

Formal Asymmetric Cycloaddition of Activated α,β -Unsaturated Ketones with α -Diazomethylphosphonate Mediated by a Chiral Silver SPINOL Phosphate Catalyst

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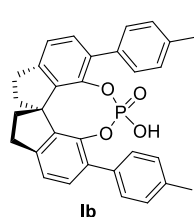
1. General methods

All solvents were purified by standard procedures and distilled prior to use. Reagents obtained from commercial source were used without further purification. Petroleum ether and ethyl acetate for flash column chromatography were distilled before use. All reactions were monitored by TLC with silica gel coated plates. Flash column chromatography was performed on silica gel H (10–40 μ). NMR spectra were recorded on 600 MHz instruments. Chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. Optical rotations were measured on a Perkin Elmer 341 Polarimeter at $\lambda = 589$ nm. Analytical high performance liquid chromatography (HPLC) was carried out on WATERS 510 instrument (2487 Dual λ Absorbance Detector and 515 HPLC Pump) using chiral column. ESI HRMS was recorded on a Bruker Apex-2.

2. Synthesis of chiral phosphoric acids

SPAs were synthesized following the procedure described in the literature.^[1]

(Ra)-12-hydroxy-1,10-bis(4-methylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide

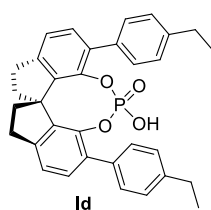


(1b)

White solid, mp 136.2–137.5 °C, $[\alpha]_D^{25} = -383.8^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.37–7.31 (m, 2H), 7.26 (d, $J = 2.4$ Hz, 2H), 7.24 (s, 2H), 7.14 (d, $J = 7.6$ Hz, 2H), 6.84 (d, $J = 7.2$ Hz, 4H), 3.16–3.06 (m, 2H), 2.88 (dd, $J = 15.9, 7.7$ Hz, 2H), 2.32 (dd, $J = 11.8, 6.3$ Hz, 2H), 2.21 (s, 2H), 2.10 (s, 6H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ

145.0, 142.4, 140.6, 136.6, 135.0, 134.5, 130.2, 129.4, 128.9, 128.5, 127.6, 127.0, 122.6, 60.1, 38.7, 30.2, 20.9 ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{31}\text{H}_{27}\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 517.1545, found 517.1548.

(Ra)-12-hydroxy-1,10-bis(4-ethylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide

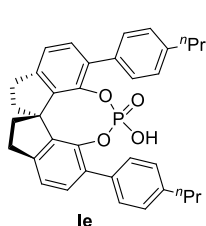


(1d)

White solid, mp 119.2–121.5 °C, $[\alpha]_D^{25} = -393.8^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.31–7.20 (m, 7H), 7.13 (d, $J = 7.6$ Hz, 2H), 6.87 (d, $J = 7.6$ Hz, 3H), 3.16–3.02 (m, 2H), 2.89 (dd, $J = 16.0, 7.8$ Hz, 2H), 2.47–2.37 (m, 4H), 2.31 (dd, $J =$

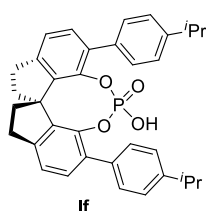
12.0, 6.4 Hz, 2H), 2.23–2.16 (m, 2H), 1.03 (t, $J = 7.5$ Hz, 6H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 144.9, 142.6, 140.6, 135.3, 134.5, 130.2, 129.4, 127.7, 122.4, 60.1, 38.7, 30.2, 28.3, 15.0 ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{33}\text{H}_{31}\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 545.1858, found 545.1859.

(Ra)-12-hydroxy-1,10-bis(4-propylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide
(1e)



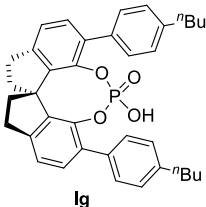
White solid, mp 132.5–134.5 °C, $[\alpha]_D^{25} = -394.8^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.36–7.32 (m, 2H), 7.24–7.22 (m, 4H), 7.13 (d, $J = 7.4$ Hz, 2H), 6.92 (d, $J = 7.9$ Hz, 4H), 3.09 (d, $J = 6.4$ Hz, 2H), 2.87 (dd, $J = 15.8$, 7.6 Hz, 2H), 2.32 (dd, $J = 16.6$, 8.0 Hz, 6H), 2.15 (d, $J = 4.2$ Hz, 2H), 1.45 (dd, $J = 13.2$, 6.2 Hz, 4H), 0.86–0.74 (m, 6H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 144.8, 142.4, 141.3, 140.5, 135.0, 134.8, 130.2, 129.2, 128.5, 128.1, 127.6, 127.0, 122.4, 60.0, 38.6, 37.7, 30.3, 24.1, 14.0 ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{35}\text{H}_{35}\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 573.2171, found 573.2170.

(Ra)-12-hydroxy-1,10-bis(4-isopropylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide (If)



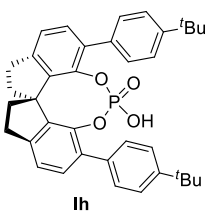
White solid, mp 128.7–130.5 °C, $[\alpha]_D^{25} = -401.3^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.19–7.14 (m, 6H), 7.06 (d, $J = 7.4$ Hz, 2H), 6.91 (d, $J = 7.3$ Hz, 4H), 3.02 (t, $J = 16.2$ Hz, 2H), 2.80 (dd, $J = 15.7$, 7.5 Hz, 2H), 2.63 (dt, $J = 13.7$, 6.8 Hz, 2H), 2.23 (dd, $J = 11.4$, 6.0 Hz, 2H), 2.12–2.00 (m, 2H), 1.05–0.97 (m, 3H), 0.98–0.88 (m, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 147.2, 144.8, 142.4, 140.5, 135.1, 134.7, 130.2, 129.3, 126.2, 122.4, 60.0, 38.6, 33.6, 30.2, 23.9, 23.4 ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{35}\text{H}_{35}\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 573.2171, found 573.2170.

(Ra)-12-hydroxy-1,10-bis(4-butylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide (Ig)



White solid, mp 122.4–123.5 °C, $[\alpha]_D^{25} = -405.8^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.34 (d, $J = 6.7$ Hz, 2H), 7.29 (d, $J = 7.1$ Hz, 2H), 7.24 (s, 2H), 7.14 (d, $J = 7.3$ Hz, 2H), 6.92 (d, $J = 7.8$ Hz, 4H), 3.10 (dd, $J = 20.0$, 11.9 Hz, 2H), 2.87 (dd, $J = 15.6$, 7.3 Hz, 2H), 2.36 (s, 2H), 2.32 (dd, $J = 17.6$, 8.4 Hz, 4H), 2.15 (s, 2H), 1.52–1.35 (m, 4H), 1.32–1.22 (m, 4H), 0.83 (ddd, $J = 9.6$, 4.8, 2.5 Hz, 6H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 144.8, 142.4, 141.5, 140.5, 134.9, 130.2, 129.2, 128.5, 128.1, 127.6, 127.1, 122.4, 60.0, 38.7, 35.2, 33.2, 30.3, 22.5, 13.9 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{37}\text{H}_{39}\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 601.2484, found 601.2488.

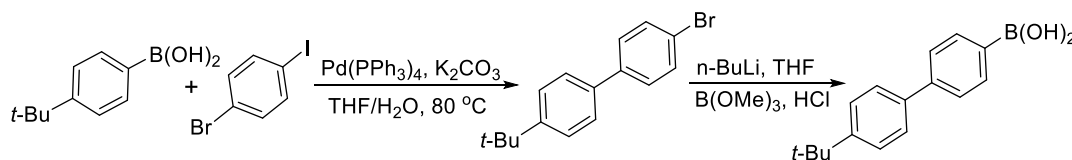
(Ra)-12-hydroxy-1,10-bis(4-tert-butylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide (Ih)



White solid, mp 139.2–141.3 °C, $[\alpha]_D^{25} = -456.7^\circ$ ($c = 1.0$, CHCl_3); ^1H NMR (600 MHz, CDCl_3) δ 7.34 (s, 2H), 7.24–7.21 (m, 4H), 7.18 (d, $J = 6.9$ Hz, 4H), 7.12 (d, $J = 7.5$ Hz, 2H), 3.13–3.03 (m, 2H), 2.86 (dd, $J = 15.7$, 7.7 Hz, 2H), 2.29 (dd, $J = 11.8$, 6.2 Hz, 2H), 2.09 (dd, $J = 20.4$, 10.1 Hz, 2H), 1.11 (s, 18H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ

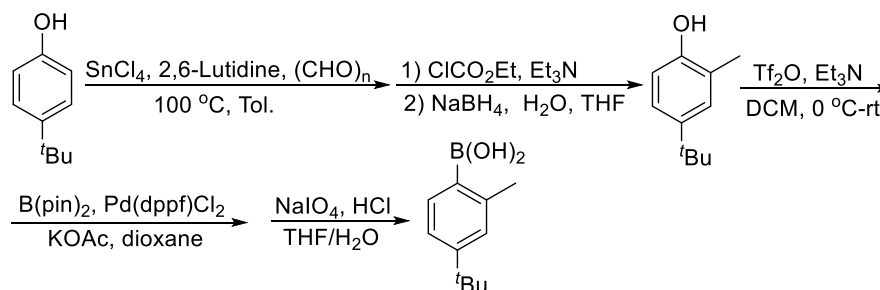
144.8, 142.4, 141.3, 140.5, 135.0, 134.8, 130.2, 129.2, 128.5, 128.1, 127.6, 127.0, 122.4, 38.6, 37.7, 30.4, 24.1, 14.0 ppm. HRMS (ESI-TOF) calcd. for $C_{37}H_{39}O_4PNa$ $[M+Na]^+$ 601.2484, found 601.2484.

Partial intermediates for the synthesis of chiral phosphoric acids were prepared as the following procedure:



$Pd(PPh_3)_4$ 115 mg (0.1 mmol) was added to the mixture of 4-*tert*-butylphenylboronic acid 3.6 g (20 mmol), *p*-bromoiodobenzene 5.6 g (20 mmol) and K_2CO_3 5.5 g (40 mmol) in 80mL degassing THF/ H_2O = 3:1 (v:v) under an Ar atmosphere in a round-bottomed flask. The reaction was stirred at 80 °C until the starting material was disappear, then the mixture was concentrated under reduce pressure and the residue was extracted with EA, combined organic layer and washed with saturated NaCl, dried over with Na_2SO_4 and concentrated under reduce pressure, the residue was purified by flash chromatography on silica gel to give 4-bromo-4'-(*tert*-butyl)-1,1'-biphenyl.

To the solution of 4-bromo-4'-(*tert*-butyl)-1,1'-biphenyl 2.9 g (10 mmol) in dry THF (50 mL), *n*-butyllithium 6.3 mL (15 mmol) was slowly added with stirring at -78 °C. The reaction was maintained at -78 °C until starting material was disappear, then trimethylborate 2.3 mL (20 mmol) was added slowly, the mixture was warmed up to rt slowly and stirred overnight. 1 N HCl was added to until pH = 1 and stirred for another 2 h. The mixture was extracted with EA, combined organic layer and washed with saturated NaCl, dried over with Na_2SO_4 and concentrated under reduce pressure, the residue was purified by flash chromatography on silica gel to afford 4-*tert*-butylbiphenyl-4-ylboronic acid.^[2]



$SnCl_4$ 2.6 mL (40 mmol in 100 mL Tol) was added slowly to the solution of 4-*tert*-Butylphenol 15 g (100 mmol) and 2,6-lutidine 16 g (150 mmol) in dry toluene (300 mL) at room temperature. The mixture was stirred for 30 min, polyoxymethylene 19.5 g (650 mmol) was added in one portion and stirred overnight at 100 °C.

The mixture was filtrated and washed with DCM, dried over with Na₂SO₄ and concentrated under reduce pressure; the residue was purified by flash chromatography on silica gel to give the product.

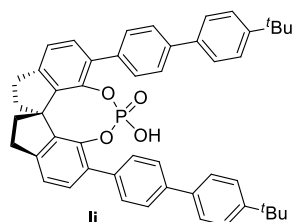
Ethyl carbonochloridate 5.7 mL (60 mmol) was added dropwise to the mixture of above obtained products 8.9 g (50 mmol) and triethylamine 9 mL (65 mmol) in 100 mL dry THF at 0 °C. The resulted mixture was strried for another 30 min, filtrated and washed with little THF. To the solution was added NaBH₄ 7.6 g (200 mmol in 75 mL H₂O) in ice bath, and stirred until the starting material was disappear, 2 N HCl was added to adjust the pH = 2. The mixture was concentrated and extracted with EA. The solution was dried over with Na₂SO₄ and concentrated under reduce pressure, and the residue was purified by flash chromatography on silica gel to give 4-*tert*-butyl-2-methylphenol.

Tf₂O 7 mL (50 mmol) was added dropwise to the solution of 4-*tert*-butyl-2-methylphenol 6.6 g (40 mmol) and Et₃N 8.3 mL (60 mmol) in 100 mL dry DCM at 0 °C. The mixture was stirred until the start material was disappeared, after working up, the desired product was achieved by flash chromatography on silica gel.

Pd(dppf)Cl₂ 366 mg (0.5 mmol) was added to the mixture of the above product 8.9 g (30 mmol), B(pin)₂ 9.1 g (36 mmol) and KOAc 20.6 g (210 mmol) in degassing dioxane 70 mL under an Ar atmosphere in a round-bottomed flask. The mixture was refluxed untill the start material was disappear, the mixture was filtrated and washed with Et₂O, combined organic layer and washed with saturated NaCl, dried over with Na₂SO₄ and concentrated under reduce pressure, and the boronate was achieved by flash chromatography on silica gel.

NaIO₄ 12.8 g (60 mmol) was added to the solution of the above obtained boronate 5.5 g (20 mmol) in THF/H₂O (v:v = 4:1) (150 mL), the mixture was stirred for 30 min at rt, then 1 N HCl (20 mL) was added. The mixture was stirred at room temperature untill the start material was disappear, THF was removed, and the residue was extracted with Et₂O, combined the organic layers and dried over with Na₂SO₄, concentrated under reduce pressure and the residue was purified by flash chromatography on silica gel to achieve the 4-*tert*-butyl-2-methylphenylboronic acid.^[3]

(Ra)-12-hydroxy-1,10-bis(4'-*tert*-butylbiphenyl-4-yl)-4,5,6,7-tetrahydrodiindeno[1,3,2]dioxaphosphocine 12-oxide (II)



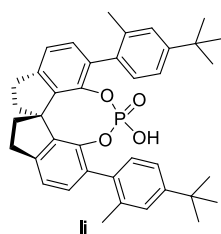
White solid, mp 207.8–209.0 °C, $[\alpha]_D^{25} = -399.7^\circ$ ($c = 1.0$, CHCl₃); ¹H NMR (600 MHz, CDCl₃) δ 7.36 (d, $J = 7.5$ Hz, 3H), 7.27 (d, $J = 7.7$ Hz, 2H), 7.24–7.19 (m, 5H), 7.17 (t, $J = 8.1$ Hz, 6H), 7.11 (d, $J = 7.8$ Hz, 4H), 3.17–3.03 (m, 2H), 2.91 (dd, $J = 16.0, 7.8$ Hz, 2H), 2.30 (dd, $J = 12.0, 6.3$ Hz, 2H),

2.18–2.13 (m, 2H), 1.29 (s, 18H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 149.6, 145.1, 142.5, 140.6, 139.7, 138.1,

136.5, 134.2, 130.3, 129.7, 128.5, 127.6, 127.2, 126.8, 125.2, 122.5, 60.1, 38.6, 34.4, 31.4, 30.3 ppm. HRMS

(ESI-TOF) calcd. for $C_{49}H_{47}O_4PNa$ $[M+Na]^+$ 753.3110, found 753.3111.

(Ra)-12-hydroxy-1,10-bis(4-(tert-butyl)-2-methylphenyl)-4,5,6,7-tetrahydrodiindeno[1,3,2]



dioxaphosphocine 12-oxide (lj)

White solid, mp 119.8–121.4 °C, $[\alpha]_D^{25} = -297.4^\circ$ ($c = 1.0$, $CHCl_3$); 1H NMR (600 MHz,

$CDCl_3$) δ 7.10 (s, 2H), 7.07 (d, $J = 6.7$ Hz, 2H), 7.02 (s, 2H), 6.98 (s, 4H), 3.15–3.04

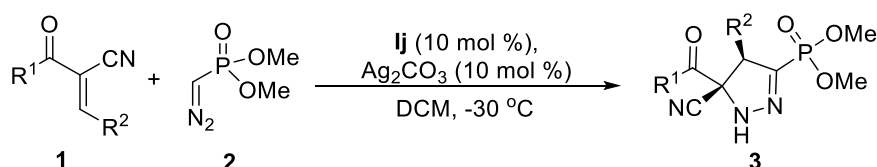
(m, 2H), 2.86 (dd, $J = 15.8, 7.8$ Hz, 2H), 2.29 (dd, $J = 11.6, 6.1$ Hz, 2H), 2.15 (d, $J =$

36.6 Hz, 2H), 2.06 (s, 6H), 1.13 (s, 18H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7,

144.7, 142.6, 139.8, 135.1, 134.9, 134.3, 131.0, 130.8, 125.6, 122.6, 122.3, 59.8, 38.6, 34.1, 31.3, 30.3, 29.7,

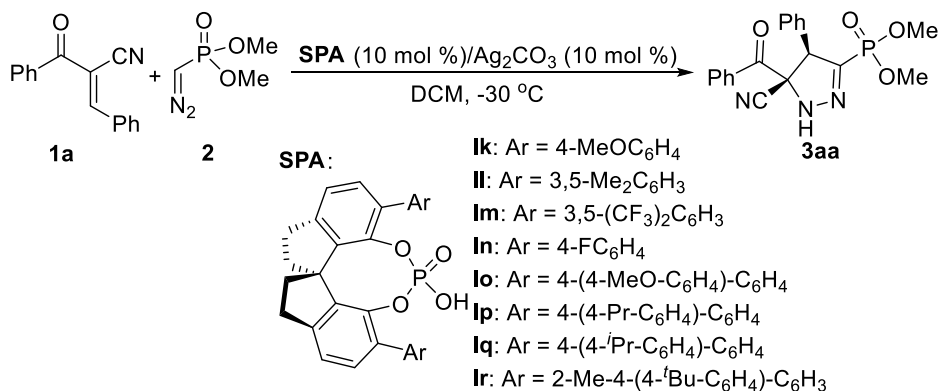
20.3 ppm. HRMS (ESI-TOF) calcd. for $C_{39}H_{43}O_4PNa$ $[M+Na]^+$ 629.2797, found 629.2793.

3. General procedure for asymmetric 1,3-dipolar cycloadditions reaction



SPA **lj** (10 mol %) and Ag_2CO_3 (10 mol %) were dissolved in anhydrous CH_2Cl_2 (1 mL) in a pre-dried tube under argon in the dark and stirred for 2 h at 30 °C. Next, α,β -unsaturated ketone **1** (0.3 mmol) was added and the system was cooled to -30 °C. Seyferth–Gilbert reagent **2** (0.2 mmol) was then added and the mixture was stirred and monitored by TLC until **2** had been completely consumed. The reaction mixture was then purified directly by flash chromatography on silica gel (30–50% $AcOEt$ /petroleum ether) to obtain the corresponding product.

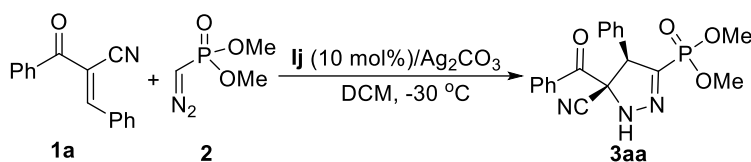
4. Asymmetric 1,3-dipolar cycloadditions reaction catalyzed by other catalysts^a



entry ^a	SPA	Time	yield(%) ^b	<i>dr</i> ^{c,d}	<i>ee</i> (%) ^d
1	Ik	3d	26	99:1	50
2	Il	3d	18	96:4	4
3	Im	3d	5	99:1	5
4	In	3d	8	99:1	26
5	Io	3d	26	99:1	64
6	Ip	3d	39	99:1	62
7	Iq	3d	39	99:1	70
8	Ir	3d	47	99:1	50

^aConditions: Unless noted otherwise, all of the reactions were carried out with **1a** (0.15 mmol), **2** (0.1 mmol), **SPA** (10 mol %) and Ag₂CO₃ (10 mol %) in 1.0 mL of DCM at -30 °C for 3 days; ^bIsolated yield; ^cRatio of the major diastereomer to the total of the other three ones; ^dDetermined by chiral HPLC

5. Partial results of reaction conditions optimization



entry ^a	solvent	con. (mol/L)	ratio (1a : 2)	ratio (Ij :Ag ₂ CO ₃)	yield (%) ^b	<i>dr</i> ^{c,d}	<i>ee</i> (%) ^d
1	DCM	0.1	2:1	1:1	65	99:1	85
2	DCM	0.1	1.5:1	1:2	55	97:3	74
3	DCM	0.1	1.5:1	1:1	60	99:1	85
4	CHCl ₃	0.1	1.5:1	1:1	40	95:5	50
5	DCE	0.1	1.5:1	1:1	47	99:1	79
6	<i>i</i> PrOH	0.1	1.5:1	1:1		Trace	
7	<i>m</i> -xylene	0.1	1.5:1	1:1	52	99:1	46
8	Toluene	0.1	1.5:1	1:1	65	99:1	65
9	F-Ph	0.1	1.5:1	1:1	60	99:1	53
10	THF	0.1	1.5:1	1:1	57	99:1	61
11	EA	0.1	1.5:1	1:1	39	99:1	64
12	CH ₃ CN	0.1	1.5:1	1:1	73	99:1	0
13	DCM	0.1	1:1	1:1	44	97:3	82
14	DCM	0.1	1.25:1	1:1	50	99:1	84
15	DCM	0.1	1.75:1	1:1	62	99:1	84
16	DCM	0.1	1:1.5	1:1	53	99:1	83
17 ^e	DCM	0.1	1.5:1	1:1	47	99:1	85
18 ^f	DCM	0.1	1.5:1	1:1	65	97:3	85
19 ^g	DCM	0.1	1.5:1	1:1	78	99:1	80

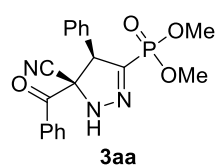
20 ^b	DCM	0.1	1.5:1	1:1	39	95:5	52
21	DCM	0.05	1.5:1	1:1	26	98:2	55
22	DCM	0.15	1.5:1	1:1	66	98:2	90
23	DCM	0.2	1.5:1	1:1	85	99:1	92
24	DCM	0.25	1.5:1	1:1	86	99:1	92
25	DCM	0.3	1.5:1	1:1	88	99:1	92

^aConditions: Unless noted otherwise, all of the reactions were carried out with **1a** (0.15 mmol), **2** (0.1 mmol), **Ij** (10 mol%) and Ag₂CO₃ (10 mol%) in 1.0 mL of DCM at –30 °C for 3 days; ^bIsolated yield; ^cRatio of the major diastereomer to the total of the other three ones; ^dDetermined by chiral HPLC; ^e5 mol% of **Ij** used; ^f15 mol% of **Ij** used; ^gConducted at –20 °C; ^hPerformed at –40 °C.

The silver phosphate from **Ij** was identified as the best catalyst for further optimization of the reaction conditions. Changing the ratio of **1a** and **2** had little effect on the reaction selectivity, but profoundly affected the yield (entries 3 and 13–16): At a 1:1 ratio of **1a/2**, **3aa** was afforded in only 44% yield (entry 13). Increasing the **1a/2** ratio to 1.25:1 improved the yield to 50% (entry 14). As the relative amount of **1a** was increased further, the yield increased. However, as increasing the **1a/2** ratio above 1.5:1 resulted in only a marginal increase in yield; 1.5:1 was selected as the optimum ratio for the reaction (entry 3). Other reaction parameters, including solvent (entries 3–11), catalyst loading (entries 3, 17 and 18), temperature (entries 3, 19 and 20), concentration (entries 3 and 21–25), were also optimized. The best results were achieved when the reaction proceeded at –30 °C in dichloromethane (DCM) at a concentration of 0.2 M with 10 mol % **Ij** and 10 mol % silver carbonate.

