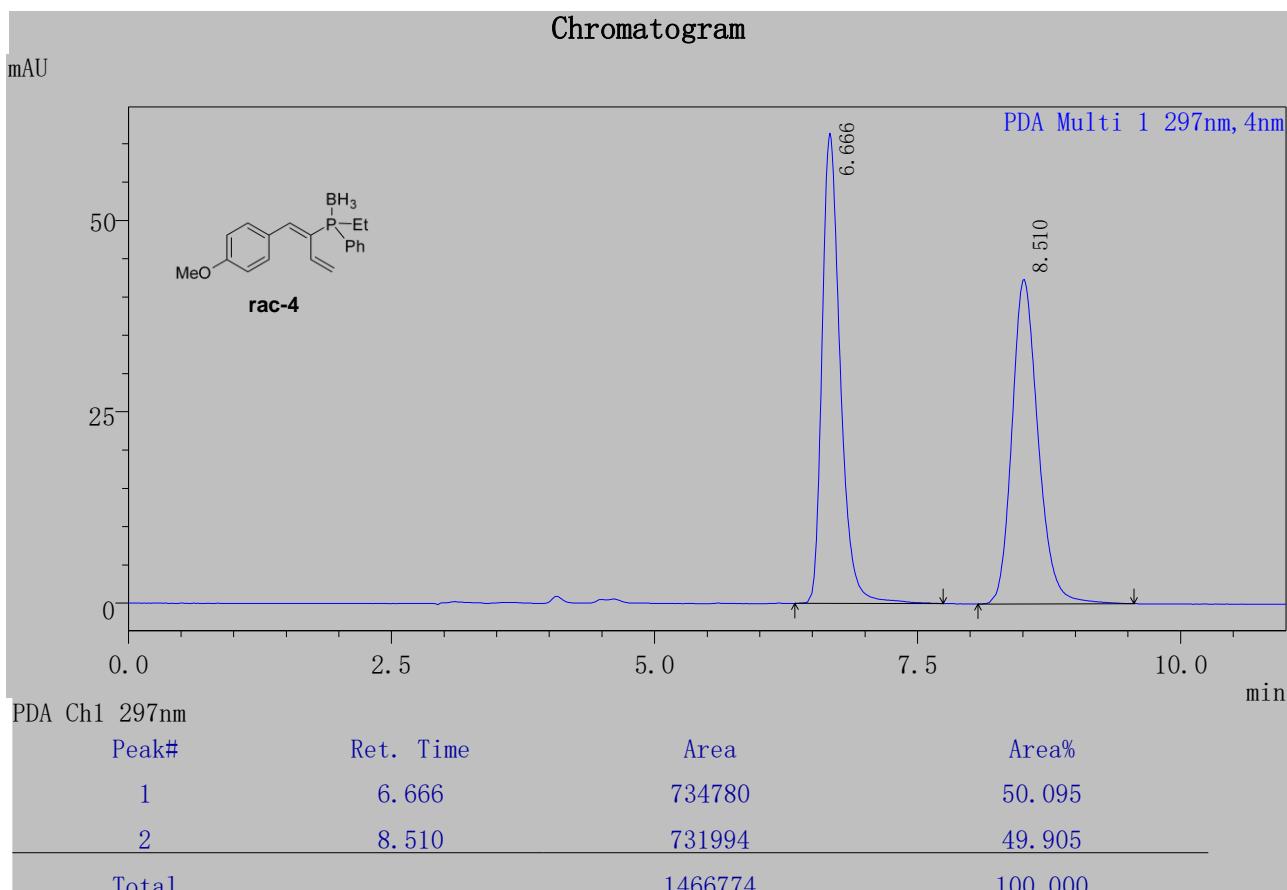


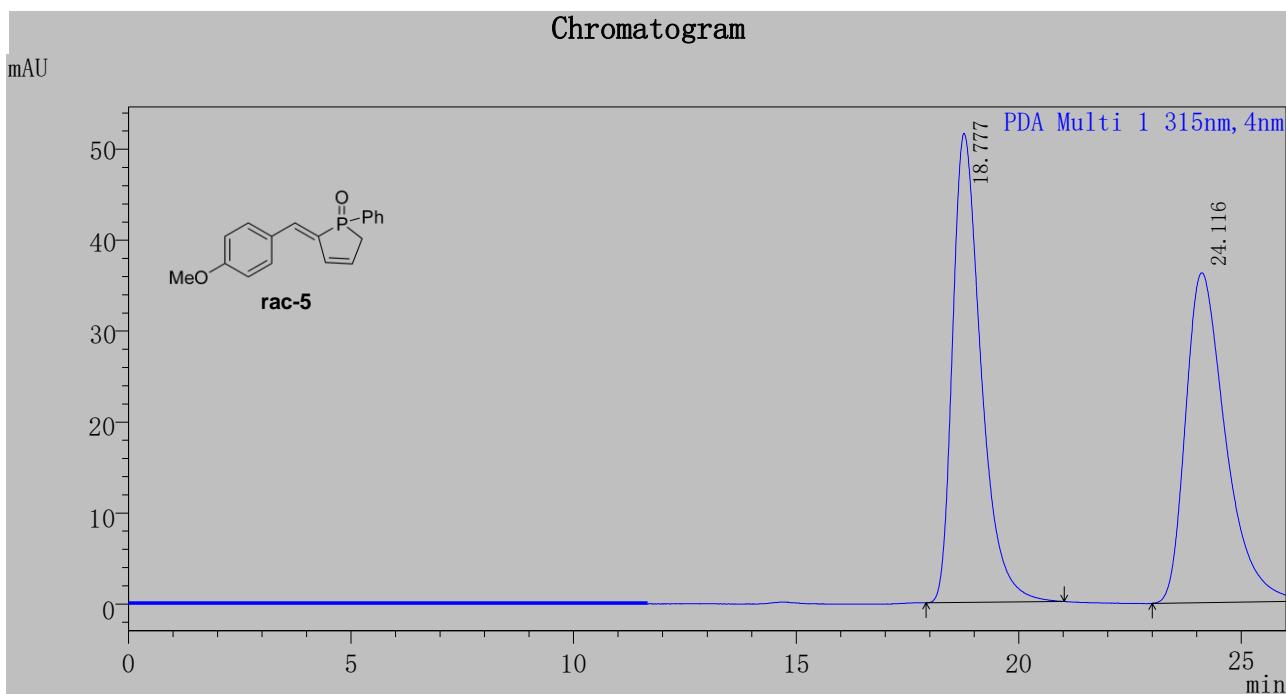
PDA Ch1 256nm

Peak#	Ret. Time	Area	Area%
1	14.870	365018	99.306
2	16.601	2552	0.694
Total		367570	100.000



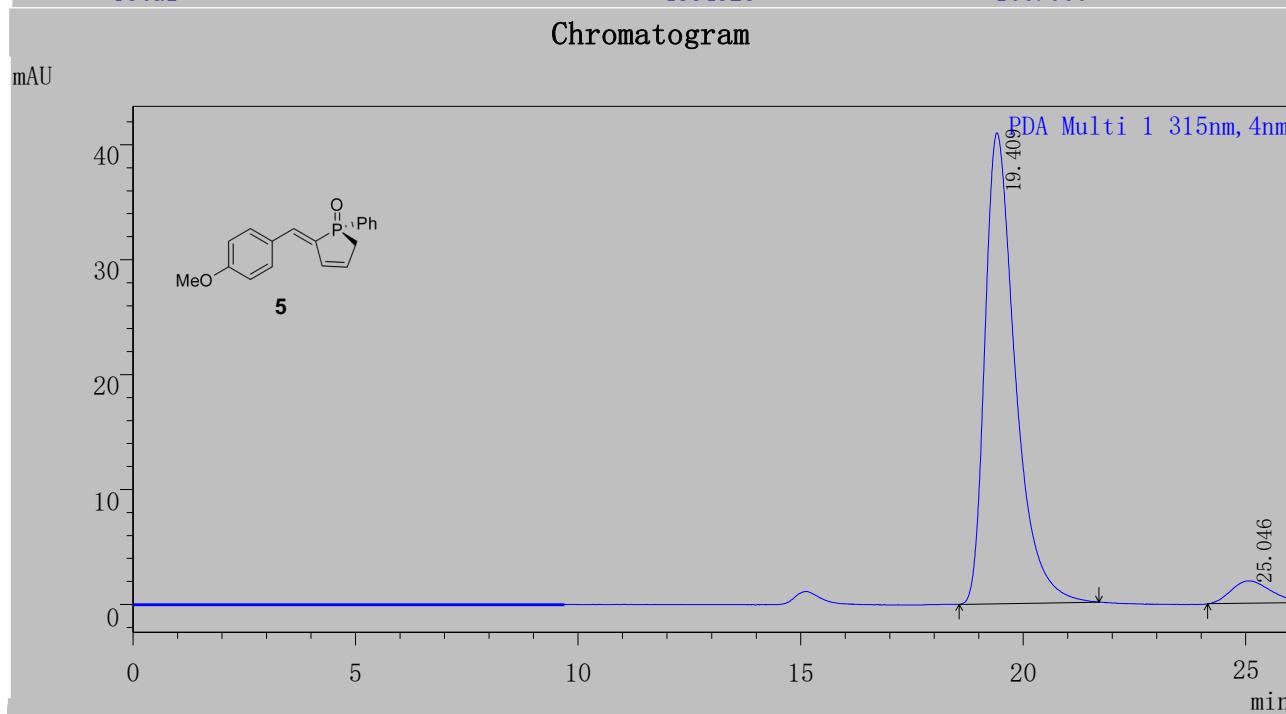






PDA Ch1 315nm

Peak#	Ret. Time	Area	Area%
1	18.777	2290014	50.282
2	24.116	2264314	49.718
Total		4554328	100.000



PDA Ch1 315nm

Peak#	Ret. Time	Area	Area%
1	19.409	1942185	94.131
2	25.046	121100	5.869
Total		2063285	100.000