6. Characterization of the asymmetric 1,3-dipolar cycloadditions reaction products

Dimethyl ((4*R*, 5*R*)-5-benzoyl-5-cyano-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (**3aa**)



White solid, 65 mg (85% yield); mp 144.4–145.5 °C, $[\alpha]_D^{25} = +208.3^\circ$ ($c = 1.0$, CHCl₃);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} =$

36.275 min, $t_{minor} = 33.681$ min, $dr = 99:1$, $ee = 92\%$; ¹H NMR (600 MHz, CDCl₃) δ 8.11

(d, $J = 7.8$ Hz, 2H), 7.72 (t, $J = 7.3$ Hz, 1H), 7.62 (s, 1H), 7.57 (t, $J = 7.6$ Hz, 2H), 7.51 (t, $J = 7.2$ Hz, 2H), 7.49–

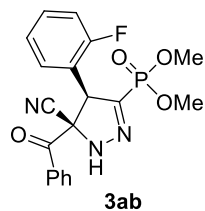
7.44 (m, 1H), 7.39 (d, $J = 7.3$ Hz, 2H), 4.87 (s, 1H), 3.63 (d, $J = 11.3$ Hz, 3H), 3.33 (d, $J = 11.4$ Hz, 3H) ppm;

¹³C NMR (151 MHz, CDCl₃) δ 188.0, 148.0, 146.4, 135.4, 132.7, 130.2, 129.8, 129.7, 129.3, 129.0, 115.3,

72.40 (d, $J = 5.4$ Hz), 62.9, 62.7, 53.75 (d, $J = 5.8$ Hz), 53.06 (d, $J = 6.0$ Hz) ppm; HRMS (ESI-TOF) calcd. for

C₁₉H₁₈N₃O₄PNa [M+Na]⁺ 406.0933, found 406.0937.

Dimethyl ((4R, 5R)-5-benzoyl-5-cyano-4-(2-fluorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3ab)



3ab

White solid, 66 mg (83% yield); mp 136.4–139.3 °C, $[\alpha]_D^{25} = +315.9^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

48.606 min, $t_{\text{minor}} = 34.018$ min, $dr = 97:3$, $ee = 82\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.12

(d, $J = 7.8$ Hz, 2H), 7.72 (t, $J = 7.4$ Hz, 1H), 7.63 (s, 1H), 7.57 (t, $J = 7.7$ Hz, 2H), 7.46

(dd, $J = 13.2, 6.4$ Hz, 1H), 7.35 (t, $J = 7.1$ Hz, 1H), 7.29 (t, $J = 7.5$ Hz, 1H), 7.24 (d, $J = 8.9$ Hz, 1H), 5.27 (s,

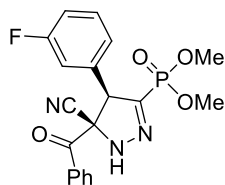
1H), 3.63 (d, $J = 11.3$ Hz, 3H), 3.50 (d, $J = 11.3$ Hz, 3H) ppm, ^{13}C NMR (151 MHz, CDCl_3) δ 187.8, 135.5,

131.7, 130.4, 129.7, 129.3, 125.3 (d, $J = 3.5$ Hz), 119.8 (d, $J = 14.0$ Hz), 116.5, 116.3, 115.1, 71.5, 55.0, 53.7

(d, $J = 5.9$ Hz), 53.2 (d, $J = 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{FN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 424.0838,

found 424.0836.

Dimethyl ((4R, 5R)-5-benzoyl-5-cyano-4-(3-fluorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3ac)



3ac

White solid, 75 mg (94% yield); mp 104.9–107.3 °C, $[\alpha]_D^{25} = +410.25^\circ$ ($c = 1.0$,

CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20,

$t_{\text{major}} = 35.449$ min, $t_{\text{minor}} = 33.617$ min, $dr = 99:1$, $ee = 90\%$; ^1H NMR (600 MHz,

CDCl_3) δ 8.03 (d, $J = 7.7$ Hz, 2H), 7.67 (t, $J = 7.4$ Hz, 1H), 7.55–7.49 (m, 3H), 7.42 (d,

$J = 6.0$ Hz, 1H), 7.11 (dd, $J = 9.2, 4.5$ Hz, 2H), 7.03 (d, $J = 9.0$ Hz, 1H), 4.80 (s, 1H), 3.60 (d, $J = 11.3$ Hz, 3H),

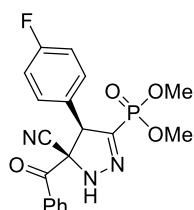
3.36 (d, $J = 11.4$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 187.6, 164.0, 162.4, 147.5, 146.0, 135.6, 134.9,

131.3, 130.1, 129.4, 124.6, 117.0, 116.8, 116.0, 115.9, 115.0, 72.2 (d, $J = 5.3$ Hz), 62.2, 62.0, 53.83 (d, $J =$

5.9 Hz), 53.18 (d, $J = 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{FN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 424.0838, found

424.0836.

Dimethyl ((4R, 5R)-5-benzoyl-4-(4-fluorophenyl)-5-cyano-4,5-dihydro-1H-pyrazol-3-yl) phosphonate (3ad)



3ad

White solid, 77 mg (96% yield); mp 119.9–120.7 °C, $[\alpha]_D^{25} = +341.6^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

42.190 min, $t_{\text{minor}} = 27.951$ min, $dr = 98:2$, $ee = 91\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.08

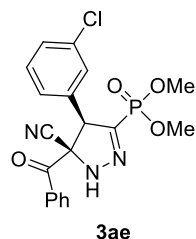
(d, $J = 7.6$ Hz, 2H), 7.70 (d, $J = 11.1$ Hz, 1H), 7.57 (t, $J = 7.5$ Hz, 2H), 7.42–7.33 (m, 2H),

7.19 (t, $J = 8.2$ Hz, 2H), 4.88 (s, 1H), 3.65 (d, $J = 11.3$ Hz, 3H), 3.42 (d, $J = 11.3$ Hz,

3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 187.7, 164.3, 162.6, 147.6, 146.1, 135.4, 130.9 (d, $J = 8.5$ Hz), 130.1,

129.7, 128.6, 116.8, 116.6, 115.3, 72.4 (d, $J = 5.1$ Hz), 61.99, 61.83, 53.74 (d, $J = 5.8$ Hz), 53.13 (d, $J = 6.0$

Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{FN}_3\text{O}_4\text{P}$ $[\text{M}]^+$ 401.0941, found 401.0840.

Dimethyl (4*R*, 5*R*)-5-benzoyl-4-(3-chlorophenyl)-5-cyano-4,5-dihydro-1*H*-pyrazol-3-ylphosphonate (3ae)

White solid, 77 mg (92% yield); mp 83.1–86.7 °C, $[\alpha]_D^{25} = +542.9^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

33.105 min, $t_{\text{minor}} = 29.116$ min, $dr = 98:2$, $ee = 87\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.10

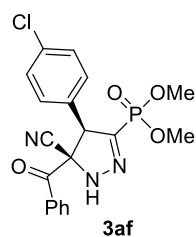
(d, $J = 7.4$ Hz, 2H), 7.74 (d, $J = 7.5$ Hz, 1H), 7.60 (t, $J = 7.9$ Hz, 2H), 7.55 (s, 1H), 7.46 (d,

$J = 5.0$ Hz, 2H), 7.37 (s, 1H), 7.31–7.28 (m, 1H), 4.85 (s, 1H), 3.67 (d, $J = 11.3$ Hz, 3H), 3.43 (d, $J = 11.4$ Hz,

3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 187.6, 147.6, 146.0, 135.55 (d, $J = 15.8$ Hz), 134.6, 130.9, 130.1 (d, J

$= 14.7$ Hz), 129.5, 129.0, 127.1, 115.0, 72.1 (d, $J = 5.3$ Hz), 62.1, 61.9, 53.9 (d, $J = 5.8$ Hz), 53.2 (d, $J = 6.1$

Hz) ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{ClN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 440.0543, found 440.0540.

Dimethyl (4*R*, 5*R*)-5-benzoyl-4-(4-chlorophenyl)-5-cyano-4,5-dihydro-1*H*-pyrazol-3-ylphosphonate (3af)

White solid, 79 mg (95% yield); mp 80.2–83.7 °C, $[\alpha]_D^{25} = +479.4^\circ$ ($c = 1.0$, CHCl_3); HPLC

condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 46.753$ min,

$t_{\text{minor}} = 25.855$ min, $dr = 98:2$, $ee = 93\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.02 (d, $J = 7.5$ Hz,

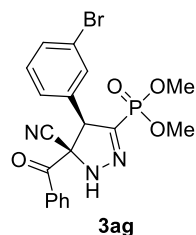
2H), 7.67 (t, $J = 7.4$ Hz, 1H), 7.52 (t, $J = 7.8$ Hz, 2H), 7.48 (s, 1H), 7.42 (d, $J = 8.4$ Hz,

2H), 7.25 (s, 1H), 7.19 (s, 1H), 4.80 (s, 1H), 3.60 (d, $J = 11.3$ Hz, 3H), 3.36 (d, $J = 11.4$ Hz, 3H) ppm; ^{13}C NMR

(151 MHz, CDCl_3) δ 187.7, 147.7, 146.2, 136.0, 135.6, 131.2, 130.2, 129.9, 129.6, 129.4, 115.1, 72.2 (d, $J =$

5.3 Hz), 62.09 (s), 61.9, 53.8 (d, $J = 5.9$ Hz), 53.2 (d, $J = 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for

$\text{C}_{19}\text{H}_{17}\text{ClN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 440.0543, found 440.0538.

Dimethyl ((4*R*, 5*R*)-5-benzoyl-4-(3-bromophenyl)-5-cyano-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ag)

White solid, 87 mg (94% yield); mp 112.5–114.0 °C, $[\alpha]_D^{25} = +303.6^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

36.652 min, $t_{\text{minor}} = 33.822$ min, $dr = 98:2$, $ee = 89\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.09

(d, $J = 7.8$ Hz, 2H), 7.73 (t, $J = 7.2$ Hz, 1H), 7.64 (s, 1H), 7.60–7.57 (m, 2H), 7.51 (s, 1H),

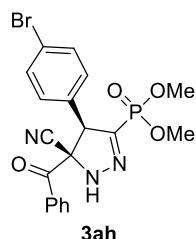
7.38 (t, $J = 7.7$ Hz, 1H), 7.33 (d, $J = 7.4$ Hz, 1H), 4.84 (s, 1H), 3.66 (d, $J = 11.3$ Hz, 3H),

3.44 (d, $J = 11.3$ Hz, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 187.6, 147.3, 145.8, 135.5, 134.9, 132.9, 131.9,

131.1, 130.1, 129.6, 129.4, 127.6, 123.4, 115.0, 72.2 (d, $J = 5.3$ Hz), 62.0 61.8, 53.8 (d, $J = 5.9$ Hz), 53.2 (d, J

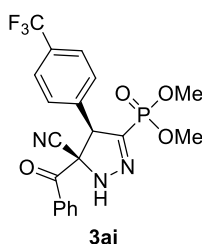
$= 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{BrN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 484.0038, found 484.0041.

Dimethyl ((4*R*, 5*R*)-5-benzoyl-4-(4-bromophenyl)-5-cyano-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ah)



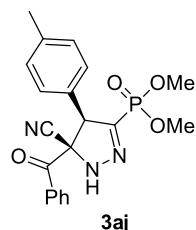
White solid, 83 mg (90% yield); mp 113.0–115.8 °C, $[\alpha]_D^{25} = +368.9^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 51.422$ min, $t_{\text{minor}} = 27.375$ min, $dr = 99:1$, $ee = 94\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.07 (d, $J = 7.8$ Hz, 2H), 7.72 (t, $J = 7.3$ Hz, 1H), 7.67 (s, 1H), 7.64 (d, $J = 8.2$ Hz, 2H), 7.57 (t, $J = 7.7$ Hz, 2H), 7.25 (s, 1H), 4.85 (s, 1H), 3.65 (d, $J = 11.3$ Hz, 3H), 3.43 (d, $J = 11.4$ Hz, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 187.6, 147.3, 145.8, 135.5, 132.8, 131.8, 130.6, 130.1, 129.7, 129.4, 124.1, 115.2, 72.2 (d, $J = 5.3$ Hz), 62.1, 62.0, 53.8 (d, $J = 5.9$ Hz), 53.2 (d, $J = 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{BrN}_3\text{O}_4\text{P Na}$ $[\text{M}+\text{Na}]^+$ 484.0038, found 484.0040.

Dimethyl ((4*R*, 5*R*)-5-benzoyl-5-cyano-4-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ai)

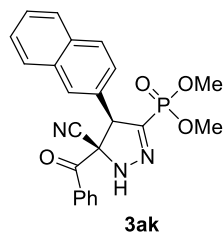


White solid, 68 mg (76% yield); mp 142.0–144.3 °C, $[\alpha]_D^{25} = +279.1^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 20.103$ min, $t_{\text{minor}} = 17.901$ min, $dr = 99:1$, $ee = 89\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.08 (d, $J = 7.6$ Hz, 2H), 7.78 (s, 1H), 7.77 (s, 1H), 7.74 (t, $J = 7.4$ Hz, 1H), 7.69 (s, 1H), 7.59 (t, $J = 7.8$ Hz, 2H), 7.52 (d, $J = 8.0$ Hz, 2H), 4.95 (s, 1H), 3.65 (d, $J = 11.3$ Hz, 3H), 3.43 (d, $J = 11.4$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 187.4, 147.2, 145.7, 136.7, 135.6, 132.2, 132.0, 131.8, 131.6, 130.1, 129.9, 129.6, 129.5 (d, $J = 3.2$ Hz), 128.0, 126.5 (t, $J = 9.7$ Hz), 124.6, 122.8, 121.0, 115.0, 72.2 (d, $J = 5.1$ Hz), 62.1, 62.0, 53.8 (d, $J = 5.8$ Hz), 53.2 (d, $J = 6.1$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{17}\text{F}_3\text{N}_3\text{O}_4\text{P Na}$ $[\text{M}+\text{Na}]^+$ 474.0806, found 474.0810.

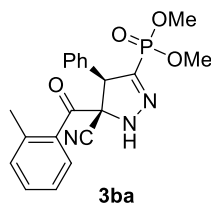
Dimethyl ((4*R*, 5*R*)-5-benzoyl-5-cyano-4-(*p*-tolyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3aj)



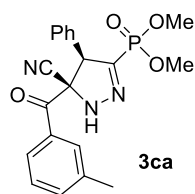
White solid, 72 mg (91% yield); mp 147.5–149.6 °C, $[\alpha]_D^{25} = +380.3^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 38.677$ min, $t_{\text{minor}} = 28.069$ min, $dr = 99:1$, $ee = 89\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.10 (d, $J = 7.9$ Hz, 2H), 7.71 (t, $J = 7.3$ Hz, 1H), 7.57 (dd, $J = 19.4, 11.8$ Hz, 3H), 7.30 (d, $J = 7.8$ Hz, 2H), 7.28 (s, 1H), 4.83 (s, 1H), 3.63 (d, $J = 11.3$ Hz, 3H), 3.36 (d, $J = 11.3$ Hz, 3H), 2.40 (s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 188.1, 148.0, 146.5, 139.8, 135.4, 130.3 (d, $J = 11.6$ Hz), 129.6, 129.3, 128.8, 115.4, 72.5 (d, $J = 5.4$ Hz), 62.7, 62.5, 53.7 (d, $J = 5.8$ Hz), 53.1 (d, $J = 6.0$ Hz), 21.3 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 420.1089, found 420.1085.

Dimethyl ((4*R*, 5*R*)-5-benzoyl-5-cyano-4-(naphthalen-2-yl)-4,5-dihydro-1*H*-pyrazol-3-yl) phosphonate (3ak)

White solid, 55 mg (64% yield); mp 150.6–152.2 °C, $[\alpha]_D^{25} = +276.2^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 57.976$ min, $t_{\text{minor}} = 33.939$ min, $dr = 98:2$, $ee = 82\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.15 (d, $J = 7.8$ Hz, 2H), 7.99 (d, $J = 8.5$ Hz, 1H), 7.93–7.88 (m, 2H), 7.73 (t, $J = 7.4$ Hz, 1H), 7.68 (s, 1H), 7.61–7.54 (m, 4H), 7.49–7.45 (m, 1H), 5.05 (s, 1H), 3.63 (d, $J = 11.3$ Hz, 3H), 3.26 (d, $J = 11.4$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 188.0, 147.9, 146.4, 135.5, 133.7, 133.5, 130.3, 130.0, 129.7, 129.4, 128.7, 128.2, 127.9, 127.1, 126.9, 125.5, 115.4, 72.38 (d, $J = 5.3$ Hz), 63.1, 62.9, 53.8 (d, $J = 5.9$ Hz), 53.0 (dd, $J = 11.7, 5.7$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{23}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 456.1089, found 456.1091.

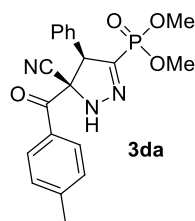
Dimethyl ((4*R*, 5*R*)-5-cyano-5-(2-methylbenzoyl)-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ba)

White solid, 73 mg (92% yield); mp 118.8–120.7 °C, $[\alpha]_D^{25} = +457.1^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 29.610$ min, $t_{\text{minor}} = 34.556$ min, $dr = 91:9$, $ee = 89\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.00 (d, $J = 8.0$ Hz, 2H), 7.62 (s, 1H), 7.50 (t, $J = 7.3$ Hz, 2H), 7.47–7.43 (m, 1H), 7.38 (dd, $J = 15.0, 7.7$ Hz, 4H), 4.85 (s, 1H), 3.62 (d, $J = 11.3$ Hz, 3H), 3.33 (d, $J = 11.3$ Hz, 3H), 2.46 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 191.1, 147.9, 146.4, 141.8 (d, $J = 9.4$ Hz), 133.6, 133.3, 132.7, 130.0, 129.5 (t, $J = 14.5$ Hz), 128.8, 126.0, 115.3, 73.3 (d, $J = 4.9$ Hz), 62.5, 62.3, 53.7 (d, $J = 5.7$ Hz), 53.1 (d, $J = 6.0$ Hz), 21.8 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 420.1089, found 420.1086.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-(3-methylbenzoyl)-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ca)

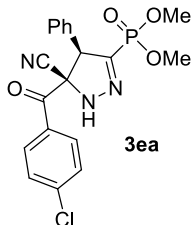
White solid, 72 mg (91% yield); mp 128.4–129.7 °C, $[\alpha]_D^{25} = +345.6^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 36.166$ min, $t_{\text{minor}} = 29.266$ min, $dr = 99:1$, $ee = 90\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.83 (s, 2H), 7.50 (s, 1H), 7.45 (dd, $J = 15.0, 7.4$ Hz, 3H), 7.42–7.35 (m, 2H), 7.32 (d, $J = 7.2$ Hz, 2H), 7.19 (s, 1H), 4.79 (s, 1H), 3.57 (d, $J = 11.2$ Hz, 3H), 3.26 (d, $J = 11.3$ Hz, 3H), 2.37 (s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 188.2, 148.1, 146.6, 139.5, 136.2, 132.8, 130.8, 129.8, 129.6, 129.7 (d, $J = 27.2$ Hz), 129.2, 129.0, 127.4, 115.4, 72.4 (d, $J = 5.4$ Hz), 63.0, 62.8, 53.7 (d, $J = 5.0$ Hz), 53.0 (d, $J = 5.8$ Hz), 21.3 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 420.1089, found 420.1068.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-(4-methylbenzoyl)-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3da)



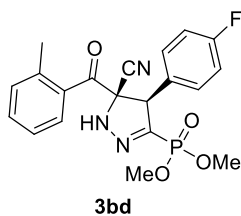
White solid, 68 mg (86% yield); mp 117.2–119.7 °C, $[\alpha]_D^{25} = +345.0^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 37.615$ min, $t_{\text{minor}} = 35.813$ min, $dr = 99:1$, $ee = 91\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.00 (d, $J = 8.0$ Hz, 2H), 7.62 (s, 1H), 7.50 (t, $J = 7.3$ Hz, 2H), 7.47–7.43 (m, 1H), 7.38 (dd, $J = 15.0$, 7.7 Hz, 4H), 4.85 (s, 1H), 3.62 (d, $J = 11.3$ Hz, 3H), 3.33 (d, $J = 11.3$ Hz, 3H), 2.46 (s, 3H) ppm. ^{13}C NMR (151 MHz, CDCl_3) δ 187.6, 148.0, 146.9, 146.5, 132.8, 130.3, 130.0, 129.7, 129.6, 129.0, 127.0, 115.5, 72.3, 63.0, 62.8, 53.71 (d, $J = 5.6$ Hz), 53.03 (d, $J = 5.9$ Hz), 21.8 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 420.1089, found 420.1067.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-(4-chlorobenzoyl)-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ea)



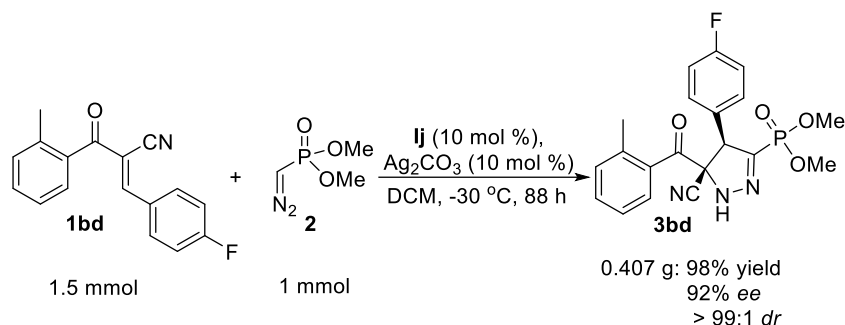
White solid, 61 mg (73% yield); mp 126.3–128.0 °C, $[\alpha]_D^{25} = +397.4^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 43.524$ min, $t_{\text{minor}} = 36.172$ min, $dr = 99:1$, $ee = 83\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.04 (d, $J = 8.4$ Hz, 2H), 7.62 (s, 1H), 7.55 (d, $J = 8.4$ Hz, 2H), 7.50 (d, $J = 7.2$ Hz, 2H), 7.37 (d, $J = 6.9$ Hz, 2H), 4.81 (s, 1H), 3.64 (d, $J = 11.3$ Hz, 3H), 3.33 (d, $J = 11.3$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 187.0, 147.8, 146.3, 142.3, 132.5, 131.5, 129.9, 129.8, 129.7, 128.9, 128.0, 115.2, 72.4 (d, $J = 5.3$ Hz), 62.9, 62.8, 53.8 (d, $J = 5.8$ Hz), 53.1 (d, $J = 6.0$ Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{17}\text{ClN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 440.0543, found 440.0538.

Dimethyl ((4*R*, 5*R*)-5-cyano-4-(4-fluorophenyl)-5-(2-methylbenzoyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3bd)



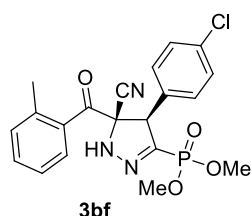
White solid, 78 mg (94% yield); mp 109.5–113.0 °C, $[\alpha]_D^{25} = +495.31^\circ$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 30.205$ min, $t_{\text{minor}} = 28.140$ min, $dr = 99:1$, $ee = 90\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.93 (d, $J = 7.9$ Hz, 1H), 7.67 (s, 1H), 7.55 (t, $J = 7.5$ Hz, 1H), 7.42 (d, $J = 7.7$ Hz, 1H), 7.37 (t, $J = 7.6$ Hz, 1H), 7.32–7.28 (m, 2H), 7.17 (t, $J = 8.5$ Hz, 2H), 4.85 (s, 1H), 3.66 (d, $J = 11.3$ Hz, 3H), 3.46 (d, $J = 11.3$ Hz, 3H), 2.50 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 191.0, 164.2, 162.5, 147.7, 146.1, 141.7, 133.6, 133.3, 130.7, 129.2, 128.6, 126.0, 116.6, 116.5, 115.2, 73.3 (d, $J = 5.3$ Hz), 61.6, 61.4, 53.7 (d, $J = 5.9$ Hz), 53.2 (d, $J = 6.1$ Hz), 21.6 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{19}\text{FN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 438.0995, found 438.0999.

In the case of **1bd**, the asymmetric 1,3-dipolar cycloadditions reaction was successfully conducted on a mmol scale.



Procedure as: SPA **Ij** (60.6 mg, 10 mol %) and Ag_2CO_3 (27.4 mg, 10 mol %) were dissolved in anhydrous CH_2Cl_2 (5 mL) in a pre-dried tube under argon in the dark and stirred for 2 h at 30 °C. Next, **1bd** (0.398 g, 1.5 mmol) was added and the system was cooled to -30 °C. Seyferth–Gilbert reagent **2** (0.15 g, 1 mmol) was then added, the mixture was stirred and monitored by TLC until **2** had been completely consumed. The reaction mixture was then purified directly by flash chromatography on silica gel (30-50% AcOEt/petroleum ether) to obtain the corresponding product **3bd** (0.407 g, 98% yield) with 92% ee, >99:1 dr.

Dimethyl ((4R, 5R)-4-(4-chlorophenyl)-5-cyano-5-(2-methylbenzoyl)-4,5-dihydro-1H-pyrazol-3-yl) phosphonate (3bf)



White solid, 82 mg (95% yield); mp 61.6–62.4 °C, $[\alpha]_{\text{D}}^{25} = +476.9^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

33.019 min, $t_{\text{minor}} = 27.691$ min, $dr = 92:8$, $ee = 95\%$; ^1H NMR (600 MHz, CDCl_3) δ

7.83 (d, $J = 7.9$ Hz, 1H), 7.59 (s, 1H), 7.47 (t, $J = 7.5$ Hz, 1H), 7.37 (d, $J = 8.4$ Hz,

2H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.28 (t, $J = 7.8$ Hz, 1H), 7.17 (d, $J = 8.4$ Hz, 2H), 4.74 (s, 1H), 3.57 (d, $J = 11.3$

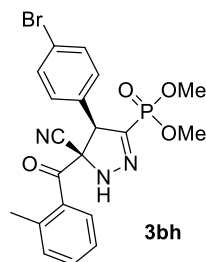
Hz, 3H), 3.39 (d, $J = 11.3$ Hz, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 190.9, 147.4, 145.9, 141.7,

135.7, 133.7, 133.4, 131.2, 130.2, 129.7, 129.1, 128.9, 126.0, 125.7, 115.1, 73.18 (d, $J = 5.3$ Hz), 61.6, 61.4,

53.7 (d, $J = 5.9$ Hz), 53.2 (d, $J = 6.1$ Hz), 21.6 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{19}\text{ClN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$

454.0699, found 454.0698.

Dimethyl ((4R, 5R)-4-(4-bromophenyl)-5-cyano-5-(2-methylbenzoyl)-4,5-dihydro-1H-pyrazol-3-yl) phosphonate (3bh)



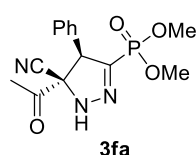
White solid, 89 mg (94% yield); mp 102.9–109.3 °C, $[\alpha]_{\text{D}}^{25} = +410.25^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IE, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

52.614 min, $t_{\text{minor}} = 47.051$ min, $dr = 91:9$, $ee = 94\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.83

(d, $J = 8.0$ Hz, 1H), 7.58 (s, 1H), 7.52 (d, $J = 8.3$ Hz, 2H), 7.46 (t, $J = 7.5$ Hz, 1H), 7.33 (d, $J = 7.7$ Hz, 1H), 7.28 (t, $J = 7.6$ Hz, 1H), 7.10 (d, $J = 8.2$ Hz, 2H), 4.73 (s, 1H), 3.57 (d, $J = 11.2$ Hz, 3H), 3.39 (d, $J = 11.3$ Hz, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 190.9, 147.4, 145.9, 141.7, 133.6, 133.3, 132.7, 131.9, 131.7, 130.4, 129.1, 128.3, 126.0, 125.7, 123.9, 115.1, 73.1 (d, $J = 5.3$ Hz), 61.7, 61.5, 53.7 (d, $J = 6.0$ Hz), 53.2 (d, $J = 6.0$ Hz), 21.6 ppm. HRMS (ESI-TOF) calcd. for $\text{C}_{20}\text{H}_{19}\text{BrN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 498.0194, found 498.0196.

Dimethyl ((4*R*, 5*R*)-5-acetyl-5-cyano-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3fa)

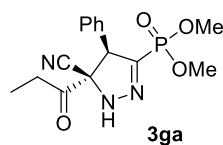


White solid, 25 mg (36% yield); mp 106.4–108.2 °C, $[\alpha]_D^{25} = +133.8^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 32.285$ min, $t_{\text{minor}} = 19.165$ min, $dr = 97:3$, $ee = 53\%$, ^1H NMR (600 MHz, CDCl_3) ^1H NMR

(600 MHz, CDCl_3) δ 7.38 (d, $J = 7.9$ Hz, 4H), 7.23 (s, 1H), 4.59 (s, 1H), 3.57 (d, $J = 8.1$ Hz, 3H), 3.39 (d, $J = 7.6$ Hz, 3H), 2.80 (s, 2H), 1.14 (d, $J = 4.5$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 195.6, 132.7, 129.7, 129.4, 128.7, 127.7, 114.3, 75.4, 61.5, 61.3, 53.8 (d, $J = 5.7$ Hz), 53.2 (d, $J = 5.8$ Hz), 23.9, 8.0 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{16}\text{H}_{20}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 343.0698, found 343.0702.

Dimethyl ((4*R*, 5*R*)-5-cyano-4-phenyl-5-propionyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ga)

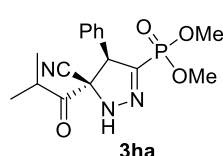


White solid, 25 mg (37% yield); mp 104.7–106.3 °C, $[\alpha]_D^{25} = +189.29^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 35.279$ min, $t_{\text{minor}} = 17.880$ min, $dr = 99:1$, $ee = 73\%$, ^1H NMR (600 MHz, CDCl_3) δ 7.38

(d, $J = 7.9$ Hz, 2H), 7.27–7.19 (m, 2H), 4.59 (s, 1H), 3.57 (d, $J = 8.1$ Hz, 3H), 3.39 (d, $J = 7.6$ Hz, 3H), 2.80 (s, 2H), 1.14 (d, $J = 4.5$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 199.1, 146.6, 145.0, 132.9, 129.6, 129.4, 128.8, 114.7, 75.1, 61.6, 61.4, 53.8, 53.3, 30.2, 8.0 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{15}\text{H}_{18}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 358.0933, found 358.0938.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-isobutyryl-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ha)



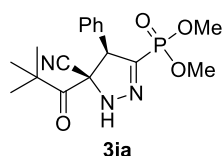
White solid, 43 mg (61% yield); mp 106.5–108.2 °C, $[\alpha]_D^{25} = +267.34^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 57.174$ min, $t_{\text{minor}} = 36.156$ min, $dr = 98:2$, $ee = 77\%$, ^1H NMR (600 MHz, CDCl_3) δ

7.35 (tt, $J = 7.3, 5.1$ Hz, 3H), 7.23 (d, $J = 6.7$ Hz, 2H), 4.57 (s, 1H), 3.55 (d, $J = 11.3$ Hz, 3H), 3.40 (d, $J = 11.3$ Hz, 3H), 3.17 (dt, $J = 13.4, 6.7$ Hz, 1H), 1.22 (dd, $J = 6.7, 4.4$ Hz, 6H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 202.4, 146.8, 145.3, 132.7, 129.6, 129.3, 128.7, 114.5, 74.8 (d, $J = 5.3$ Hz), 61.2, 61.0, 53.6 (d, $J = 5.8$ Hz),

53.2 (d, $J = 5.9$ Hz), 36.5, 20.3, 19.8 ppm; HRMS (ESI-TOF) calcd. for $C_{16}H_{20}N_3O_4PNa$ $[M+Na]^+$ 372.1089, found 372.1091.

Dimethyl ((4*R*, 5*R*)-5-cyano-4-phenyl-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ia)

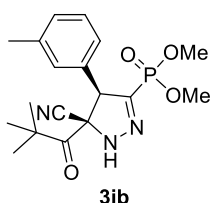


White solid, 58 mg (80% yield); mp 143.5–144.7 °C, $[\alpha]_D^{25} = +457.1^\circ$ ($c = 1.0$, $CHCl_3$);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 24.426$ min, $t_{minor} = 19.037$ min, $dr = 99:1$, $ee = 92\%$; 1H NMR (600 MHz, $CDCl_3$) δ

7.45–7.41 (m, 2H), 7.32 (d, $J = 7.5$ Hz, 2H), 7.20 (s, 1H), 4.73 (s, 1H), 3.62 (d, $J = 11.3$ Hz, 3H), 3.41 (d, $J = 11.3$ Hz, 3H), 1.46–1.38 (m, 9H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 202.0, 147.3, 145.8, 132.5, 129.6, 129.3, 129.0, 115.3, 73.0 (d, $J = 5.4$ Hz), 61.6, 61.4, 53.6 (d, $J = 5.7$ Hz), 53.1 (d, $J = 5.9$ Hz), 45.1, 28.2 ppm; HRMS (ESI-TOF) calcd. for $C_{17}H_{22}N_3O_4PNa$ $[M+Na]^+$ 386.1246, found 386.1247.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-pivaloyl-4-(*m*-tolyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ib)



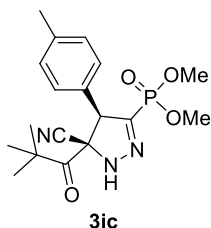
White solid, 56 mg (74% yield); mp 110.0–114.4 °C, $[\alpha]_D^{25} = +393.2^\circ$ ($c = 1.0$, $CHCl_3$);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 31.750$ min, $t_{minor} = 39.080$ min, $dr = 90:10$, $ee = 84\%$; 1H NMR (600 MHz, $CDCl_3$) δ

7.24 (t, $J = 7.8$ Hz, 1H), 7.20 (s, 1H), 7.14 (d, $J = 7.5$ Hz, 1H), 7.04 (d, $J = 6.4$ Hz, 2H),

4.61 (s, 1H), 3.55 (d, $J = 11.3$ Hz, 3H), 3.34 (d, $J = 11.3$ Hz, 3H), 2.31 (s, 3H), 1.37 (s, 9H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 202.1, 147.2, 145.7, 139.0, 132.4, 130.3, 129.6, 129.1, 126.1, 115.3, 73.1 (d, $J = 5.4$ Hz), 61.5, 61.4, 53.6 (d, $J = 5.7$ Hz), 53.1 (d, $J = 5.9$ Hz), 45.0, 28.2, 21.4 ppm; HRMS (ESI-TOF) calcd. for $C_{18}H_{24}N_3O_4PNa$ $[M+Na]^+$ 400.1402, found 400.1396.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-pivaloyl-4-(*p*-tolyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ic)



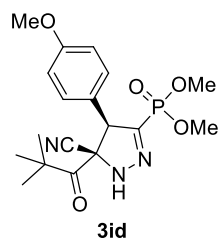
White solid, 53 mg (70% yield); mp 113.7–116.1 °C, $[\alpha]_D^{25} = +388.3^\circ$ ($c = 1.0$, $CHCl_3$);

HPLC condition: chiralpak IE, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 41.332$ min, $t_{minor} = 50.565$ min, $dr = 99:1$, $ee = 97\%$; 1H NMR (600 MHz, $CDCl_3$) δ 7.27

(s, 1H), 7.23 (s, 1H), 7.20 (d, $J = 8.0$ Hz, 2H), 7.17 (s, 1H), 4.69 (s, 1H), 3.63 (d, $J =$

11.3 Hz, 3H), 3.43 (d, $J = 11.3$ Hz, 3H), 2.36 (s, 3H), 1.44 (s, 9H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ 202.1, 147.4, 145.9, 139.5, 130.0, 129.4, 128.9, 115.4, 73.1 (d, $J = 5.5$ Hz), 61.4, 61.2, 53.6 (d, $J = 5.8$ Hz), 53.2 (d, $J = 5.9$ Hz), 45.0, 28.2, 21.3 ppm; HRMS (ESI-TOF) calcd. for $C_{18}H_{24}N_3O_4PNa$ $[M+Na]^+$ 400.1402, found 400.1406.

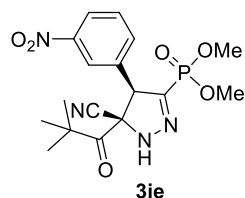
Dimethyl ((4*R*, 5*R*)-5-cyano-5-pivaloyl-4-(4-methoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3id)



White solid, 42 mg (53% yield); mp 132.8–134.8 °C, $[\alpha]_D^{25} = +302.75^\circ$ ($c = 1.0$, CHCl_3);
HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 90/10, $t_{\text{major}} =$
53.677 min, $t_{\text{minor}} = 41.316$ min, $dr = 99:1$, $ee = 93\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.24
(d, $J = 8.5$ Hz, 2H), 7.21 (s, 1H), 6.95 (d, $J = 8.5$ Hz, 2H), 4.69 (s, 1H), 3.82 (s, 3H),

3.64 (d, $J = 11.3$ Hz, 3H), 3.45 (d, $J = 11.3$ Hz, 3H), 1.44 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 202.1,
160.4, 147.3, 145.8, 130.3, 124.3, 115.4, 114.7 (s), 73.1 (d, $J = 5.4$ Hz), 61.1 (s), 61.0 (s), 55.3 (s), 53.6 (d, $J =$
5.7 Hz), 53.2 (d, $J = 5.9$ Hz), 45.1, 28.1 ppm; HRMS (ESI-TOF) calcd. For $\text{C}_{18}\text{H}_{24}\text{N}_3\text{O}_5\text{PNa}$ $[\text{M}+\text{Na}]^+$ 416.1351,
found 416.1353.

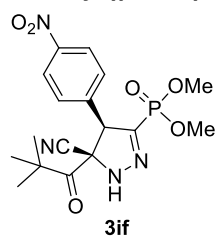
Dimethyl ((4*R*, 5*R*)-5-cyano-4-(3-nitrophenyl)-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ie)



White solid, 76 mg (93% yield); mp 144.7–146.0 °C, $[\alpha]_D^{25} = +320.0^\circ$ ($c = 1.0$,
 CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20,
 $t_{\text{major}} = 24.428$ min, $t_{\text{minor}} = 19.037$ min, $dr = 95:5$, $ee = 93\%$; ^1H NMR (600 MHz,
 CDCl_3) δ 8.29 (d, $J = 6.6$ Hz, 1H), 8.17 (s, 1H), 7.73 (d, $J = 8.2$ Hz, 1H), 7.67 (d, $J =$

6.4 Hz, 2H), 4.97 (s, 1H), 3.68 (d, $J = 11.3$ Hz, 3H), 3.61 (d, $J = 11.3$ Hz, 3H), 1.43 (s, 9H) ppm; ^{13}C NMR (151
MHz, CDCl_3) δ 201.0, 148.6, 135.3, 134.9, 130.3, 124.4, 124.1, 115.1, 73.03 (d, $J = 5.2$ Hz), 60.8, 60.6, 53.7
(d, $J = 5.9$ Hz), 53.5 (d, $J = 6.1$ Hz), 45.3, 27.8 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_6\text{PNa}$ $[\text{M}+\text{Na}]^+$
431.1096, found 431.1101.

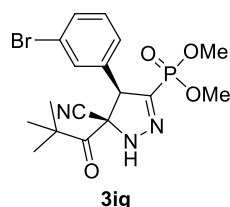
Dimethyl ((4*R*, 5*R*)-5-cyano-4-(4-nitrophenyl)-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3if)



White solid, 77 mg (95% yield); mp 143.2–145.3 °C, $[\alpha]_D^{25} = +440.3^\circ$ ($c = 1.0$, CHCl_3);
HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$
50.433 min, $t_{\text{minor}} = 16.842$ min, $dr = 99:1$, $ee = 96\%$; ^1H NMR (600 MHz, CDCl_3) δ 8.31
(d, $J = 8.6$ Hz, 2H), 7.64 (s, 1H), 7.52 (d, $J = 8.6$ Hz, 2H), 4.93 (s, 1H), 3.67 (d, $J =$

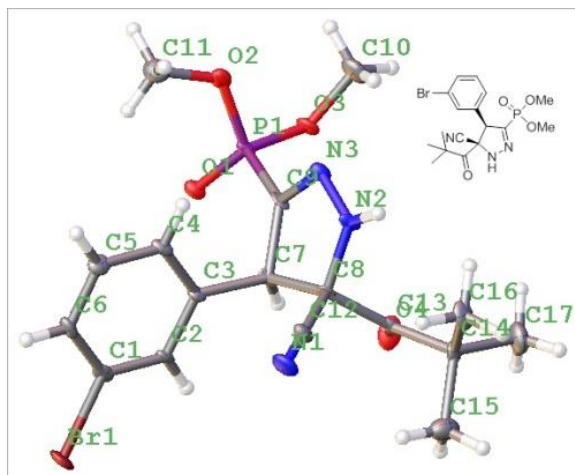
11.3 Hz, 3H), 3.60 (d, $J = 11.3$ Hz, 3H), 1.43 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.0, 148.5, 139.7,
130.3, 124.3, 115.1, 73.0 (d, $J = 5.0$ Hz), 60.8, 60.6, 53.7 (d, $J = 5.8$ Hz), 53.4 (d, $J = 6.0$ Hz), 45.3, 27.8 ppm;
HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_6\text{PNa}$ $[\text{M}+\text{Na}]^+$ 431.1096, found 431.1096.

Dimethyl ((4*R*, 5*R*)-4-(3-bromophenyl)-5-cyano-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ig)



White solid, 82 mg (93% yield); mp 152.0–153.5 °C, $[\alpha]_D^{25} = +293.1^\circ$ ($c = 1.0$, CHCl_3);
HPLC condition: chiralpak IE, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

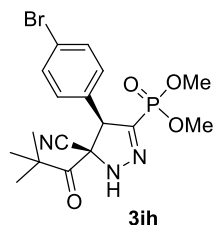
23.536 min, t_{minor} = 29.192 min, dr = 98:2, ee = 93%; ^1H NMR (600 MHz, CDCl_3) δ 7.49 (d, J = 7.8 Hz, 1H), 7.38 (s, 1H), 7.26 (t, J = 7.8 Hz, 1H), 7.20 (s, 1H), 7.12 (s, 1H), 4.65 (s, 1H), 3.59 (d, J = 11.3 Hz, 3H), 3.44 (d, J = 11.3 Hz, 3H), 1.37 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.5, 146.1, 144.6, 134.8, 132.6, 132.0, 130.8, 127.8, 123.1, 115.1, 73.0, 60.8, 60.6, 53.7 (d, J = 5.4 Hz), 53.3, 45.2 (d, J = 3.6 Hz), 28.0 (d, J = 5.1 Hz) ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{21}\text{BrN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 464.0351, found 464.0351.

Table 2. Crystal data and structure refinement for **3ig**.

Empirical formula	$\text{C}_{17}\text{H}_{21}\text{BrN}_3\text{O}_4\text{P}$
Formula weight	442.25
Temperature	290.84(10) K
Wavelength	1.54184 Å
Crystal system, space group	orthorhombic, P 21 21 21
Unit cell dimensions	a = 7.2078(2) Å alpha = 90 deg. b = 13.6652(5) Å beta = 90 deg. c = 19.4644(5) Å gamma = 90 deg.
Volume	1917.17(10) Å ³
Z, Calculated density	4, 1.532 Mg/m ³
Absorption coefficient	3.955 mm ⁻¹
F(000)	904.0
Crystal size	0.38 x 0.25 x 0.14 mm
Theta range for data collection	5.5300 to 71.1500 deg.
Limiting indices	-5 <= h <= 8, -16 <= k <= 16, -23 <= l <= 23
Reflections collected / unique	17944 / 3679 [R(int) = 0.1748]
Completeness to theta = 26.00	99.85 %
Absorption correction	multi-scan
Max. and min. transmission	1.00000 and 0.53318
Goodness-of-fit on F ²	1.051
Final R indices [I > 2sigma(I)]	R1 = 0.0795, wR2 = 0.1866
R indices (all data)	R1 = 0.0775, wR2 = 0.1846

Absolute structure parameter	-0.01(2)
Largest diff. peak and hole	1.893 and -1.322 e.Å ⁻³

Dimethyl ((4*R*, 5*R*)-4-(4-bromophenyl)-5-cyano-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl) phosphonate (3ih)



White solid, 64 mg (81% yield); mp 146.6–148.7 °C, $[\alpha]_D^{25} = +383.6^\circ$ ($c = 1.0$, CHCl₃);

HPLC condition: chiralpak IE, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 27.954$ min, $t_{minor} = 29.993$ min, $dr = 99:1$, $ee = 94\%$; ¹H NMR (600 MHz, CDCl₃) δ 7.57

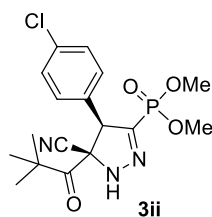
(d, $J = 8.2$ Hz, 2H), 7.41 (s, 1H), 7.20 (d, $J = 8.2$ Hz, 2H), 4.74 (s, 1H), 3.65 (d, $J =$

11.3 Hz, 3H), 3.51 (d, $J = 11.3$ Hz, 3H), 1.42 (s, 9H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 201.6, 146.3, 144.8,

132.5, 131.6, 130.7, 123.8, 115.2, 72.9 (d, $J = 5.3$ Hz), 60.9, 60.8, 53.7 (d, $J = 5.8$ Hz), 53.3 (d, $J = 6.0$ Hz),

45.2, 28.0 ppm; HRMS (ESI-TOF) calcd. for C₁₇H₂₁BrN₃O₄PNa [M+Na]⁺ 464.0351, found 464.0350.

Dimethyl ((4*R*, 5*R*)-4-(4-chlorophenyl)-5-cyano-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl) phosphonate (3ii)



White solid, 74 mg (93% yield); mp 137.9–140.1 °C, $[\alpha]_D^{25} = +385.3^\circ$ ($c = 1.0$, CHCl₃);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 19.393$ min, $t_{minor} = 13.397$ min, $dr = 99:1$, $ee = 93\%$; ¹H NMR (600 MHz, CDCl₃) δ

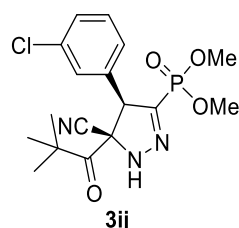
7.46 (s, 1H), 7.42 (d, $J = 8.0$ Hz, 2H), 7.26 (d, $J = 7.9$ Hz, 2H), 4.75 (s, 1H), 3.65 (d, J

= 11.3 Hz, 3H), 3.51 (d, $J = 11.4$ Hz, 3H), 1.42 (s, 9H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 201.6, 146.3, 144.8,

135.6, 131.2, 130.4, 129.5, 115.3, 73.0 (d, $J = 5.3$ Hz), 60.9, 60.7, 53.6 (d, $J = 5.8$ Hz), 53.3 (d, $J = 6.0$ Hz),

45.2, 28.0 ppm; HRMS (ESI-TOF) calcd. for C₁₇H₂₁ClN₃O₄PNa [M+Na]⁺ 420.0856, found 420.0853.

Dimethyl ((4*R*, 5*R*)-4-(3-chlorophenyl)-5-cyano-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3ij)



White solid, 75 mg (94% yield); mp 149.5–152.4 °C, $[\alpha]_D^{25} = +293.1^\circ$ ($c = 1.0$, CHCl₃);

HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} = 32.001$ min, $t_{minor} = 26.199$ min, $dr = 99:1$, $ee = 94\%$; ¹H NMR (600 MHz, CDCl₃) δ

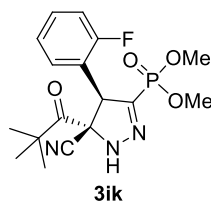
7.48 (s, 1H), 7.39 (d, $J = 5.3$ Hz, 2H), 7.30 (s, 1H), 7.24–7.19 (m, 1H), 4.74 (s, 1H),

3.65 (d, $J = 11.3$ Hz, 3H), 3.52 (d, $J = 11.3$ Hz, 3H), 1.43 (d, $J = 3.9$ Hz, 9H) ppm;

¹³C NMR (151 MHz, CDCl₃) δ 201.5, 146.1, 144.6, 135.1, 134.6 (d, $J = 4.6$ Hz), 130.5, 129.7, 129.1, 127.3,

115.1, 72.9 (d, $J = 5.2$ Hz), 60.9, 60.7, 53.7 (d, $J = 5.8$ Hz), 53.2 (d, $J = 6.0$ Hz), 45.2, 28.0 ppm; HRMS (ESI-

TOF) calcd. for C₁₇H₂₁ClN₃O₄PNa [M+Na]⁺ 420.0856, found 420.0854.

Dimethyl ((4R, 5R)-4-(2-fluorophenyl)-5-cyano-5-pivaloyl-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3ik)

White solid, 63 mg (83% yield); mp 148.2–150.1 °C, $[\alpha]_D^{25} = +332.82^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

22.461 min, $t_{\text{minor}} = 18.026$ min, $dr = 91:9$, $ee = 86\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.41

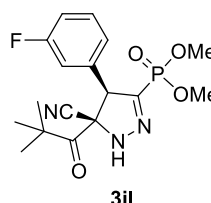
(dt, $J = 7.2, 3.8$ Hz, 1H), 7.34–7.28 (m, 2H), 7.24 (t, $J = 7.5$ Hz, 1H), 7.17 (t, $J = 9.2$ Hz,

1H), 5.13 (s, 1H), 3.63 (d, $J = 11.3$ Hz, 3H), 3.56 (d, $J = 11.3$ Hz, 3H), 1.44 (s, 9H) ppm; ^{13}C NMR (151 MHz,

CDCl_3) δ 201.9, 161.0, 159.4, 145.9, 144.3, 131.5, 130.7, 125.0, 120.0, 116.2, 116.0, 115.1, 72.0(d, $J = 5.2$

Hz), 53.5 (d, $J = 5.9$ Hz), 53.2 (d, $J = 6.0$ Hz), 45.0, 27.9 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{21}\text{ClN}_3\text{O}_4\text{PNa}$

$[\text{M}+\text{Na}]^+$ 404.1151, found 404.1155.

Dimethyl ((4R, 5R)-5-cyano-4-(3-fluorophenyl)-5-pivaloyl-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3il)

White solid, 72 mg (94% yield); mp 120.6–122.2 °C, $[\alpha]_D^{25} = +370.1^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

37.532 min, $t_{\text{minor}} = 28.393$ min, $dr = 99:1$, $ee = 92\%$; ^1H NMR (600 MHz, CDCl_3) δ

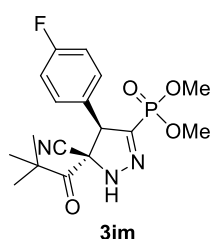
7.42 (dd, $J = 13.6, 7.4$ Hz, 2H), 7.11 (dd, $J = 11.2, 4.8$ Hz, 2H), 7.04 (d, $J = 9.2$ Hz,

1H), 4.76 (s, 1H), 3.65 (d, $J = 11.3$ Hz, 3H), 3.51 (d, $J = 11.4$ Hz, 3H), 1.43 (s, 9H) ppm; ^{13}C NMR (151 MHz,

CDCl_3) δ 201.6, 163.8, 162.2, 146.2, 144.7, 134.9, 130.9, 124.8, 116.7, 116.5, 116.2, 116.0, 115.1, 73.0 (d, J

= 5.3 Hz), 61.0, 60.8, 53.6 (d, $J = 5.8$ Hz), 53.2 (d, $J = 6.0$ Hz), 45.2, 28.0 ppm; HRMS (ESI-TOF) calcd. for

$\text{C}_{17}\text{H}_{21}\text{FN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 404.1151, found 404.1156.

Dimethyl ((4R, 5R)-5-cyano-4-(4-fluorophenyl)-5-pivaloyl-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3im)

White solid, 71 mg (93% yield); mp 140.1–141.5 °C, $[\alpha]_D^{25} = +362.1^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

18.442 min, $t_{\text{minor}} = 13.956$ min, $dr = 99:1$, $ee = 96\%$; ^1H NMR (600 MHz, CDCl_3) δ

7.32 (s, 1H), 7.26–7.21 (m, 2H), 7.06 (t, $J = 8.2$ Hz, 2H), 4.69 (s, 1H), 3.57 (d, $J =$

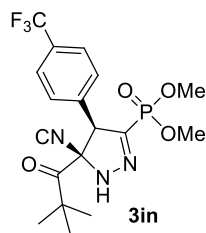
11.2 Hz, 3H), 3.43 (d, $J = 11.3$ Hz, 3H), 1.36 (s, 9H) ppm; ^{13}C NMR (151 MHz,

CDCl_3) δ 201.7, 164.1, 162.4, 146.6, 145.1, 131.0, 128.5, 116.4, 116.2, 115.3, 73.06 (d, $J = 5.2$ Hz), 60.8,

60.7, 53.8–53.5(m), 53.4–53.1(m), 45.1, 28.0 (d, $J = 2.2$ Hz) ppm; HRMS (ESI-TOF) calcd. for

$\text{C}_{17}\text{H}_{21}\text{FN}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 404.1151, found 404.1154.

Dimethyl ((4*R*, 5*R*)-5-cyano-5-pivaloyl-4-(4-(trifluoromethyl)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)phosphonate (3in)



White solid, 81 mg (92% yield); mp 144.4–146.1 °C, $[\alpha]_D^{25} = +322.6^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

17.371 min, $t_{\text{minor}} = 10.849$ min, $dr = 99:1$, $ee = 93\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.49

(d, $J = 7.8$ Hz, 1H), 7.38 (s, 1H), 7.26 (t, $J = 7.8$ Hz, 1H), 7.20 (s, 1H), 7.12 (s, 1H),

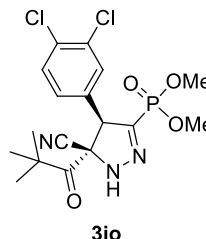
4.65 (s, 1H), 3.59 (d, $J = 11.3$ Hz, 3H), 3.44 (d, $J = 11.3$ Hz, 3H), 1.37 (s, 9H) ppm; ^{13}C NMR (151 MHz,

CDCl_3) δ 201.4, 146.2, 144.7, 136.7, 131.8, 131.6, 129.7, 126.2 (d, $J = 3.5$ Hz), 124.7, 122.9, 115.2, 73.0 (d, J

$= 5.2$ Hz), 61.1, 60.9, 53.7, 53.3, 45.3, 28.0 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{19}\text{H}_{21}\text{F}_3\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$

466.1119, found 466.1116.

Dimethyl (4*R*, 5*R*)-5-cyano-4-(3,4-dichlorophenyl)-5-pivaloyl-4,5-dihydro-1H-pyrazol-3-ylphosphonate (3io)



White solid, 82 mg (95% yield); mp 59.6–60.2 °C, $[\alpha]_D^{25} = +348.59^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

23.076 min, $t_{\text{minor}} = 20.166$ min, $dr = 98:2$, $ee = 96\%$; ^1H NMR (600 MHz, CDCl_3) δ

7.45 (d, $J = 8.3$ Hz, 1H), 7.33 (d, $J = 2.0$ Hz, 1H), 7.10 (dd, $J = 8.3, 2.0$ Hz, 1H), 4.69

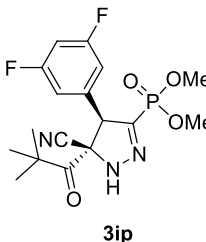
(s, 1H), 3.61 (d, $J = 11.3$ Hz, 3H), 3.51 (d, $J = 11.4$ Hz, 3H), 1.36 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ

201.2, 145.9, 144.4, 134.0, 133.4, 132.7, 131.2, 130.9, 128.4, 115.0, 72.9 (d, $J = 5.2$ Hz), 60.3, 60.1, 53.7 (d, J

$= 5.9$ Hz), 53.4 (d, $J = 6.1$ Hz), 45.2, 28.0 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{20}\text{Cl}_2\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$

454.0466, found 454.0466.

Dimethyl (4*R*, 5*R*)-5-cyano-4-(3,5-difluorophenyl)-5-pivaloyl-4,5-dihydro-1H-pyrazol-3-ylphosphonate (3ip)



White solid, 71 mg (89% yield); mp 128.3–129.5 °C, $[\alpha]_D^{25} = +421.96^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 90/10, $t_{\text{major}} =$

80.006 min, $t_{\text{minor}} = 43.225$ min, $dr = 94:6$, $ee = 92\%$; ^1H NMR (600 MHz, CDCl_3) δ

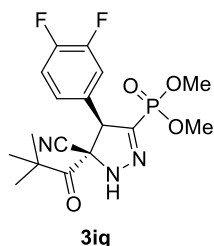
7.49 (s, 1H), 6.87 (d, $J = 7.1$ Hz, 3H), 4.77 (s, 1H), 3.69 (d, $J = 11.3$ Hz, 3H), 3.59 (d, J

$= 11.4$ Hz, 3H), 1.43 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.2, 164.2 (d, $J = 12.7$ Hz), 162.5 (d, $J =$

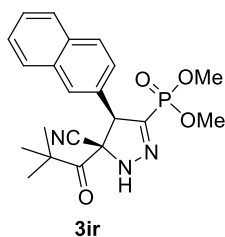
12.6 Hz), 145.7, 144.2, 136.2 (t, $J = 9.1$ Hz), 114.9, 112.3 (dd, $J = 20.6, 5.7$ Hz), 105.4, 105.2, 105.1, 72.9 (d,

$J = 5.2$ Hz), 60.6, 60.5, 53.8 (d, $J = 5.9$ Hz), 53.4 (d, $J = 6.1$ Hz), 45.3, 28.0 ppm; HRMS (ESI-TOF) calcd. for

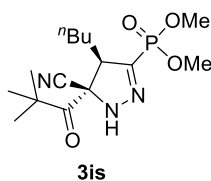
$\text{C}_{17}\text{H}_{20}\text{F}_2\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 422.1057, found 422.1061.

Dimethyl (4*R*, 5*R*)-5-cyano-4-(3,4-difluorophenyl)-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-ylphosphonate (3iq)

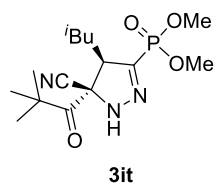
White solid, 75 mg (94% yield); mp 120.2–121.1 °C, $[\alpha]_{\text{D}}^{25} = +363.98^{\circ}$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak IA, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 16.606$ min, $t_{\text{minor}} = 12.569$ min, $dr = 98:2$, $ee = 96\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.40 (s, 1H), 7.24 (dd, $J = 17.9, 8.5$ Hz, 1H), 7.18–7.12 (m, 1H), 7.08 (d, $J = 8.4$ Hz, 1H), 4.77 (s, 1H), 3.68 (d, $J = 11.3$ Hz, 3H), 3.58 (d, $J = 11.3$ Hz, 3H), 1.43 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.4, 151.9 (d, $J = 8.0$ Hz), 151.4 (d, $J = 15.9$ Hz), 150.2 (d, $J = 7.9$ Hz), 149.8 (d, $J = 15.8$ Hz), 146.2, 144.7, 129.7–129.5 (m), 125.6, 118.3, 115.1, 73.0 (d, $J = 5.3$ Hz), 60.5, 60.4, 53.7 (d, $J = 5.9$ Hz), 53.4 (d, $J = 6.1$ Hz), 45.3, 28.0 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{17}\text{H}_{20}\text{F}_2\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 422.1057, found 422.1060.

Dimethyl (4*R*, 5*R*)-5-cyano-4-(naphthalen-2-yl)-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-ylphosphonate (3ir)

White solid, 78 mg (94% yield); mp 63.2–66.9 °C, $[\alpha]_{\text{D}}^{25} = +430.8^{\circ}$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak ID, 254 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 45.723$ min, $t_{\text{minor}} = 38.656$ min, $dr = 99:1$, $ee = 91\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.92 (d, $J = 8.5$ Hz, 1H), 7.89–7.83 (m, 2H), 7.82 (s, 1H), 7.52 (dd, $J = 5.5, 3.7$ Hz, 2H), 7.41–7.38 (m, 1H), 4.92 (s, 1H), 3.60 (d, $J = 11.3$ Hz, 3H), 3.35 (d, $J = 11.4$ Hz, 3H), 1.46 (s, 9H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 202.0, 146.8, 145.3, 133.6, 133.3, 129.9, 129.3, 128.8, 128.2, 127.9, 127.0, 126.7, 125.7, 115.4, 73.1 (d, $J = 5.2$ Hz), 61.7, 61.6, 53.7 (d, $J = 5.7$ Hz), 53.2 (d, $J = 6.0$ Hz), 45.1, 28.2 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{21}\text{H}_{24}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 436.1402, found 436.1400.

Dimethyl ((4*R*, 5*R*)-4-butyl-5-cyano-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3is)

White solid, 63 mg (92% yield); mp 107.8–109.1 °C, $[\alpha]_{\text{D}}^{25} = +126.62^{\circ}$ ($c = 1.0$, CHCl_3); HPLC condition: chiralpak ID, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} = 23.410$ min, $t_{\text{minor}} = 21.036$ min, $dr = 99:1$, $ee = 97\%$; ^1H NMR (600 MHz, CDCl_3) δ 6.99 (s, 1H), 3.84 (d, $J = 11.3$ Hz, 3H), 3.82 (s, 1H), 3.80 (d, $J = 11.3$ Hz, 3H), 2.10 (ddd, $J = 15.3, 10.1, 4.4$ Hz, 1H), 2.02–1.92 (m, 1H), 1.50 (ddd, $J = 24.0, 13.5, 9.1$ Hz, 2H), 1.42 (s, 9H), 1.41–1.35 (m, 2H), 0.95 (t, $J = 7.1$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.8, 147.2, 145.7, 115.8, 71.85 (d, $J = 5.8$ Hz), 55.2, 55.0, 53.6 (t, $J = 6.6$ Hz), 45.2, 28.8, 28.1, 27.8, 22.5, 13.6 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{15}\text{H}_{26}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 366.1559, found 366.1564.

Dimethyl ((4*R*, 5*R*)-5-cyano-4-isobutyl-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3it**)**

White solid, 63 mg (92% yield); mp 106.3–108.0 °C, $[\alpha]_D^{25} = +76.84^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak IA, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

12.360 min, $t_{\text{minor}} = 11.057$ min, $dr = 99:1$, $ee = 98\%$; ^1H NMR (600 MHz, CDCl_3) δ 6.94

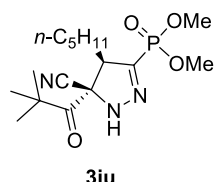
(s, 1H), 3.88 (dd, $J = 8.5, 5.4$ Hz, 1H), 3.75 (d, $J = 11.4$ Hz, 3H), 3.73 (d, $J = 11.3$ Hz,

3H), 1.83 (ddd, $J = 14.0, 8.5, 5.3$ Hz, 1H), 1.74 (ddd, $J = 14.2, 8.7, 5.3$ Hz, 1H), 1.71–1.65 (m, 1H), 1.33 (s,

9H), 0.92 (d, $J = 6.5$ Hz, 3H), 0.89 (d, $J = 6.4$ Hz, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.6, 147.9, 146.4,

116.0, 72.9 (d, $J = 5.8$ Hz), 53.8 (d, $J = 6.1$ Hz), 53.4 (d, $J = 5.7$ Hz) (m), 53.3, 45.5, 38.4, 27.5, 25.9, 22.9,

21.6 ppm; HRMS (ESI-TOF) calcd. for $\text{C}_{15}\text{H}_{26}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 366.1559, found 366.1563.

Dimethyl ((4*R*, 5*R*)-5-cyano-4-pentyl-5-pivaloyl-4,5-dihydro-1*H*-pyrazol-3-yl)phosphonate (3iu**)**

White solid, 63 mg (88% yield); mp 76.4–77.8 °C, $[\alpha]_D^{25} = +120.26^\circ$ ($c = 1.0$, CHCl_3);

HPLC condition: chiralpak ID, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{\text{major}} =$

20.520 min, $t_{\text{minor}} = 19.048$ min, $dr = 99:1$, $ee = 97\%$; ^1H NMR (600 MHz, CDCl_3) δ 7.12

(s, 1H), 3.75 (d, $J = 11.3$ Hz, 4H), 3.71 (d, $J = 11.3$ Hz, 3H), 2.00 (dd, $J = 9.0, 5.0$ Hz,

1H), 1.86 (ddd, $J = 18.7, 12.6, 6.1$ Hz, 1H), 1.42 (d, $J = 9.8$ Hz, 1H), 1.31 (d, $J = 16.0$ Hz, 9H), 1.27 (s, 5H),

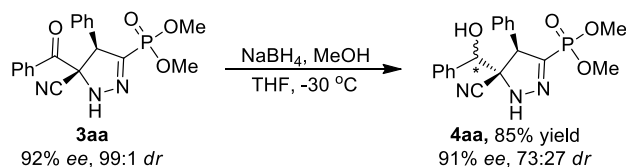
0.82 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 201.8, 146.8, 145.3, 115.8, 71.9 (d, $J = 5.8$ Hz), 55.3, 55.1,

53.7 (d, $J = 5.8$ Hz), 53.4 (d, $J = 6.1$ Hz), 45.2, 31.6, 29.1, 27.7, 25.7, 22.2, 13.8 ppm; HRMS (ESI-TOF) calcd.

for $\text{C}_{16}\text{H}_{28}\text{N}_3\text{O}_4\text{PNa}$ $[\text{M}+\text{Na}]^+$ 380.1715, found 380.1727.

7. Synthesis of hydroxyl containing-phosphonylpyrazolines

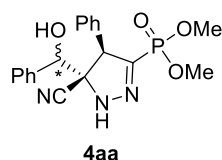
To demonstrate the potential further utility of these reaction products, **3aa** was treated with NaBH_4 at -30°C to obtain hydroxyl-containing phosphonylpyrazolines with almost the same enantioselectivity (91%) and 73:27 dr .



Procedure as: **3aa** 88 mg (0.23 mmol, 1 equiv.) was dissolved in THF (10 mL), NaBH_4 18 mg (0.46 mmol, 2 equiv.) was added carefully at -30°C . Then MeOH (2 mL) was added drop by drop, the resulting solution was stirred at -30°C until the starting material disappearance. Saturated NH_4Cl was added to quench the reaction. The mixture was concentrated and diluted with DCM, and washed with saturated NaCl (2×10 mL). The

organic layers were dried over Na₂SO₄, filtered, and concentrated in vacuum. The residue was purified by chromatography on silica gel to afford **4aa**.

Dimethyl (4*R*, 5*R*)-5-cyano-5-(hydroxy(phenyl)methyl)-4-phenyl-4,5-dihydro-1*H*-pyrazol-3-ylphosphonate (4aa)



White solid, 75 mg (85% yield); mp 208.4–210.9 °C, $[\alpha]_D^{25} = +113.3^\circ$ ($c = 1.0$, CHCl₃);

HPLC condition: chiralpak ID, 244 nm, 0.5 mL/min, hexane/*i*-PrOH = 80/20, $t_{major} =$

37.105 min, $t_{minor} = 33.374$ min, $dr = 72:28$, $ee = 90\%$; ¹H NMR (600 MHz, MeOD) ¹H

NMR (600 MHz, MeOD) δ 7.60 (d, $J = 7.3$ Hz, 2H), 7.46–7.39 (m, 3H), 7.39–7.33 (m, 3H), 7.18 (d, $J = 6.8$ Hz, 2H), 4.83 (s, 1H), 4.73 (s, 1H), 3.54 (dd, $J = 11.1, 9.9$ Hz, 6H) ppm; ¹³C NMR (151 MHz, MeOD) δ 142.4, 140.9, 137.9, 135.2, 128.8, 128.6, 128.4, 128.2, 128.0, 127.7, 116.3, 75.2, 74.5, 74.5, 59.8, 59.7, 52.7, 52.7, 52.5, 52.47 ppm; HRMS (ESI-TOF) calcd. for C₁₉H₂₀N₃O₄PNa [M+Na]⁺ 408.1089, found 408.1091.

8. Complete references for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

9. Computational methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. DFT method B3-LYP^[4] with a standard 6-31G(d) basis set was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to confirm them as a local minima or transition structures, and to derive the thermochemical corrections for the enthalpies and free energies. The M11 functional in combination with the 6-311+G(d,p) basis set was used to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with an SMD^[5] solvation model in the dichloromethane solvent.

10. Free energy profiles for silver-catalyzed asymmetric 1,3-dipolar cycloaddition.

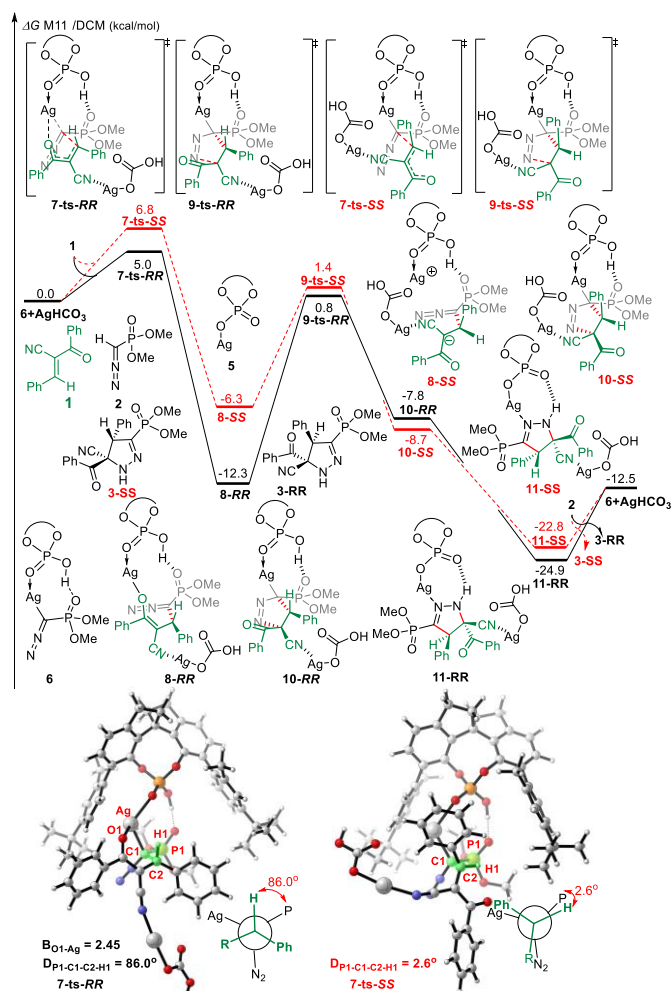
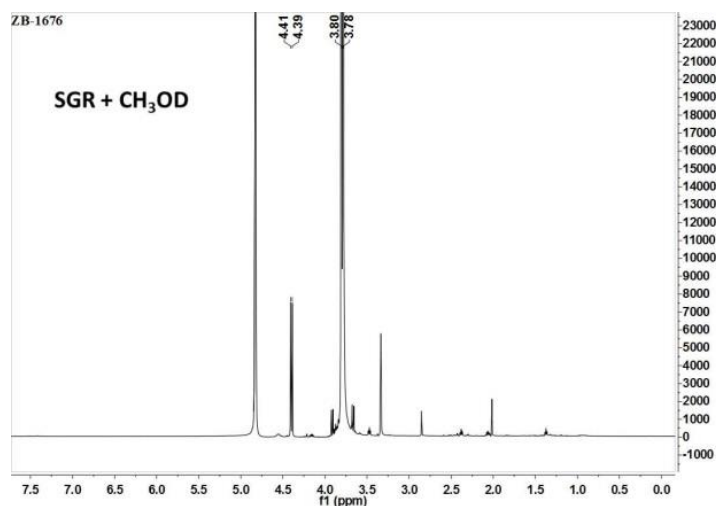
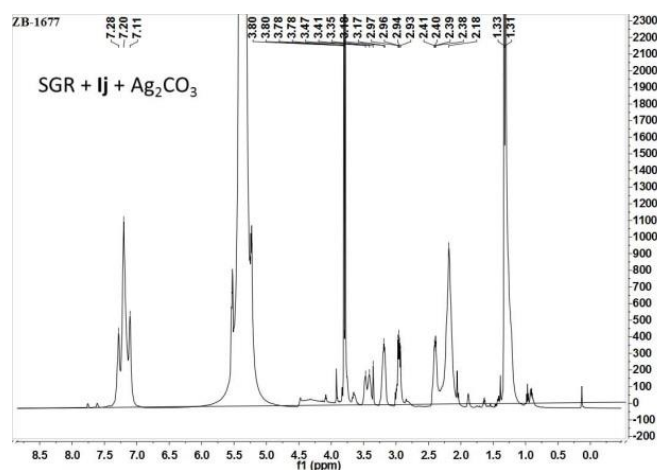


Fig S1. Free energy profiles for silver-catalyzed asymmetric 1,3-dipolar cycloaddition. Values given in kcal/mol are the relative free energies calculated using the M11 method in DCM solvent.

Density functional M11 with a standard 6–311+G(d,p) basis set (SDD basis set for Ag) was employed to gain insight into the mechanism and the origin of enantioselectivity of this asymmetric 1,3-dipolar cycloaddition (Figure S1). Deprotonation of diazophosphonate **2** by the silver phosphate catalyst would reversibly yield diazomethyl silver complex **6**. The theoretical study showed that the [3+2] cycloaddition could take place *via* a stepwise process. Intermolecular nucleophilic addition of the carbon atom of the diazomethane moiety in complex **6** to the *si* face of the β -carbon atom in α,β -unsaturated ketone **1**, activated by silver bicarbonate salt *via* transition state **7-ts-RR**, leads to generation of a new C–C bond in intermediate **8-RR**. The calculated activation free energy of this step was only 5.0 kcal/mol. Generation of intermediate **8-RR** was exergonic (12.3 kcal/mol), which indicated an irreversible process. Therefore, the enantioselectivity would be controlled by this step. Subsequent cyclization with C–N bond formation generates five-membered ring-type intermediate **10-RR** *via* transition state **9-ts-RR** with a free energy barrier of 13.1 kcal/mol. The active catalyst, diazomethyl silver complex **6**, is rapidly regenerated following proton transfer, ligand exchange, and the release of product (*R,R*)-**3**.

Alternatively, corresponding nucleophilic addition to the *re* face of α,β -unsaturated ketone **1** would occur *via* transition state **7-ts-SS** to generate the enantiomer **8-SS**. The calculated activation free energy of this process was 6.8 kcal/mol. Subsequent cyclization and proton transfer would generate enantiomer **3-SS**. Based on our theoretical calculations, the enantioselectivity could be explained by the energy difference between transition states **7-ts-RR** and **7-ts-SS**. The relative free energy of **7-ts-SS** was 1.8 kcal/mol higher than that of **7-ts-RR**, which predicted a 92% ee. This theoretical calculation was in agreement with experimental observations. In transition state **7-ts-RR**, the dihedral angle $D_{P1-C1-C2-H1}$ was 86.0°, while the corresponding $D_{P1-C1-C2-H1}$ dihedral angle in transition state **7-ts-SS** was only 2.6°. This showed that the C2–C3 bond would adopt an eclipsed conformation in transition state **7-ts-SS**. Furthermore, we found that the oxygen atom in α,β -unsaturated ketone was close to Ag ($B_{Ag-O1} = 2.45 \text{ \AA}$) in **7-ts-RR**, which represented significant coordination in that geometry. Therefore, both the configuration of the forming C–C bond in the nucleophilic addition step and the coordination of the α,β -unsaturated ketone oxygen atom with Ag influenced the enantioselectivity of this asymmetric 1,3-dipolar cycloaddition.

1a) ^1H NMR of SGR in the CH_3OD 

1b) SPA **Ij** 30 mg (0.05 mmol) and 13.7 mg Ag_2CO_3 (0.05 mmol, 1 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.25 mL) in a dried NMR sample tube in the dark and shaking for 1 h at rt. 7.5 mg SGR (0.05 mmol, 1 equiv.) was added and continuing shaking for 40 min. CD_3OD was added and conducted the ^1H NMR experiment, and found that the peak (4.41 ppm, d) of the α -proton of SGR was disappear.

Fig S2. Deuterium exchange experiment of the SGR with CH_3OD in the reaction conditions.

11. Other proposed pathways for the 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate

a) Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate in the absence of silver phosphate and silver bicarbonate

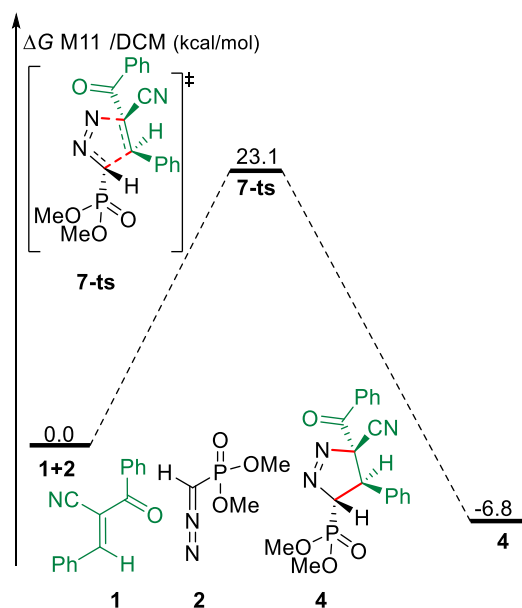


Fig S3. Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate in the absence of silver phosphate and silver bicarbonate. The values given by kcal/mol represent the relative free energies calculated by M11 method in dichloromethane solvent.

The 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate in the absence of silver phosphate and silver bicarbonate was taken into consideration firstly. As shown in Figure S3, the 1,3-dipolar cycloaddition of diazophosphonate **2** with α,β -unsaturated ketone **1** occurs via transition state **7-ts** to generate a five-membered ring intermediate **4** with an activation free energy of 23.1 kcal/mol. The calculated results indicate that the reaction pathway, in the absence of chiral silver phosphate and silver bicarbonate as co-catalysts, is energetically unfavorable.

b) Free energy profiles for the 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate in the absence of silver bicarbonate.

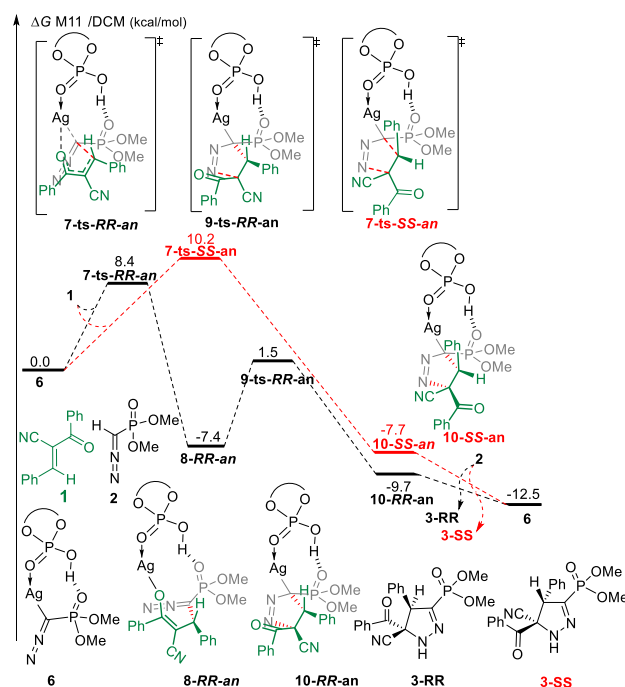


Fig S4. Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate in the absence of silver bicarbonate. The values given by kcal/mol represent the relative free energies calculated by M11 method in dichloromethane solvent.

The free energy profiles for the 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with unactivated α -diazomethylphosphonate is depicted in Figure S4. The intermolecular nucleophilic addition from the carbon atom of diazomethane moiety in complex **6** to the *si* face of the β -carbon atom in α,β -unsaturated ketone **1** via transition state **7-ts-RR-an** leads to the formation of new C-C bond in intermediate **8-RR-an**. The calculated activation free energy of this step is 8.4 kcal/mol. Subsequent cyclization with the formation of C-N bond generates intermediate **10-RR-an** via transition state **9-ts-RR-an** with a free energy barrier of 8.9 kcal/mol. The active catalyst diazomethylsilver **6** could be regenerated by following proton transfer, ligand exchange with the release of (R,R)-product **3**. The activation energy of transition state **7-ts-RR-an** is 3.4 kcal/mol higher than that of **7-ts-RR**, because the cyano group in the α,β -unsaturated ketone **1** is not activated by silver bicarbonate salt. The theoretical results suggested that silver bicarbonate, as a catalyst, plays a vital role in this reactions, which is consistent with the experimentally optimized conditions (the ratio of **1j** to Ag_2CO_3 equal to 1:1). In another case, the corresponding 1,3-dipolar cycloaddition to the *re* face of α,β -unsaturated ketone **1** would occur via transition state **7-ts-SS-an**, which would generate the enantiomer **10-SS-an**. The calculated activation free energy of this process is 10.2 kcal/mol. The enantiomer **3-SS** would be given by following proton transfer and ligand exchange. Therefore, the reaction pathway of 1,3-dipolar

cycloaddition for α -diazomethylphosphonate with α,β -unsaturated ketone, not activated by silver bicarbonate salt, is energetically unfavorable.

c) Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate activated by silver phosphate.

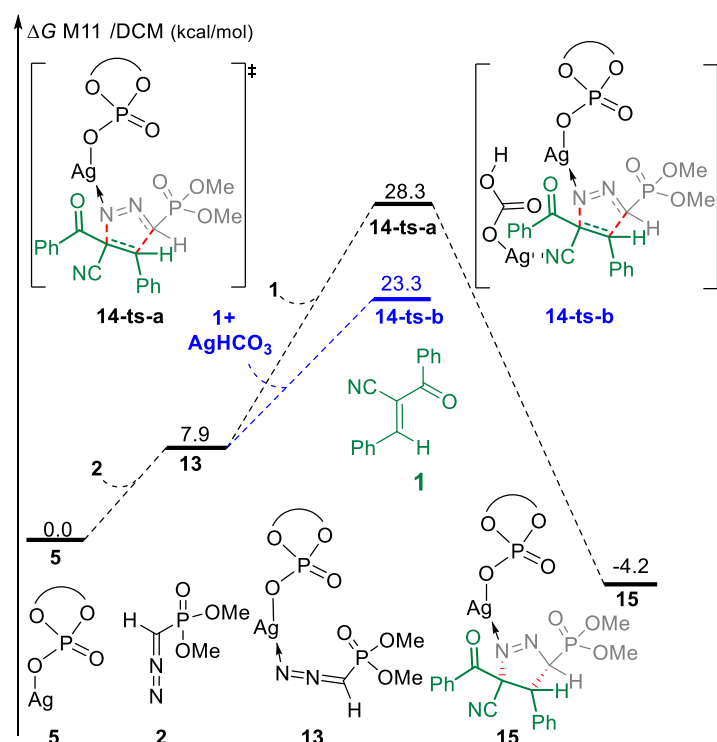


Fig S5. Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate activated by silver phosphate. The values given by kcal/mol represent the relative free energies calculated by M11 method in dichloromethane solvent.

1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone with α -diazomethylphosphonate activated by silver phosphate was also considered, in which the terminal nitrogen atom in diazo coordinates with Ag. The calculated free energy profiles were shown in Figure S5. The coordination of diazophosphonate **2** to the silver phosphate catalyst forms the intermediate **13** in an endothermic process with 7.9 kcal/mol free energy. The following 1,3-dipolar cycloaddition would yield five-membered ring intermediate **15** via transition state **14-ts-a**. The calculated activation free energy of this step is up to 28.3 kcal/mol. In addition, the intermediate **13** cycloaddition with unsaturated ketone **1** activated by silver bicarbonate salt was also calculated, the activation free energy of **14-ts-b** was also up to 23.3 kcal/mol. Therefore, 1,3-dipolar cycloaddition through silver-activation of diazo is energetically unfavorable.

d) Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone activated by silver phosphate with α -diazomethylphosphonate.

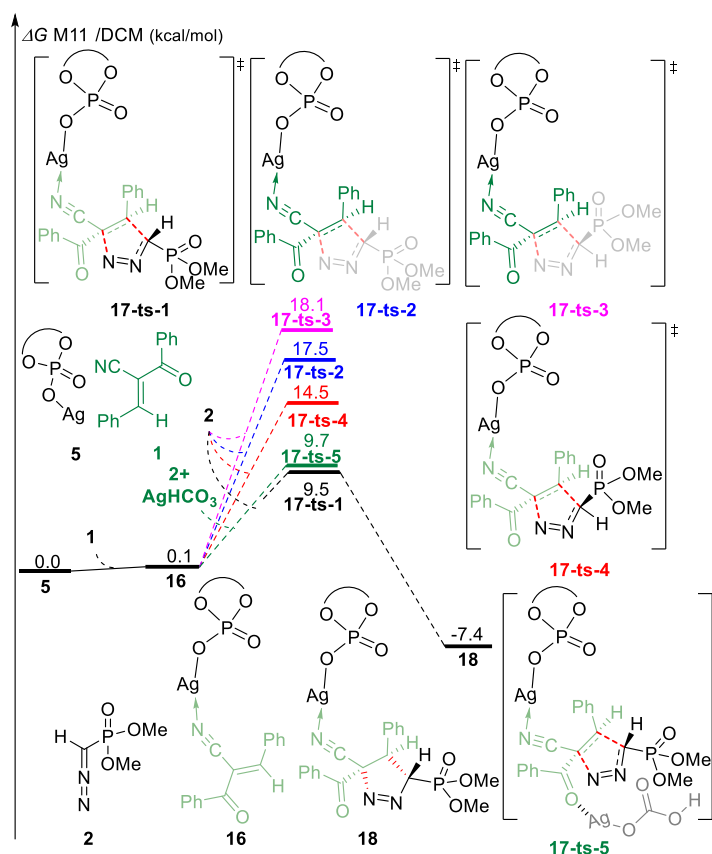


Fig S6. Free energy profiles for 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone activated by silver phosphate with α -diazomethylphosphonate. The values given by kcal/mol represent the relative free energies calculated by M11 method in dichloromethane solvent.

Moreover, as depicted in Figure S6, we also conducted the calculation of 1,3-dipolar cycloaddition reaction of substituted α,β -unsaturated ketone activated by silver phosphate with α -diazomethylphosphonate. The coordination of α,β -unsaturated ketone **1** with silver phosphate catalyst would yield complex **16** reversibly. The intermolecular cycloaddition from *re* face of diazophosphonate **2** to the *si* face of the complex **16** via transition state **17-ts-1** leads to five-membered ring intermediate **18**. The calculated activation free energy of this step is 9.5 kcal/mol. The corresponding 1,3-dipolar cycloaddition from *si* face of diazophosphonate **2** to the *si* face of the complex **16** via transition state **17-ts-4** would leads to the (*R,R*)-product. the enantiomer could yield via transition state **17-ts-2** or transition state **17-ts-3**, the calculated activation free energy of these steps are 17.5 kcal/mol and 18.1 kcal/mol, respectively. Furthermore, the (*R,R*)-product would be formed by diazophosphonate **2** activated by silver phosphate cycloaddition with complex **16** via transition state **17-ts-5** with a free energy barrier of 9.7 kcal/mol. These calculated results indicate that the reaction pathways, in which the cyano group in α,β -unsaturated ketone was activated by silver phosphate, is energetically unfavorable.

12. Absolute calculation energies, enthalpies, and free energies

Geometry	$E_{\text{(elec-B3LYP)}}^1$	$G_{\text{(corr-B3LYP)}}^2$	$H_{\text{(corr-B3LYP)}}^3$	$E_{\text{(solv, M11)}}^4$	IF ⁵
1	-746.260001	0.180435	0.240096	-746.040483	-
2	-795.037977	0.077817	0.128233	-794.993854	-
3-RR	-1541.315272	0.286135	0.372774	-1541.081832	-
3-SS	-1541.315272	0.286128	0.372775	-1541.081832	-
4	-1541.3122	0.285264	0.37188	-1541.072182	-
5	-2300.829009	0.646437	0.765917	-2300.158225	-
6	-3095.905424	0.745414	0.895954	-3095.172854	-
7-ts	-1541.266541	0.28198	0.369346	-1541.021243	-421.98
7-ts-RR	-4253.615968	0.970516	1.173515	-4252.519136	-238.80
7-ts-SS	-4253.611345	0.97338	1.173336	-4252.51919	-234.69
8-RR	-4253.638569	0.971512	1.175745	-4252.547729	-
8-SS	-4253.624882	0.971885	1.175889	-4252.53855	-
9-ts-RR	-4253.622109	0.97498	1.173329	-4252.530382	-114.58
9-ts-SS	-4253.614005	0.973858	1.173807	-4252.528255	-139.44
10-RR	-4253.627714	0.977064	1.174602	-4252.546135	-
10-SS	-4253.634143	1.175257	0.977605	-4252.548149	-
11-RR	-4253.646005	0.976546	1.177652	-4252.57292	-
11-SS	-4253.638741	0.974258	1.176841	-4252.567283	-
AgHCO ₃	-411.404592	-0.002444	0.034197	-411.266647	-
7-ts-RR-an	-3842.152158	0.954488	1.136721	-3841.228318	-261.41
7-ts-SS-an	-3842.140483	0.951652	1.136605	-3841.222528	-256.24
8-RR-an	-3842.172162	0.95341	1.138889	-3841.252387	-
9-ts-RR-an	-3842.157269	0.954896	1.136764	-3841.239637	-141.53
10-RR-an	-3842.174822	0.95857	1.137998	-3841.261205	-
10-SS-an	-812.293322	0.959859	1.138556	-3841.259332	-
13	-3095.890441	0.748289	0.895849	-3095.1636	-
14-ts-a	-3842.124978	0.952758	1.137529	-3841.1956	-428.88

14-ts-b	-4253.581433	0.969748	1.17392	-4252.489523	-396.10
15	-3842.172533	0.95545	1.140516	-3841.249998	-
16	-3047.128606	0.847419	1.008528	-3046.219172	-
17-ts-1	-3842.154605	0.954748	1.138103	-3841.227521	-266.35
17-ts-2	-3842.144655	0.954459	1.137555	-3841.214366	-258.85
17-ts-3	-3842.136199	0.948027	1.137279	-3841.206995	-376.43
17-ts-4	-3842.145894	0.952493	1.137761	-3841.217231	-311.02
17-ts-5	-4253.604038	0.970387	1.173998	-4252.511935	-228.61
18	-3842.174187	0.957803	1.140323	-3841.257451	-

¹The electronic energy calculated by B3LYP in gas phase. ²The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ³The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁴The electronic energy calculated by M11 in dichloromethane solvent. ⁵The B3LYP calculated imaginary frequencies for the transition states.

13. B3LYP geometries for all the optimized compounds and transition state.

1				C	-4.65134700	0.05887300	-1.30857500
C	-5.14375900	-0.59630700	0.31768300	C	-4.02111100	-0.56640700	0.94529600
C	-4.06746600	-1.31307900	0.84287400	C	-5.97022800	-0.28894000	-1.03898200
C	-2.76538800	-0.83596800	0.69059400	H	-4.36100100	0.43790600	-2.28231900
C	-2.53163500	0.37435100	0.01926400	C	-5.34563700	-0.90888300	1.21442100
C	-3.62453800	1.10200200	-0.48319300	H	-3.29240800	-0.64992900	1.74345400
C	-4.91983900	0.61384700	-0.34677700	C	-6.32062600	-0.77492100	0.22448600
H	-6.15568400	-0.97677200	0.42848000	H	-6.72639700	-0.18230300	-1.81147200
H	-4.23859600	-2.24650700	1.37134600	H	-5.61524900	-1.27512300	2.20067600
H	-1.94290100	-1.40185000	1.11259500	H	-7.35127200	-1.04518800	0.43739100
H	-3.43344500	2.04842100	-0.97804300	C	0.97528900	1.58590700	-0.15433800
H	-5.75632700	1.17628500	-0.75221500	C	1.67699200	1.79451100	1.04146500
C	-1.17802900	0.99116100	-0.12567000	C	0.86206800	2.64299000	-1.06725100
O	-1.06327000	2.20762300	-0.21387000	C	2.25591800	3.03425800	1.31420700
C	0.07229700	0.13332800	-0.16995900	H	1.77845500	0.98556800	1.75748800
C	1.25861500	0.77384300	0.04014000	C	1.44106600	3.88265500	-0.79452600
H	1.12999000	1.83759700	0.23261500	H	0.31193500	2.49038800	-1.99134300
C	2.63970000	0.31766300	0.05488000	C	2.14008100	4.08112500	0.39735300
C	3.62136100	1.29109600	0.34618800	H	2.79345600	3.18246000	2.24697800
C	3.06585300	-1.00552600	-0.19603900	H	1.34631400	4.69137900	-1.51398800
C	4.97236900	0.96343200	0.38837800	H	2.59161400	5.04617900	0.61152800
H	3.30710000	2.31357900	0.53964800	N	0.33076300	-1.96142000	0.31764700
C	4.41836200	-1.32834700	-0.15274700	N	-0.97921800	-1.53075500	0.36981800
H	2.34447600	-1.77922500	-0.42594700	H	-1.47932900	-1.94620800	1.14854000
C	5.37498600	-0.35063800	0.13879200	P	2.78573300	-1.36213500	-0.64925000
H	5.70910100	1.72892300	0.61440400	O	3.08132300	-0.90526700	-2.02621500
H	4.72924600	-2.35055200	-0.34881700	O	3.01539600	-2.94015200	-0.44925900
H	6.42897400	-0.61290900	0.17012200	O	3.63802800	-0.65043800	0.53078500
C	-0.02043200	-1.25298300	-0.49549800	C	3.04827800	-3.59109700	0.83295800
N	-0.09292900	-2.38074700	-0.78095500	H	3.53006200	-4.55730200	0.67142600
2				H	3.62793900	-3.00562700	1.55257300
N	2.28449500	0.28388700	0.05909800	H	2.02929700	-3.73594600	1.19887800
N	3.08108000	0.55142700	-0.70995900	C	4.90673100	-0.03217400	0.23351300
C	1.35184300	-0.03015300	0.91416400	H	4.92606200	0.32820400	-0.79733500
H	1.66349700	-0.21835400	1.93378100	H	5.01604000	0.80400900	0.92651300
P	-0.36873100	-0.03087200	0.45987600	H	5.71429300	-0.75425300	0.39016600
O	-1.24066300	-0.45120100	1.58402700	3-SS			
O	-0.56502100	1.44165900	-0.16274500	C	-1.05560600	-0.05141700	-0.22287400
O	-0.51253200	-0.91363400	-0.89656900	C	1.07933100	-1.02243000	0.14357700
C	-1.83933000	1.80359900	-0.73037200	C	0.32107500	0.25720800	0.47976300
H	-1.77159600	2.86374500	-0.97892400	H	0.11410000	0.24217000	1.55583300
H	-2.03064900	1.21909400	-1.63482700	C	-1.18222800	0.60671800	-1.53604000
H	-2.64120000	1.64392400	-0.00346800	N	-1.30748100	1.06717900	-2.59552400
C	-0.63230500	-2.34157000	-0.77784200	C	-2.26989800	0.30517400	0.71371900
H	-0.85557900	-2.71664600	-1.77815300	O	-2.04002100	0.83924100	1.78241600
H	0.30999900	-2.77749300	-0.42669000	C	-3.65784300	-0.07922800	0.32165500
H	-1.43805100	-2.60423400	-0.08721400	C	-4.65134700	0.05887300	1.30857500
3-RR				C	-4.02111100	-0.56640700	-0.94529600
C	-1.05560600	-0.05141700	0.22287400	C	-5.97022800	-0.28894000	1.03898200
C	1.07933100	-1.02243000	-0.14357700	H	-4.36100100	0.43790600	2.28231900
C	0.32107500	0.25720800	-0.47976300	C	-5.34563700	-0.90888300	-1.21442100
H	0.11410000	0.24217000	-1.55583300	H	-3.29240800	-0.64992900	-1.74345400
C	-1.18222800	0.60671800	1.53604000	C	-6.32062600	-0.77492100	-0.22448600
N	-1.30748100	1.06717900	2.59552400	H	-6.72639700	-0.18230300	1.81147200
C	-2.26989800	0.30517400	-0.71371900	H	-5.61524900	-1.27512300	-2.20067600
O	-2.04002100	0.83924100	-1.78241600	H	-7.35127200	-1.04518800	-0.43739100
C	-3.65784300	-0.07922800	-0.32165500	C	0.97528900	1.58590700	0.15433800

C 1.67699200 1.79451100 -1.04146500
 C 0.86206800 2.64299000 1.06725100
 C 2.25591800 3.03425800 -1.31420700
 H 1.77845500 0.98556800 -1.75748800
 C 1.44106600 3.88265500 0.79452600
 H 0.31193500 2.49038800 1.99134300
 C 2.14008100 4.08112500 -0.39735300
 H 2.79345600 3.18246000 -2.24697800
 H 1.34631400 4.69137900 1.51398800
 H 2.59161400 5.04617900 -0.61152800
 N 0.33076300 -1.96142000 -0.31764700
 N -0.97921800 -1.53075500 -0.36981800
 H -1.47932900 -1.94620800 -1.14854000
 P 2.78573300 -1.36213500 0.64925000
 O 3.08132300 -0.90526700 2.02621500
 O 3.01539600 -2.94015200 0.44925900
 O 3.63802800 -0.65043800 -0.53078500
 C 3.04827800 -3.59109700 -0.83295800
 H 3.53006200 -4.55730200 -0.67142600
 H 3.62793900 -3.00562700 -1.55257300
 H 2.02929700 -3.73594600 -1.19887800
 C 4.90673100 -0.03217400 -0.23351300
 H 4.92606200 0.32820400 0.79733500
 H 5.01604000 0.80400900 -0.92651300
 H 5.71429300 -0.75425300 -0.39016600

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N 0.30561800 -1.54810000 1.51429700
 N -0.85171300 -1.18819800 1.28368700
 C 1.33448200 -0.61379300 0.99395300
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 O 3.56552700 -2.32686500 1.23989000
 O 1.96710400 -2.57691200 -0.82492000
 O 3.36849500 -0.50398200 -0.67109900
 C 1.67844300 -3.95598000 -0.50890300
 H 0.75602300 -4.01972100 0.07535600
 H 1.54951500 -4.46752900 -1.46443700
 H 2.50274200 -4.40103800 0.05291100
 C 4.57848600 -0.81208400 -1.39080500
 H 4.92415300 0.12891900 -1.82034700
 H 5.33464700 -1.21540000 -0.71161000
 H 4.36853600 -1.53067200 -2.18893000
 C -6.08168700 -0.66865900 -0.18761700
 C -5.55143500 -0.32277100 -1.43513900
 C -4.18447700 -0.11277100 -1.57282300
 C -3.32846000 -0.23544700 -0.46175900
 C -3.86839100 -0.58741100 0.78746600
 C -5.23938200 -0.80472300 0.91725300
 H -7.15035600 -0.83305300 -0.07861900
 H -6.20543200 -0.21743700 -2.29606700
 H -3.75357100 0.15304000 -2.53207100
 H -3.22652400 -0.71695100 1.64956500
 H -5.64860000 -1.08040300 1.88468900
 C -1.88128400 0.00788500 -0.70148300
 O -1.42419300 0.11500200 -1.82546100
 C -0.88628200 0.14610100 0.51014400
 C 0.58847300 0.34734000 0.04335800
 H 0.61371000 -0.07272900 -0.96460100
 C 1.10297700 1.77218900 -0.03475300
 C 1.18762400 2.38819600 -1.29086500

C 1.48650200 2.50283500 1.09823500
 C 1.64795700 3.69921400 -1.41390000
 H 0.88192700 1.83416200 -2.17386200
 C 1.94849500 3.81375400 0.97655500
 H 1.41813100 2.06146200 2.08871800
 C 2.03245500 4.41614400 -0.27970300
 H 1.70663100 4.15874200 -2.39697300
 H 2.24009300 4.36369200 1.86703600
 H 2.39351600 5.43676600 -0.37296300
 C -1.36331900 1.15625100 1.45562400
 N -1.73126600 1.94303500 2.22681700
 H 1.76701900 -0.11659000 1.87070600

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C 1.66270100 4.16982500 -1.47837300
 C 1.06273100 3.30182500 -0.55418600
 C 1.64344900 2.06370900 -0.31176500
 C 2.90620600 1.73534500 -0.84423400
 C 3.52509500 2.65458100 -1.70024800
 C 2.89311100 3.85464300 -2.04982400
 C 0.75942000 5.36205400 -1.72791700
 C -0.57872300 4.91855200 -1.08290000
 C -0.15658400 3.96050200 0.07958300
 H 4.49382600 2.40896200 -2.12795900
 H 3.36100400 4.52464400 -2.76677000
 H 1.15198600 6.27035500 -1.24948900
 H -1.17163600 4.35269600 -1.81015000
 H -1.18822500 5.75801700 -0.73277700
 H 0.65570600 5.58965500 -2.79503500
 C 0.28560900 4.81042200 1.32229500
 H 0.84477800 5.70695900 1.03617300
 H 0.93995400 4.19597800 1.95156700
 C -1.02101300 5.11409700 2.08040000
 C -1.85461200 3.88799600 1.78277900
 C -1.32621600 3.18069000 0.68922200
 C -2.97809600 3.42881800 2.46248900
 H -3.37753600 3.98159100 3.30930400
 C -3.58323200 2.24202200 2.04893700
 H -4.46874100 1.87495900 2.56027700
 C -3.06870500 1.48774900 0.98315300
 C -1.91571300 1.96547000 0.33061300
 H -1.50179200 6.02543000 1.69629100
 H -0.86299500 5.26906400 3.15392500
 O 0.94541100 1.10930400 0.40654300
 O -1.37844400 1.21476000 -0.70686200
 P -0.12075000 0.18601600 -0.50310600
 O 0.42405900 -0.11770800 -1.86482800
 O -0.42135800 -0.98819700 0.43454700
 C 3.50494000 0.40923400 -0.48809200
 C 3.36776900 -0.68380800 -1.35684200
 C 4.11412100 0.19428800 0.76504000
 C 3.75605800 -1.98573600 -0.97069800
 C 4.53085900 -1.09941800 1.12245300
 C 4.35769000 -2.21625700 0.29617100
 H 3.72442600 -2.77906600 -1.71401400
 H 4.99299900 -1.22342000 2.09570900
 C -3.73160500 0.20593600 0.59807500
 C -3.76678900 -0.84344700 1.52151600
 C -4.37647100 0.03326200 -0.64725700
 C -4.40542200 -2.05072500 1.23542000

H	-3.26397300	-0.71845100	2.47654000
C	-5.01207800	-1.18358400	-0.90796300
C	-5.04158900	-2.25013300	0.00540400
H	-4.39216700	-2.83385000	1.98552700
H	-5.50854200	-1.29398400	-1.86927800
C	-4.40629800	1.13016600	-1.68671700
H	-4.69234200	2.09321500	-1.24774200
H	-3.42037500	1.26414500	-2.14607600
H	-5.12101000	0.89470000	-2.48204100
C	4.86076900	-3.62117000	0.67072400
C	6.07643300	-3.96442000	-0.22713100
H	6.46341200	-4.95964500	0.02189900
H	5.80879100	-3.96449900	-1.28940200
H	6.88580400	-3.23972400	-0.08432900
C	5.30175900	-3.71050200	2.14458400
H	5.61380500	-4.73561000	2.37226800
H	6.15349000	-3.05596400	2.35867100
H	4.48700100	-3.44970900	2.82986800
C	3.74941700	-4.67309400	0.43957500
H	2.86918500	-4.45702600	1.05975500
H	3.42967600	-4.71561700	-0.60700800
H	4.10998200	-5.67224000	0.71076300
C	-5.75686500	-3.56112000	-0.36864000
C	-5.11381300	-4.15513600	-1.64460200
H	-5.61727600	-5.08833600	-1.92735500
H	-5.18272300	-3.46731600	-2.49359700
H	-4.05270900	-4.37533700	-1.47998900
C	-7.25406700	-3.27572900	-0.63625300
H	-7.77679700	-4.19944400	-0.91524000
H	-7.73995200	-2.86639600	0.25707700
H	-7.39164800	-2.55599800	-1.44992700
C	-5.66374100	-4.61792600	0.74851500
H	-4.62381600	-4.88239400	0.97206500
H	-6.13548600	-4.27380600	1.67606100
H	-6.17885200	-5.53365000	0.43545700
H	2.91040700	-0.52757500	-2.32742800
C	4.27621800	1.32417400	1.75248900
H	4.67527600	2.22359600	1.27281400
H	3.30494900	1.59594100	2.18472100
H	4.94252100	1.04039500	2.57287400
Ag	1.43334500	-2.08501500	-0.22249800

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C	-0.77861200	5.20074800	-1.24075900
C	-0.91397500	4.13491200	-0.33703300
C	0.15761700	3.26501800	-0.15739800
C	1.40686200	3.49190300	-0.76180700
C	1.51828800	4.59970500	-1.61811300
C	0.43294100	5.43690200	-1.88244900
C	-2.09206300	5.93824200	-1.38961600
C	-3.10059900	4.95390200	-0.75649000
C	-2.28003800	4.19262800	0.33917100
H	2.47601800	4.78596100	-2.09563800
H	0.53827500	6.26084300	-2.58370700
H	-2.07501000	6.89551600	-0.84962000
H	-3.43582900	4.23287300	-1.51067000
H	-3.98874800	5.44444300	-0.34590900
H	-2.32762900	6.17036300	-2.43436900
C	-2.23164100	5.04668700	1.65125700
H	-2.08427600	6.11236000	1.44949700
H	-1.39069800	4.70330200	2.26449800

C	-3.56256600	4.73548500	2.37053000
C	-3.84698400	3.31510000	1.93210200
C	-3.03287100	2.96410400	0.84290000
C	-4.74020900	2.39784100	2.47602000
H	-5.36975000	2.66978400	3.31955600
C	-4.82176600	1.11789100	1.92583900
H	-5.53270400	0.40006100	2.32466200
C	-3.98751200	0.71068500	0.87150700
C	-3.07079500	1.65406800	0.37359300
H	-4.36057500	5.41928000	2.04836700
H	-3.48647700	4.83180600	3.45955900
O	-0.03571800	2.10387900	0.61228400
O	-2.14706800	1.25033800	-0.60634000
P	-0.65869100	0.81500000	-0.15987700
O	0.08828600	0.44234300	-1.41049200
O	-0.82401900	-0.23456400	0.97992400
C	2.58458000	2.59988500	-0.54915800
C	3.13195400	1.91889200	-1.64432800
C	3.21202000	2.46868800	0.70928700
C	4.26468900	1.11085100	-1.51397000
C	4.35182300	1.66376400	0.80924600
C	4.90497800	0.96548200	-0.27541900
H	4.64492200	0.60600600	-2.39516600
H	4.82964400	1.59296800	1.78276400
C	-4.08115200	-0.68538700	0.35282700
C	-3.86437300	-1.74962700	1.23569100
C	-4.44609600	-0.97726600	-0.98114100
C	-3.98679400	-3.07815600	0.82730400
H	-3.57617100	-1.52998700	2.25995300
C	-4.56144300	-2.31697400	-1.36405800
C	-4.33681200	-3.39342100	-0.49096300
H	-3.80828000	-3.86168000	1.55545100
H	-4.85186500	-2.52062000	-2.39182900
C	-4.73647100	0.11005100	-1.99071300
H	-5.36195900	0.90144400	-1.56223700
H	-3.81260900	0.58282200	-2.34347300
H	-5.25789500	-0.29861200	-2.86207100
C	6.18389300	0.12950700	-0.08524800
C	7.36566500	1.08928600	0.19767600
H	8.29200600	0.52110400	0.34866600
H	7.52293100	1.77901700	-0.63993700
H	7.18908800	1.68985600	1.09686800
C	6.01835800	-0.83952900	1.10914200
H	6.91955200	-1.45520900	1.21794600
H	5.87175000	-0.30525100	2.05384900
H	5.16217000	-1.50673900	0.96729400
C	6.52547500	-0.70650500	-1.33402700
H	5.72027000	-1.40503700	-1.58778200
H	6.72658300	-0.07746600	-2.20880800
H	7.42801500	-1.29825200	-1.14426700
C	-4.49003500	-4.83846400	-0.99928300
C	-3.49385100	-5.08652900	-2.15723100
H	-3.59427300	-6.11141000	-2.53549900
H	-3.66479700	-4.40272100	-2.99494700
H	-2.45939300	-4.94789100	-1.82123700
C	-5.93395300	-5.05662200	-1.51246800
H	-6.05574900	-6.08119900	-1.88518400
H	-6.66278200	-4.89784700	-0.70936000
H	-6.18376900	-4.37273700	-2.33023200
C	-4.21468300	-5.87917300	0.10297300

H	-3.19316200	-5.80076300	0.49308700	C	-5.23339400	0.53453400	-0.65063100
H	-4.90955800	-5.77624700	0.94426700	C	-5.97464000	2.76109800	-1.28437200
H	-4.33532300	-6.88968600	-0.30373700	H	-6.61766700	3.41340800	-1.86933300
H	2.65406200	2.01793500	-2.61559800	C	-5.06399600	3.30515500	-0.37860900
C	2.70068100	3.19215500	1.93420300	H	-5.01604400	4.38109900	-0.24070600
H	2.49311500	4.24725400	1.72171400	C	-4.17167100	2.49887800	0.34847000
H	1.76831200	2.74559600	2.29899200	C	-4.26054200	1.10542600	0.16706800
H	3.43323000	3.14722000	2.74621500	H	-7.96574100	0.54624900	-2.00613800
Ag	1.66159500	-1.08661800	-1.24267100	H	-6.94159100	0.97706700	-3.37077700
N	3.34981400	-3.62674300	-0.82166600	O	-2.62844400	-1.12890200	-1.19741100
N	4.10210900	-4.33350100	-1.31778300	O	-3.34484200	0.27671800	0.83615900
C	2.50271700	-2.78238800	-0.32592300	P	-2.04352300	-0.29212000	0.07071700
P	1.90605400	-2.99262300	1.29421100	O	-1.17224700	-1.05835900	0.99172500
O	0.95318000	-1.89827000	1.71747300	O	-1.41463400	0.96092500	-0.67999400
O	1.24197500	-4.46415900	1.51044800	H	-0.43290900	0.93272100	-0.74750000
O	3.18919900	-3.13176600	2.25931500	C	-4.32934000	2.10316400	3.26343200
C	-0.05224600	-4.72801300	0.94732200	C	-3.31763700	2.93429900	2.68310300
H	-0.78459400	-3.99104200	1.29132000	C	-4.41866000	1.92678000	4.61965600
H	-0.00396500	-4.71391500	-0.14743800	C	-3.19609300	3.13890500	1.28500700
H	-0.33864600	-5.72572800	1.28613200	C	-2.41300800	3.61031300	3.58580500
C	3.00665400	-3.28764700	3.67888500	C	-3.50485500	2.57152800	5.50118200
H	4.00402800	-3.25015400	4.12005300	H	-5.19960400	1.29293200	5.03069400
H	2.39246800	-2.47400600	4.07596000	C	-2.20906300	4.02250600	0.77976800
H	2.53838100	-4.25174200	3.89760100	C	-1.45530900	4.48859500	3.07091900
H	-0.06381300	-0.88928100	1.22093400	C	-2.53421300	3.39245800	4.99436500
7-ts				H	-3.59143300	2.41841200	6.57323500
H	6.72733600	-1.61443700	-2.10956100	C	-2.02231300	4.26525900	-0.62137800
C	4.99125700	-1.58738300	-0.84061400	C	-1.34090200	4.72496900	1.69855800
C	6.46805700	-1.44935900	-1.05229800	H	-0.79581900	5.01559700	3.75756900
C	7.00393500	-2.51236300	-0.13758400	H	-1.84041000	3.90615400	5.65552300
C	5.97953000	-3.14322200	0.44223100	C	-1.10206200	5.17660900	-1.07386700
O	4.74505400	-2.59054500	-0.00423600	H	-2.62657200	3.71394300	-1.33174100
H	6.80677800	-0.42902100	-0.81630200	C	-0.39079300	5.66468600	1.18580100
H	8.05059300	-2.74005000	0.00813300	C	-0.28327700	5.90116200	-0.15872500
C	5.83994000	-4.25095500	1.41862500	H	-0.99842500	5.35366100	-2.14136400
H	5.28605900	-3.91712600	2.30343500	H	0.23240300	6.20310600	1.89620300
H	5.29426300	-5.09421000	0.97975000	H	0.41977900	6.64115400	-0.53309800
H	6.82726100	-4.59975200	1.73008500	C	-1.57239300	-3.11981500	-3.51031700
C	3.94261900	-0.76741000	-1.25957200	C	-0.77371900	-3.54582100	-2.40055800
C	-5.50552900	-3.24055600	-0.28066400	C	-1.03047400	-2.95240700	-4.75787500
C	-4.75793000	-2.12198400	-0.68394500	C	-1.30634900	-3.73175300	-1.10050200
C	-3.39197500	-2.26860100	-0.91092900	C	0.62454400	-3.82051300	-2.64838300
C	-2.76634900	-3.52829800	-0.84585300	C	0.35166900	-3.20525800	-4.99131800
C	-3.56546900	-4.63705300	-0.51798800	H	-1.66109600	-2.63145200	-5.58210200
C	-4.91918500	-4.50020500	-0.21091100	C	-0.47208800	-4.19526600	-0.05184900
C	-6.92214400	-2.83557400	0.06240500	C	1.42685400	-4.29847800	-1.60691300
C	-6.80964400	-1.29932300	0.17034000	C	1.15148100	-3.63001100	-3.96486000
C	-5.67638400	-0.91445700	-0.84183000	H	0.76114700	-3.07343600	-5.98902500
H	-3.09884300	-5.61683600	-0.47772900	C	-0.93826200	-4.36805500	1.29371500
H	-5.50129700	-5.36877500	0.08535800	C	0.91305800	-4.50792300	-0.32321200
H	-7.62379300	-3.13221000	-0.72928800	H	2.46916800	-4.54039900	-1.80743600
H	-6.48979800	-1.02262900	1.18158500	H	2.20344000	-3.84835000	-4.13520400
H	-7.74919000	-0.77872200	-0.03636700	C	-0.12138000	-4.87049900	2.27638800
H	-7.27790200	-3.30089400	0.98823400	H	-1.95853200	-4.09273600	1.53054500
C	-6.27633100	-0.83143100	-2.28590900	C	1.72837300	-5.03617800	0.72778400
H	-6.97676100	-1.64538700	-2.49544000	C	1.22900800	-5.22771000	1.98788400
H	-5.45897700	-0.89763200	-3.01337700	H	-0.51084000	-5.01206300	3.28135600
C	-6.92394900	0.56880100	-2.35418700	H	2.75819400	-5.29581800	0.49387200
C	-6.04949200	1.37906600	-1.42205500	H	1.85497100	-5.64617600	2.77139600

H	-5.04474800	1.61410900	2.61265000
H	-2.62891000	-2.93644700	-3.35442100
C	6.36753300	3.56444900	0.26568400
C	6.78871700	2.37192600	0.85753900
C	5.92599300	1.27029500	0.91977600
C	4.63562900	1.37652700	0.40002100
C	4.24490400	2.58169100	-0.21741400
C	5.08744200	3.68356200	-0.28908700
H	7.04374000	4.41284300	0.22277000
H	7.78952600	2.29555100	1.27060100
H	6.26874100	0.34430900	1.36860800
H	4.77571500	4.60248000	-0.77117400
C	2.43722800	1.21225900	-0.50421300
C	3.50411500	0.41502700	0.28838800
N	2.93566600	2.46264800	-0.72110100
C	2.19570100	3.50718100	-1.44541100
H	1.14386200	3.21607800	-1.39953900
H	2.29449300	4.43901000	-0.88186700
C	2.65348600	3.68129900	-2.88117800
C	2.50489100	2.63243900	-3.80103200
C	3.20241300	4.89255300	-3.31489300
C	2.91238400	2.79218100	-5.12474800
H	2.04921300	1.69816200	-3.48132500
C	3.60652900	5.05569100	-4.64247300
H	3.30348100	5.72070100	-2.61628300
C	3.46635800	4.00407800	-5.54815500
H	2.78559200	1.97624500	-5.83100000
H	4.02764000	6.00318300	-4.96639200
H	3.77838800	4.12914900	-6.58105000
O	1.34966500	0.79667400	-0.89815900
C	3.72891500	-1.75941300	5.32694200
C	4.69860000	-0.89456200	4.79605400
C	4.58660400	-0.37476200	3.50689100
C	3.48553900	-0.72875900	2.70852200
C	2.50564000	-1.58024200	3.29235400
C	2.60655600	-2.10550900	4.57826900
H	3.84337700	-2.14600600	6.33491100
H	5.55157800	-0.61229900	5.40620000
H	5.33561800	0.32169400	3.15694700
H	1.83112300	-2.74893000	4.98277300
C	1.74673200	-1.04871300	1.25633100
C	2.98720200	-0.38977700	1.37155100
N	1.47831800	-1.73573700	2.36883500
H	0.61990100	-2.26578100	2.48671400
H	1.03651500	-1.04718800	0.44902100
H	2.95857400	-1.21920700	-1.33313600
H	4.18523700	-0.06824600	-2.05615100
7-ts-RR			
C	6.00671700	-2.55054400	-2.26985600
C	5.69844000	-1.69522700	-1.19975500
C	4.60065000	-1.98597100	-0.39650800
C	3.88356100	-3.18756400	-0.53935500
C	4.25993200	-4.05034900	-1.58212500
C	5.29124200	-3.72721700	-2.46559900
C	7.13291400	-1.97181400	-3.09998500
C	7.21203700	-0.51408600	-2.59126600
C	6.74301400	-0.59119400	-1.10023000
H	3.71348800	-4.98110400	-1.70519500
H	5.52730100	-4.39098500	-3.29325700
H	8.07454900	-2.51043600	-2.92412100

H	6.50911000	0.11281400	-3.15147700
H	8.20798000	-0.07155800	-2.69193200
H	6.93242100	-2.03294300	-4.17551300
C	7.93825200	-1.04534200	-0.19326400
H	8.54997200	-1.81799500	-0.66922400
H	7.53618200	-1.46382700	0.73657300
C	8.71325600	0.25262600	0.11447700
C	7.61841100	1.29633500	0.09448100
C	6.45960900	0.78682000	-0.51275000
C	7.64442900	2.59156300	0.60002000
H	8.54100100	2.98650900	1.07104900
C	6.50168000	3.38299000	0.49381100
H	6.51386600	4.40458500	0.86203300
C	5.30809200	2.89741600	-0.06900900
C	5.30841500	1.57182000	-0.53897300
H	9.47142700	0.45765200	-0.65456000
H	9.24110900	0.21251400	1.07397900
O	4.15979900	-1.03001700	0.53630800
O	4.11625900	1.01516900	-1.03669100
P	3.17512900	0.12187500	-0.06762400
O	2.02346200	-0.38983900	-0.86805900
O	2.85973500	0.93349400	1.24120900
C	2.74962500	-3.57109800	0.35128100
C	1.48128800	-3.79613900	-0.21721900
C	2.92185500	-3.81971500	1.73025700
C	0.40252500	-4.26772300	0.55266400
C	1.83133600	-4.29753100	2.47007900
C	0.56415600	-4.54431600	1.92137500
H	-0.53658000	-4.46513600	0.04889800
H	1.99905000	-4.51072100	3.52277300
C	4.12407500	3.80431000	-0.11738900
C	3.64502500	4.34198700	1.08735800
C	3.54311700	4.23569100	-1.32692600
C	2.62524100	5.28604900	1.10837400
H	4.08410500	4.00433800	2.02226700
C	2.51705700	5.19143100	-1.27706900
C	2.03870900	5.74271400	-0.08228800
H	2.29312700	5.67424600	2.06710200
H	2.10016000	5.51984500	-2.22338700
C	4.01834500	3.73060300	-2.67040000
H	5.11227500	3.74103000	-2.74051400
H	3.69423800	2.69854200	-2.84674200
H	3.62240200	4.35023800	-3.48109300
C	-0.55678800	-5.13436600	2.79640100
C	-0.09066000	-6.49766900	3.36426900
H	-0.88067300	-6.93742300	3.98455300
H	0.13879200	-7.20258100	2.55698900
H	0.80471500	-6.39812300	3.98712800
C	-0.86524900	-4.17404700	3.96974300
H	-1.64697900	-4.59809600	4.61102800
H	0.01676600	-3.99722200	4.59499200
H	-1.22236100	-3.20506900	3.60329800
C	-1.85803100	-5.36531600	2.00437000
H	-2.26580200	-4.43309200	1.59880000
H	-1.71334900	-6.06797200	1.17574500
H	-2.61866200	-5.79213700	2.66740400
C	0.94593000	6.82607600	-0.03784800
C	0.39312500	7.16161900	-1.43580500
H	-0.39280000	7.92058400	-1.35086500
H	1.16940000	7.56407500	-2.09655800

H	-0.04470000	6.28213100	-1.92161300
C	1.54139400	8.12048200	0.56763300
H	0.77788700	8.90683000	0.61578800
H	1.91779100	7.95674300	1.58300300
H	2.37381500	8.49108900	-0.04161700
C	-0.23064700	6.34616300	0.84498000
H	-0.67747500	5.42980900	0.44409800
H	0.09075700	6.14327400	1.87237500
H	-1.01181800	7.11524600	0.88874600
H	1.35051900	-3.66785000	-1.28942900
C	4.25624800	-3.62675500	2.41303300
H	5.06757700	-4.09633400	1.84535100
H	4.50318000	-2.56320500	2.50787300
H	4.24729500	-4.06337200	3.41640700
Ag	0.20249200	-1.55791400	0.06943600
N	-2.43428100	-1.08782700	1.50429200
N	-3.32805500	-1.77659300	1.68506000
C	-1.48020500	-0.34268500	1.01184900
P	-0.81325300	0.90522200	2.08648600
O	0.38025900	1.61521300	1.51030300
O	-2.05351000	1.84827800	2.43783300
O	-0.51611500	0.22736400	3.52980400
C	-1.87449400	3.08411500	3.16080100
H	-1.63023400	2.87258100	4.20592600
H	-1.08590600	3.68278900	2.69798900
H	-2.82886400	3.60680500	3.09505100
C	0.75836100	-0.36673700	3.83674900
H	0.75139200	-0.55863900	4.91112900
H	0.88181300	-1.31293700	3.29915300
H	1.57681800	0.31161200	3.58364600
H	1.89119800	1.24854700	1.30444400
C	-4.70322600	-5.57287000	-3.05496300
C	-5.14013900	-4.87879900	-1.92550300
C	-4.45380200	-3.74455100	-1.48878400
C	-3.31327700	-3.30102900	-2.17610000
C	-2.86281200	-4.02352000	-3.29338900
C	-3.56173400	-5.14279000	-3.73821300
H	-5.24566600	-6.44955900	-3.39866200
H	-6.01492500	-5.21991600	-1.37896100
H	-4.79130000	-3.22607300	-0.59770500
H	-1.96748500	-3.68809100	-3.80722100
H	-3.21575300	-5.68264500	-4.61553400
C	-2.50132100	-2.12348400	-1.72931400
O	-1.25310500	-2.21991200	-1.78872200
C	-3.13323600	-0.90065500	-1.26405700
C	-2.30074200	0.20272700	-0.86875000
C	-2.80968900	1.58488900	-0.72187600
C	-2.08626500	2.61541700	-1.34895500
C	-3.99496800	1.91408800	-0.03865700
C	-2.56607800	3.92462000	-1.34109600
H	-1.15656500	2.38143300	-1.86151400
C	-4.47391300	3.22270600	-0.02446600
H	-4.55060900	1.15367100	0.49763200
C	-3.76190700	4.22886600	-0.68527200
H	-2.00996700	4.70438200	-1.85413700
H	-5.41319500	3.43174200	0.47969300
H	-4.13908600	5.24816300	-0.68719500
C	-4.53103700	-0.74186300	-1.32049100
N	-5.68006100	-0.54758600	-1.38541100

H	-1.31412800	0.15272400	-1.31729300
C	-8.71783100	2.40078400	0.52429300
O	-9.16450600	1.53818200	-0.33611100
O	-9.67116800	3.25505600	1.00237600
H	-10.49891700	2.99895200	0.56229500
O	-7.55891000	2.51279600	0.93211100
Ag	-7.46161300	0.42002400	-0.90054400

7-ts-SS

C	5.46021200	-3.09475100	-1.88603800
C	5.19749200	-2.16752000	-0.86437500
C	4.03226800	-2.30288600	-0.11496900
C	3.16423500	-3.39665700	-0.29011000
C	3.48793500	-4.33124700	-1.28709700
C	4.61345100	-4.17773900	-2.09829900
C	6.69615700	-2.69153800	-2.66067500
C	6.89494900	-1.22268300	-2.22681300
C	6.33824000	-1.15951800	-0.76376500
H	2.82665400	-5.18061200	-1.43371100
H	4.81597900	-4.89426000	-2.89009800
H	7.55945800	-3.31202300	-2.38173200
H	6.29131400	-0.56534500	-2.86284900
H	7.93431300	-0.88615700	-2.29111200
H	6.56741800	-2.79940200	-3.74341600
C	7.44320000	-1.63074900	0.24091400
H	8.00488600	-2.49246400	-0.13329500
H	6.96393600	-1.92663900	1.18118800
C	8.31857500	-0.37914900	0.47353300
C	7.32693900	0.75136600	0.30014900
C	6.14989900	0.28347100	-0.30465000
C	7.44857200	2.08589700	0.67481200
H	8.35986500	2.45043800	1.14220200
C	6.38321100	2.95763900	0.44523300
H	6.47398000	4.00626200	0.71337200
C	5.16850900	2.51618400	-0.10699300
C	5.07220000	1.15388300	-0.44339000
H	9.12897800	-0.31475600	-0.26617300
H	8.79349100	-0.37438400	1.46113200
O	3.68915400	-1.29058800	0.79750900
O	3.84245800	0.64829500	-0.89632600
P	2.84088400	-0.04703500	0.17106500
O	1.59186400	-0.43353500	-0.54082200
O	2.72506700	0.86827700	1.44303100
C	1.91925700	-3.58873100	0.51355900
C	0.66989800	-3.55647300	-0.13478800
C	1.95207000	-3.89399900	1.88880900
C	-0.53371800	-3.81101800	0.55270400
C	0.74374300	-4.15680800	2.55328400
C	-0.51040600	-4.12776100	1.92891500
H	-1.45485300	-3.85055200	-0.02496200
H	0.80112900	-4.41867100	3.60687200
C	4.03926400	3.47822700	-0.26973400
C	3.57400700	4.16401800	0.86370500
C	3.46390800	3.78064900	-1.52098600
C	2.56366500	5.11483600	0.77688700
H	4.00857600	3.93033500	1.83186000
C	2.44535000	4.74455300	-1.58019800
C	1.96938400	5.42979200	-0.45552100
H	2.24006500	5.61600400	1.68463000
H	2.03138000	4.96882400	-2.55802400

C	3.92739500	3.12241000	-2.80084100
H	5.01994600	3.05103500	-2.84603300
H	3.53391400	2.10297400	-2.88840700
H	3.59046200	3.69109900	-3.67361900
C	-1.77972300	-4.48652500	2.72280200
C	-1.66683100	-5.95116800	3.21349700
H	-2.56193000	-6.22831200	3.78283100
H	-1.57687500	-6.64281600	2.36806100
H	-0.79723400	-6.09926400	3.86312600
C	-1.91550300	-3.55015000	3.94741100
H	-2.81602500	-3.80581500	4.51815400
H	-1.06015300	-3.63348300	4.62712200
H	-2.00033200	-2.50185300	3.63887500
C	-3.05954700	-4.35934300	1.87455000
H	-3.20006700	-3.34415000	1.48873400
H	-3.06444100	-5.04290100	1.01941600
H	-3.93087000	-4.60160100	2.49316300
C	0.87890700	6.51419500	-0.53429500
C	0.28719100	6.65543000	-1.94984500
H	-0.49356400	7.42436700	-1.94704400
H	1.04336700	6.95816200	-2.68314800
H	-0.17098700	5.72137300	-2.29510600
C	1.49760200	7.87537300	-0.13178300
H	0.73865900	8.66669400	-0.17029800
H	1.90365600	7.84968400	0.88520400
H	2.31281500	8.15216100	-0.81030100
C	-0.27798300	6.17761700	0.43581900
H	-0.75631500	5.22579000	0.18000600
H	0.06706200	6.10981500	1.47291500
H	-1.04531400	6.95999100	0.39375700
H	0.63937000	-3.38227400	-1.20761700
C	3.25536200	-3.97530700	2.64970600
H	3.98659200	-4.59985100	2.12421500
H	3.70751600	-2.98360200	2.76901100
H	3.10080300	-4.39880300	3.64687400
Ag	-0.45329400	-1.23032200	0.34979500
N	-2.94765200	0.01423200	1.65916400
N	-4.05912700	-0.19942800	1.79451500
C	-1.75981500	0.38877700	1.23942900
P	-0.83660100	1.31384900	2.46591400
O	0.41192000	1.92833700	1.89569100
O	-1.87600300	2.34316300	3.09294100
O	-0.57266700	0.34370900	3.73479900
C	-1.54613000	3.70443400	3.44215900
H	-1.51647600	3.78320200	4.53235600
H	-0.58144100	3.98724100	3.01553600
H	-2.33717700	4.32496200	3.02299700
C	0.62419100	-0.44160200	3.87656400
H	0.62386700	-0.80489700	4.90572900
H	0.61004100	-1.29702700	3.19290600
H	1.51399500	0.16550500	3.69512600
H	1.82343100	1.33090700	1.55263300
C	-8.36858800	4.06116300	0.20956900
C	-7.78640900	3.54724900	-0.94997100
C	-6.44871100	3.14782700	-0.94628700
C	-5.67728600	3.26797400	0.21871300
C	-6.26343300	3.81505700	1.37108700
C	-7.60272200	4.19527400	1.37151000
H	-9.41280000	4.36252400	0.20712500
H	-8.37074000	3.45923200	-1.86180000

H	-6.00627300	2.76902900	-1.86153500
H	-5.65177300	3.93107900	2.25983100
H	-8.05006100	4.60090800	2.27508400
C	-4.21970100	2.91187900	0.28423600
O	-3.46077200	3.61127400	0.96296900
C	-3.69173200	1.74794600	-0.45081400
C	-2.27602000	1.53326200	-0.43189800
C	-1.57051700	0.83977900	-1.55001000
C	-0.59052400	1.55752100	-2.25252800
C	-1.86204500	-0.47530300	-1.96267900
C	0.05192800	0.99555200	-3.35669700
H	-0.32873400	2.56202900	-1.93072800
C	-1.20710600	-1.04157400	-3.05944700
H	-2.61314400	-1.07150000	-1.45534500
C	-0.25414700	-0.30311000	-3.76554100
H	0.80323000	1.57267500	-3.88883700
H	-1.46134900	-2.05785700	-3.34648400
H	0.25137500	-0.74009200	-4.62243500
C	-4.52564600	0.83485300	-1.11129700
N	-5.16517700	0.04009000	-1.68874900
H	-1.75679000	2.41702400	-0.07032200
C	-3.99605400	-4.45405600	-1.87638700
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H	-2.85355400	-5.93090000	-1.73867100
O	-5.20718000	-4.11641600	-2.10857400
Ag	-5.36811400	-2.02087500	-1.96556700

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C	6.90401800	-1.37789000	-2.15235300
C	6.26895100	-0.74368400	-1.07231000
C	5.19606200	-1.38003900	-0.45590200
C	4.81625700	-2.69113500	-0.79431900
C	5.51537800	-3.31408400	-1.84260500
C	6.53101200	-2.66030500	-2.54075300
C	7.94561400	-0.46637800	-2.76430900
C	7.59451500	0.90486300	-2.14602100
C	6.98257400	0.56291300	-0.74526800
H	5.23522600	-4.32702800	-2.11642300
H	7.02280800	-3.15288600	-3.37560200
H	8.96158100	-0.78229100	-2.48893900
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H	8.45137500	1.58151600	-2.07206400
H	7.90460500	-0.45888200	-3.85924700
C	8.13404100	0.33110000	0.29104800
H	8.96905200	-0.23400700	-0.13438700
H	7.73790800	-0.24411200	1.13575300
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C	6.29736400	1.77629100	-0.12552400
C	6.87569300	3.73795300	1.18292600
H	7.59103500	4.30529500	1.77286900
C	5.59776500	4.24655800	0.95444900
H	5.32753500	5.22399300	1.34259900
C	4.62418300	3.52550200	0.23947200
C	4.99977200	2.26428600	-0.25771400
H	9.30168300	2.18435000	0.11895500
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O	4.44222600	-0.67402100	0.50438300
O	4.03023700	1.46016900	-0.88928900
P	3.28032900	0.30538600	-0.05026900

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 H -10.57144600 2.93293900 -0.06840500
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 Ag -7.45376300 0.12059800 -0.68006500
9-ts-RR
 C -6.17751800 -2.88329700 1.57574000
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 C -4.43486100 -2.21534000 0.05043200
 C -3.68706400 -3.36520500 0.36326600
 C -4.22037900 -4.25152200 1.31354500
 C -5.44125700 -4.00465200 1.94339500
 C -7.50218800 -2.39459500 2.12157900
 C -7.56508800 -0.94165400 1.59914900
 C -6.76488800 -0.96901700 0.25365000
 H -3.65171400 -5.14226700 1.56544600
 H -5.80817900 -4.68549500 2.70708200

H	-8.33668000	-2.99607400	1.73461100	H	-0.93022500	5.94488100	2.94834800
H	-7.05317500	-0.27342000	2.30083600	H	0.15538500	5.39584600	1.66069500
H	-8.58633000	-0.57016100	1.46895100	C	-2.19936200	7.96209500	1.50865500
H	-7.55225000	-2.45338400	3.21465500	H	-1.51468300	8.77570700	1.77907900
C	-7.69109500	-1.47229600	-0.90548000	H	-2.90449000	8.34562300	0.76207000
H	-8.34579500	-2.29142400	-0.59152100	H	-2.77261700	7.69503000	2.40299000
H	-7.06252600	-1.84273600	-1.72349300	C	-0.59085600	7.22498400	-0.26339000
C	-8.45860100	-0.21501800	-1.36822000	H	-0.00218400	6.40914700	-0.69751200
C	-7.46971900	0.89442500	-1.08319700	H	-1.23077700	7.64335800	-1.04866900
C	-6.44351600	0.43552900	-0.24221300	H	0.10722700	8.01200400	0.04436800
C	-7.46932500	2.20322700	-1.55383900	H	-1.31374300	-3.64326900	1.59995600
H	-8.26115100	2.55868900	-2.20840000	C	-3.46176400	-3.89826400	-2.57703100
C	-6.43922800	3.06198100	-1.16914000	H	-4.33717400	-4.40636100	-2.15704300
H	-6.44077400	4.09566800	-1.50236000	H	-3.74784700	-2.85491200	-2.75263600
C	-5.37241300	2.62842200	-0.36384300	H	-3.23659100	-4.35512900	-3.54566600
C	-5.38081400	1.28581600	0.05224900	Ag	-0.06335500	-1.48841700	0.36258800
H	-9.38568300	-0.07892100	-0.79347600	N	2.68642400	-1.08564600	-0.87599900
H	-8.74738100	-0.26165400	-2.42437300	N	3.56946000	-1.59800700	-0.28674500
O	-3.87524600	-1.23735200	-0.78908100	C	1.78048300	-0.14386700	-0.51181000
O	-4.27858700	0.78168900	0.76747300	P	0.88417500	0.68556800	-1.81707100
P	-3.11215600	-0.00597000	-0.03502900	O	-0.20298200	1.57998200	-1.29046000
O	-2.06407700	-0.42417900	0.94409900	O	1.79495900	1.53453600	-2.82984900
O	-2.66720600	0.85009800	-1.27277500	O	0.36999500	-0.58701100	-2.68610300
C	-2.37731100	-3.68622000	-0.27536500	C	2.86720200	0.97415500	-3.62985300
C	-1.22792800	-3.80861300	0.52791200	H	2.74371700	-0.10502900	-3.75863500
C	-2.27161700	-3.98793900	-1.65012200	H	2.80544900	1.46526600	-4.60330900
C	0.00337200	-4.22864400	-0.00865800	H	3.83432400	1.19314000	-3.17237500
C	-1.03730700	-4.41834200	-2.15300300	C	-0.44968600	-0.36011900	-3.85275800
C	0.11720500	-4.55927800	-1.36998700	H	0.04337300	0.32653000	-4.54760200
H	0.84388600	-4.34821100	0.66559500	H	-0.57789200	-1.33543500	-4.32337400
H	-0.99136900	-4.67628300	-3.20801800	H	-1.42211300	0.04248000	-3.55722500
C	-4.30239200	3.59931600	0.00863200	H	-1.69978800	1.19315000	-1.22855200
C	-3.53617200	4.19157100	-1.00089700	C	5.01984700	-4.21480200	4.64886400
C	-4.10821100	4.02029600	1.34366900	C	5.54326100	-3.72439100	3.45128900
C	-2.59502600	5.18187900	-0.71914600	C	4.80518000	-2.83058600	2.67449200
H	-3.67406800	3.86120200	-2.02684800	C	3.52521600	-2.42908000	3.08788600
C	-3.16810600	5.02265700	1.59641500	C	2.99402000	-2.94951500	4.28004900
C	-2.39626300	5.62880400	0.59181000	C	3.74241500	-3.82526400	5.06196500
H	-2.02148500	5.59882700	-1.53892700	H	5.60225700	-4.90278400	5.25586900
H	-3.04901300	5.34890300	2.62672600	H	6.52750700	-4.03930300	3.11604900
C	-4.90615100	3.43924200	2.48881400	H	5.21392100	-2.47750000	1.73464400
H	-5.97990300	3.42486500	2.26773500	H	1.99577900	-2.65016600	4.58275100
H	-4.60472700	2.40648600	2.69967400	H	3.32943500	-4.20744900	5.99152900
H	-4.75764200	4.02413300	3.40199800	C	2.65971400	-1.50539700	2.29054600
C	1.41411900	-5.09848900	-1.99985500	O	1.42585200	-1.70275800	2.29017200
C	1.15449700	-6.52408900	-2.54584400	C	3.22428900	-0.39533100	1.52376000
H	2.06671500	-6.92386900	-3.00477700	C	2.26057400	0.56452200	0.83609500
H	0.85252300	-7.20528200	-1.74186700	C	2.80790200	1.97341800	0.64331500
H	0.36694200	-6.53339700	-3.30690300	C	2.38720400	2.99479400	1.50559300
C	1.84934400	-4.17868400	-3.16583700	C	3.76145000	2.27087900	-0.33783700
H	2.78011800	-4.55007700	-3.61099700	C	2.91630600	4.28213400	1.39508500
H	1.09425700	-4.14386300	-3.95895500	H	1.64463100	2.78012700	2.27102800
H	2.02002500	-3.15466300	-2.81828800	C	4.28442300	3.55936700	-0.45724900
C	2.57015700	-5.17835500	-0.98440600	H	4.13175500	1.50523900	-1.01011300
H	2.82395500	-4.19806400	-0.56799900	C	3.86460600	4.56911100	0.41034100
H	2.33984300	-5.85748300	-0.15507600	H	2.58499200	5.05991600	2.07722400
H	3.46652500	-5.56433500	-1.48257600	H	5.02251700	3.75341500	-1.22984200
C	-1.40845500	6.75265300	0.95377500	H	4.27185800	5.57274500	0.32078000
C	-0.41821300	6.25219100	2.03055000	C	4.55342100	0.02651800	1.71010900
H	0.28767300	7.04949600	2.29555100	N	5.65674500	0.41398600	1.77764100

H 1.37351100 0.63086000 1.47262800
 C 7.27688200 1.56809600 -2.45728100
 O 8.11361300 1.54302500 -1.46902000
 O 7.83651400 1.92125600 -3.65232700
 H 8.77868300 2.07418400 -3.46866700
 O 6.06814400 1.31464300 -2.42344500
 Ag 7.00993400 0.98215500 0.25103300

9-ts-SS

C 3.07896200 -4.48876800 -1.43429700
 C 3.41511900 -3.47416700 -0.52306100
 C 2.45085600 -3.03672900 0.37719700
 C 1.19794200 -3.66465800 0.48671000
 C 0.91322000 -4.71074200 -0.40801900
 C 1.83167800 -5.10322200 -1.38360900
 C 4.20859400 -4.70445600 -2.41908900
 C 5.08835100 -3.45184500 -2.20293000
 C 4.87562900 -3.07565200 -0.69869400
 H -0.06790200 -5.17321200 -0.38451300
 H 1.54690400 -5.86461900 -2.10418300
 H 4.76275700 -5.62663700 -2.19442300
 H 4.72144800 -2.63002400 -2.82821900
 H 6.14344300 -3.61228800 -2.44644800
 H 3.85091400 -4.79592600 -3.45057900
 C 5.80441300 -3.95800500 0.20421400
 H 5.86564100 -4.99203300 -0.14853100
 H 5.39385000 -3.97602000 1.22036900
 C 7.16221900 -3.22621600 0.20665900
 C 6.74888900 -1.77844900 0.06106900
 C 5.41515700 -1.68561900 -0.36986500
 C 7.49555100 -0.63391300 0.31930200
 H 8.52794100 -0.70813000 0.65158900
 C 6.90179900 0.61648800 0.15185300
 H 7.47673900 1.51938100 0.33557800
 C 5.55808000 0.75459500 -0.23658300
 C 4.82866400 -0.42544200 -0.46992300
 H 7.78988000 -3.54578100 -0.63725300
 H 7.74203800 -3.40994000 1.11825000
 O 2.69367700 -1.86180700 1.12525300
 O 3.46442000 -0.33148300 -0.80353000
 P 2.33046700 -0.49340700 0.33500000
 O 0.99442500 -0.47575500 -0.33476800
 O 2.57280800 0.56403500 1.47935000
 C 0.15880600 -3.23782800 1.46849100
 C -1.13399000 -2.92452500 0.99018300
 C 0.37315200 -3.24657400 2.86358700
 C -2.19298100 -2.63330200 1.87327100
 C -0.70629200 -2.96007500 3.71489400
 C -2.00149800 -2.66664400 3.26765000
 H -3.18200600 -2.48997600 1.45159000
 H -0.52094700 -3.01696000 4.78479100
 C 4.97430600 2.12434500 -0.33843500
 C 4.99067200 2.93988000 0.79944800
 C 4.48687700 2.66453900 -1.54986200
 C 4.53386800 4.25678000 0.76549700
 H 5.36168500 2.52717200 1.73384300
 C 4.03357800 3.98731900 -1.55562200
 C 4.04218800 4.81377400 -0.42040900
 H 4.57101600 4.84123300 1.67810700
 H 3.66853900 4.38640000 -2.49852000

C 4.47506200 1.86773800 -2.83463700
 H 5.42131100 1.33597600 -2.98693000
 H 3.67972600 1.11352500 -2.83104800
 H 4.31384100 2.52284100 -3.69658000
 C -3.14594700 -2.48081800 4.28132800
 C -3.26047800 -3.75490600 5.15483100
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 C 3.53829300 6.26485600 -0.51861300
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 H 1.68238000 7.29693800 -1.03514000
 H 1.91793400 5.79002500 -1.93555200
 H 1.43014900 5.72509200 -0.24475500
 C 4.38528100 7.03754500 -1.55836700
 H 4.03514400 8.07393300 -1.64127700
 H 5.44190400 7.05780200 -1.26731300
 H 4.32133200 6.58439900 -2.55301100
 C 3.64056400 7.01012400 0.82605500
 H 3.03898500 6.52815600 1.60598400
 H 4.67501300 7.07038200 1.18341600
 H 3.27069300 8.03527100 0.70979800
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 C 1.70370300 -3.62551600 3.47233200
 H 2.13370000 -4.50061300 2.97320000
 H 2.43274700 -2.81297100 3.37959000
 H 1.59136400 -3.86157300 4.53515700
 Ag -1.09176600 -0.40091500 0.71362600
 N -3.02317900 1.36561600 2.01951100
 N -4.12352200 1.11672000 2.17181000
 C -1.98665900 1.72047900 1.20637800
 P -0.65833500 2.53643000 2.13110600
 O 0.72812100 2.42472900 1.57574400
 O -1.20196400 4.03914100 2.24108500
 O -0.79123900 1.96042100 3.63538900
 C -0.35897700 5.09411900 2.75252800
 H 0.58135600 5.13028900 2.19700600
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 H -0.16608700 4.93637800 3.81803200
 C 0.21341100 1.10514300 4.22550600
 H 0.09583500 1.20451900 5.30553900
 H 0.04002600 0.06616000 3.93014800
 H 1.21548600 1.41591100 3.92407400
 H 1.91013800 1.32449100 1.45267500
 C -8.85763100 0.84559000 -1.91949200
 C -7.92002300 0.02063600 -1.29586900
 C -6.70567500 0.54875000 -0.85336900
 C -6.41794700 1.91027600 -1.02678100
 C -7.37892100 2.73631400 -1.62978000
 C -8.58450800 2.20683500 -2.08347900
 H -9.80017900 0.43199100 -2.26873400

H	-8.13497200	-1.03411200	-1.14576000
H	-5.99645200	-0.09930100	-0.34920600
H	-7.15888900	3.79415100	-1.72982600
H	-9.31475200	2.85491300	-2.56113200
C	-5.14867700	2.55917300	-0.54489700
O	-5.18330200	3.74179900	-0.17607700
C	-3.89470400	1.81132600	-0.53869800
C	-2.67068100	2.51944100	-0.01781500
C	-3.69235100	0.61804000	-1.21444800
N	-3.41638100	-0.39813400	-1.73566900
C	-1.79570100	-4.68857300	-2.83809200
O	-2.03526300	-3.77945500	-3.72682800
O	-1.20455300	-5.81666800	-3.34286400
H	-1.11736400	-5.66318600	-4.29885000
O	-2.03020900	-4.63897000	-1.62736800
Ag	-2.79986900	-2.08510600	-2.75055900
H	-3.07070900	3.43621100	0.42731300
C	-1.68484000	2.94433100	-1.10281100
C	-1.85463600	4.23481800	-1.63189500
C	-0.71462500	2.11088000	-1.67014700
C	-1.08655600	4.67044500	-2.71055100
H	-2.62125400	4.88088100	-1.21267000
C	0.06056000	2.54974000	-2.74641500
H	-0.53534700	1.11498600	-1.28226600
C	-0.12581500	3.82709300	-3.27489500
H	-1.24308100	5.66801900	-3.11274600
H	0.80756700	1.88301800	-3.16817800
H	0.46980100	4.16289400	-4.11987900

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C	-6.27242200	-2.70704500	1.60125600
C	-5.77109300	-1.83767700	0.61913200
C	-4.52261600	-2.09349300	0.05992200
C	-3.81841500	-3.27596100	0.35372100
C	-4.37627800	-4.15039900	1.30094200
C	-5.57856700	-3.86148500	1.94812800
C	-7.56836000	-2.17012600	2.17027000
C	-7.57782500	-0.71036700	1.66346800
C	-6.79791800	-0.75688200	0.30674600
H	-3.84088800	-5.06576500	1.53718700
H	-5.96384900	-4.53495200	2.70934800
H	-8.43218300	-2.73233700	1.78865600
H	-7.02894900	-0.07140200	2.36445400
H	-8.58444600	-0.29549400	1.55151500
H	-7.60623600	-2.23866300	3.26330000
C	-7.76009100	-1.21222100	-0.84328400
H	-8.44269200	-2.00726800	-0.52674000
H	-7.15822300	-1.60024800	-1.67312900
C	-8.48236900	0.07873400	-1.28460400
C	-7.44508800	1.14436000	-1.00531300
C	-6.42729400	0.63844000	-0.18144900
C	-7.39775600	2.45502000	-1.46799000
H	-8.18317000	2.84680600	-2.10944300
C	-6.32779900	3.26766200	-1.09315900
H	-6.29076900	4.30226400	-1.42133900
C	-5.26859500	2.78610400	-0.30479600
C	-5.32680500	1.44266700	0.10545000
H	-9.39492000	0.24749200	-0.69536000
H	-8.78782400	0.05295000	-2.33679400
O	-3.93511300	-1.13001800	-0.77575000
O	-4.23945900	0.88818600	0.80470100

P	-3.11171300	0.06169300	-0.01670400
O	-2.08018100	-0.42063100	0.95131800
O	-2.64083500	0.91265200	-1.24444600
C	-2.52536100	-3.64058100	-0.29543000
C	-1.37684000	-3.80850200	0.50334700
C	-2.43351700	-3.93337300	-1.67239900
C	-0.16098400	-4.26249600	-0.04313400
C	-1.21415200	-4.39695900	-2.18466300
C	-0.06076400	-4.57995700	-1.40971100
H	0.67801400	-4.42279700	0.62464000
H	-1.17921400	-4.64123400	-3.24325300
C	-4.15517600	3.71379700	0.05026500
C	-3.39449500	4.28605900	-0.97506700
C	-3.91461200	4.12151400	1.38175900
C	-2.41786800	5.24674300	-0.71330500
H	-3.56669000	3.96400400	-1.99841100
C	-2.93847000	5.09407100	1.61486800
C	-2.17497500	5.68298900	0.59374300
H	-1.85210700	5.64940400	-1.54552800
H	-2.78439000	5.41217900	2.64316600
C	-4.70216900	3.56067900	2.54402000
H	-5.78102600	3.58270100	2.34978200
H	-4.42994100	2.51738700	2.74204400
H	-4.51194800	4.13569400	3.45579200
C	1.22202300	-5.13864400	-2.05077800
C	0.92710300	-6.54808600	-2.61963000
H	1.82896100	-6.96115600	-3.08716500
H	0.61029500	-7.23642300	-1.82715200
H	0.13875300	-6.52656500	-3.37973800
C	1.67879300	-4.20474600	-3.19723200
H	2.58820900	-4.60353400	-3.66306600
H	0.91690100	-4.11937400	-3.98028900
H	1.89687400	-3.20150400	-2.81825100
C	2.37840100	-5.25945800	-1.03956400
H	2.66145100	-4.28852400	-0.62018700
H	2.13353300	-5.94170500	-0.21638100
H	3.26099100	-5.66554900	-1.54642700
C	-1.15088200	6.78078100	0.93440500
C	-0.14364800	6.25268500	1.98154400
H	0.58461100	7.03402800	2.23340900
H	-0.63864600	5.94917800	2.91003600
H	0.40366700	5.38798200	1.59203300
C	-1.89780300	8.00600600	1.51512400
H	-1.18667700	8.80216500	1.76894400
H	-2.61420500	8.40888300	0.78976600
H	-2.45207800	7.74897500	2.42425600
C	-0.35526300	7.24058500	-0.30212000
H	0.20223700	6.41376000	-0.75607800
H	-1.00599400	7.67810200	-1.06783600
H	0.36906000	8.00934000	-0.00903400
H	-1.45563000	-3.65339100	1.57749200
C	-3.62254700	-3.79366100	-2.59434900
H	-4.51532100	-4.27018700	-2.17397800
H	-3.86854900	-2.73891000	-2.76255800
H	-3.41796900	-4.25276200	-3.56643800
Ag	-0.15735300	-1.57420500	0.23325800
N	2.53726700	-1.30252000	-0.88831100
N	3.43764200	-1.65739900	-0.07565800
C	1.69237000	-0.29244400	-0.48868400
P	0.86613800	0.61200300	-1.79319900

O	-0.17705700	1.58012000	-1.29834500	H	5.52571800	-5.10264300	-2.13676000
O	1.86683200	1.41322100	-2.76684000	H	5.25554700	-2.10554000	-2.70556900
O	0.27424300	-0.60013800	-2.69910200	H	6.72900300	-2.96645500	-2.23679400
C	2.95431400	0.77416200	-3.48175900	H	4.64204500	-4.32221400	-3.44493900
H	3.11884700	-0.24888900	-3.13477000	C	6.24351900	-3.39108400	0.37444000
H	2.69865300	0.76465600	-4.54511300	H	6.44509600	-4.40332500	0.01009000
H	3.85815400	1.36413600	-3.31904800	H	5.76614900	-3.47955300	1.35713200
C	-0.49103400	-0.28062000	-3.87858700	C	7.50974800	-2.51455800	0.48901200
H	0.05559000	0.41625000	-4.52163300	C	6.95606400	-1.11636700	0.31864400
H	-0.64433600	-1.22421600	-4.40379600	C	5.65216600	-1.16340600	-0.19904000
H	-1.45507700	0.15177600	-3.59717500	C	7.55622500	0.10155300	0.62291900
H	-1.65407000	1.22468100	-1.21261100	H	8.56611000	0.13734500	1.02387900
C	5.01853600	-4.71680100	4.25443800	C	6.84615300	1.28340200	0.40790800
C	5.49158100	-4.18192100	3.05421100	H	7.31000400	2.24203700	0.62163700
C	4.74639800	-3.22212500	2.37022500	C	5.52341000	1.27700500	-0.06584800
C	3.50755900	-2.80023000	2.88323700	C	4.93932600	0.02556000	-0.33193600
C	3.02642300	-3.36183900	4.08005700	H	8.23440600	-2.75292200	-0.30233300
C	3.78348200	-4.30599400	4.76611300	H	8.03147100	-2.64800500	1.44355500
H	5.60864300	-5.45641200	4.78880300	O	2.89231500	-1.67985200	1.13123000
H	6.44113000	-4.51458200	2.64508700	O	3.59100600	-0.02837200	-0.72435300
H	5.10116600	-2.84256100	1.41892700	P	2.44030300	-0.31105300	0.37828100
H	2.06402900	-3.03621600	4.46128200	O	1.12935700	-0.38281700	-0.33559200
H	3.41306500	-4.72321700	5.69824400	O	2.57210100	0.72210700	1.55536400
C	2.65042400	-1.78882600	2.21044300	C	0.49196300	-3.31692500	1.26850400
O	1.43135700	-1.77938100	2.37595100	C	-0.79380900	-3.07987300	0.73391300
C	3.25838800	-0.77298000	1.22281200	C	0.62999800	-3.40309000	2.67041700
C	2.24131400	0.35587400	0.81694700	C	-1.91795200	-2.93139700	1.56921100
C	2.81977100	1.75824200	0.71668300	C	-0.51396700	-3.25884900	3.47285900
C	2.45308200	2.71518500	1.67358800	C	-1.80143700	-3.03227300	2.96826600
C	3.74920200	2.11641700	-0.26907400	H	-2.89145900	-2.82527900	1.10369300
C	3.00632000	3.99676000	1.65007200	H	-0.38252500	-3.36257300	4.54728600
H	1.72926200	2.45405300	2.44248300	C	4.78995500	2.56587400	-0.23041500
C	4.29809400	3.39962700	-0.30086300	C	4.61167200	3.38722900	0.88864300
H	4.07679000	1.39992700	-1.01386700	C	4.31693000	3.01793500	-1.48316100
C	3.92851400	4.34332300	0.65977000	C	3.96340000	4.61887000	0.79822600
H	2.71501400	4.72274000	2.40388800	H	4.97086000	3.04238600	1.85452600
H	5.01586700	3.63794100	-1.07937700	C	3.67175800	4.25638600	-1.54574100
H	4.35555600	5.34247000	0.63725800	C	3.46887100	5.08014600	-0.42683400
C	4.58384500	-0.28200600	1.54852100	H	3.84503700	5.20878500	1.70031100
N	5.66634100	0.12920000	1.65611200	H	3.31668500	4.58755100	-2.51843100
H	1.46651800	0.37022000	1.58539000	C	4.50891500	2.21480600	-2.74968500
C	7.41530200	1.97350400	-2.28483800	H	5.52962500	1.82325200	-2.82825600
O	8.19593300	1.89537400	-1.25168500	H	3.83027600	1.35461200	-2.78428300
O	8.01154100	2.49929400	-3.39433500	H	4.31498000	2.83155200	-3.63306200
H	8.92797200	2.69554300	-3.13668600	C	-3.01019600	-2.96089300	3.91949300
O	6.23011100	1.63262200	-2.35217100	C	-3.10353000	-4.28441100	4.71750300
Ag	7.02151800	1.05724400	0.29972000	H	-3.96474300	-4.25375200	5.39576200
10-SS				H	-3.23009300	-5.14170200	4.04615500
C	3.69128400	-4.14535000	-1.48861000	H	-2.20972400	-4.46341200	5.32473500
C	3.86790500	-3.14346500	-0.52093100	C	-2.83424800	-1.77846400	4.90192700
C	2.80884600	-2.83569100	0.32577700	H	-3.67821000	-1.74440200	5.60177300
C	1.61778500	-3.58346000	0.32636800	H	-1.91793600	-1.87829200	5.49526900
C	1.48607400	-4.59780900	-0.63797400	H	-2.79874700	-0.82487300	4.36495000
C	2.50095400	-4.86265900	-1.55891900	C	-4.33849800	-2.76399900	3.16262000
C	4.90734500	-4.22852100	-2.38599800	H	-4.35608400	-1.82417200	2.60136800
C	5.64822500	-2.90891000	-2.07198900	H	-4.54016500	-3.59219900	2.47252400
C	5.28919000	-2.59577500	-0.57989000	H	-5.16366900	-2.73121100	3.88318700
H	0.54923800	-5.14116200	-0.70307800	C	2.73122700	6.42146900	-0.58424200
H	2.34111200	-5.61029600	-2.33085300	C	1.30437700	6.16212200	-1.12376000

H	0.76437100	7.10968900	-1.24514400
H	1.31830100	5.65914000	-2.09573000
H	0.73350800	5.52764800	-0.43664100
C	3.50058600	7.32406500	-1.57843000
H	2.98188700	8.28275300	-1.70300000
H	4.51497600	7.53054300	-1.21768100
H	3.58540100	6.86115700	-2.56707200
C	2.60826200	7.17984600	0.75117100
H	2.04492300	6.60359500	1.49458600
H	3.58891100	7.42094600	1.17761400
H	2.07540500	8.12425400	0.59225000
H	-0.93898900	-3.15367300	-0.34240000
C	1.95647700	-3.69987900	3.33133200
H	2.49491300	-4.49598700	2.80581500
H	2.60761000	-2.81826000	3.33237700
H	1.81122500	-4.01517100	4.36939000
Ag	-0.95774700	-0.54940200	0.75661700
N	-3.09797600	0.75559600	1.98606300
N	-4.19507800	0.67551800	1.36793300
C	-2.06191000	1.41055800	1.30594800
P	-0.85449000	2.21067200	2.36508100
O	0.55189900	2.31486300	1.83269800
O	-1.51128700	3.66015900	2.62521200
O	-0.91685900	1.50729100	3.81568200
C	-0.75317100	4.69130200	3.28376300
H	0.20513100	4.84117200	2.77859500
H	-1.35574500	5.59883000	3.22428200
H	-0.58792800	4.42657100	4.33312200
C	0.14254900	0.67062100	4.31652700
H	0.05031300	0.68183100	5.40416100
H	0.01579700	-0.35261200	3.95094100
H	1.12110500	1.05450300	4.01929000
H	1.79862700	1.38433900	1.60851900
C	-9.03832300	0.32567400	-1.24291300
C	-8.03016100	-0.43136200	-0.64263700
C	-6.81111500	0.15987800	-0.31146800
C	-6.59900000	1.52402200	-0.57432400
C	-7.62806900	2.28433000	-1.15845700
C	-8.83639400	1.68612700	-1.49866500
H	-9.98325700	-0.14163600	-1.50674400
H	-8.19335400	-1.48307600	-0.42577500
H	-6.04947000	-0.42489300	0.19162400
H	-7.45466400	3.33956800	-1.34135300
H	-9.62221100	2.27650000	-1.96132600
C	-5.33175800	2.23184100	-0.24548100
O	-5.28085900	3.44538800	-0.15084100
C	-4.03483200	1.40689000	0.00561200
C	-2.74621300	2.26319500	0.20492400
C	-3.81217400	0.38222700	-1.01366400
N	-3.56182100	-0.44589600	-1.78537400
C	-1.29458000	-4.25998700	-3.37261400
O	-1.70818000	-3.34114500	-4.18655700
O	-0.56301500	-5.24833600	-3.96595700
H	-0.52674900	-5.02335600	-4.91094000
O	-1.49404200	-4.31961900	-2.15505300
Ag	-2.70294600	-1.91931300	-2.98807400
H	-3.11308600	3.18035200	0.68305700
C	-2.01464200	2.67771700	-1.06361500
C	-2.52535800	3.76312600	-1.79790400
C	-0.87527000	2.02519500	-1.54921200

C	-1.93217700	4.15934300	-2.99561000
H	-3.39724000	4.29120300	-1.42473300
C	-0.27866900	2.42333900	-2.74902000
H	-0.41889800	1.21729900	-0.99069300
C	-0.80784300	3.48577100	-3.48119700
H	-2.34706400	4.99868000	-3.54778100
H	0.60632800	1.89870700	-3.09812800
H	-0.34527400	3.79354500	-4.41539900

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C	3.65149600	5.50167300	-0.68870100
C	2.68987900	4.67841300	-0.08139300
C	2.96232800	3.32267400	0.09151800
C	4.23878800	2.80298200	-0.20876500
C	5.19521000	3.66436000	-0.76907600
C	4.90308700	5.00272200	-1.03588900
C	3.10015500	6.89551200	-0.89627800
C	1.58541600	6.69084000	-0.67609300
C	1.48365800	5.50767700	0.34646500
H	6.17969300	3.26800200	-1.00440600
H	5.64682900	5.64163100	-1.50523400
H	3.51997300	7.60044300	-0.16462400
H	1.11371900	6.38261000	-1.61599700
H	1.07130300	7.59087900	-0.32485400
H	3.33450200	7.29616200	-1.88919000
C	1.65563800	6.05395800	1.80364900
H	2.44318100	6.81120500	1.87646200
H	1.93133500	5.22073100	2.46047700
C	0.25649800	6.58285000	2.19038900
C	-0.66634800	5.68945500	1.38909900
C	0.05555700	4.97444000	0.42214900
C	-2.04216700	5.51954400	1.51253100
H	-2.60714000	6.07137600	2.25978300
C	-2.69712800	4.64501500	0.64595200
H	-3.77664700	4.54096400	0.70028100
C	-2.00164800	3.87109000	-0.30176300
C	-0.59998500	4.01326900	-0.34762700
H	0.13640400	7.63838100	1.90778700
H	0.06791600	6.52493900	3.26884800
O	1.96451000	2.47726700	0.54868100
O	0.15525000	3.18351300	-1.17302800
P	0.87926700	1.85053900	-0.55252300
O	1.62237200	1.26796300	-1.74114200
O	-0.03892800	0.99554600	0.28210500
C	4.59564700	1.37613600	0.03927600
C	4.93696800	0.55062400	-1.05244300
C	4.66657100	0.82777900	1.33691400
C	5.32237300	-0.79510500	-0.87031600
C	5.07382500	-0.50652800	1.49136600
C	5.40694600	-1.34917300	0.42390100
H	5.64435500	-1.36391000	-1.73609100
H	5.13856800	-0.89282100	2.50507800
C	-2.77018300	2.95835000	-1.19655200
C	-3.72133900	2.10007000	-0.62502800
C	-2.66690500	2.99817000	-2.60822900
C	-4.53361800	1.27646200	-1.40601900
H	-3.84383500	2.07704600	0.45470900
C	-3.48231200	2.14793100	-3.36394300
C	-4.41912900	1.26900000	-2.80170100
H	-5.27195300	0.65801000	-0.90731200
H	-3.39088300	2.20296200	-4.44647800

C -1.75112400 3.95533200 -3.33794300
 H -1.72302900 4.93595000 -2.84985100
 H -0.72157500 3.58324700 -3.36755600
 H -2.09133800 4.10134600 -4.36860200
 C 5.87704300 -2.79055400 0.68995800
 C 7.16908600 -2.75324200 1.54218700
 H 7.51748300 -3.77313900 1.74395800
 H 7.97037100 -2.21731200 1.02043300
 H 7.00742700 -2.25935400 2.50593100
 C 4.78021700 -3.56552100 1.45858900
 H 5.11688800 -4.58702900 1.67074600
 H 4.53279600 -3.09062100 2.41320900
 H 3.85992200 -3.63140900 0.86720600
 C 6.18015300 -3.55548800 -0.61261200
 H 5.29427300 -3.62809400 -1.25336500
 H 6.98892500 -3.08666800 -1.18558500
 H 6.49712400 -4.57654000 -0.37411000
 C -5.28841700 0.38138700 -3.71029200
 C -4.37822700 -0.50539000 -4.59322800
 H -4.98463200 -1.14235200 -5.24946200
 H -3.71461100 0.09181800 -5.22775900
 H -3.75065600 -1.15680600 -3.97248000
 C -6.16403700 1.27632000 -4.62023700
 H -6.78789200 0.65943800 -5.27929300
 H -6.82729600 1.90992300 -4.02059800
 H -5.55611500 1.93280100 -5.25220900
 C -6.22150900 -0.54451300 -2.90590100
 H -5.65913500 -1.22376400 -2.25427400
 H -6.92080000 0.01642100 -2.27711800
 H -6.81429500 -1.15938900 -3.59340900
 H 4.96816200 0.98959000 -2.04726000
 C 4.33111000 1.64820500 2.55893900
 H 4.81304000 2.63128300 2.52386600
 H 3.25073600 1.82034800 2.62345700
 H 4.65187300 1.13919700 3.47300700
 Ag 2.77713900 -0.64291700 -1.40200600
 N 1.21091200 -2.07508900 -0.43972400
 N 0.77476500 -1.57640800 0.75682000
 C 0.92418800 -3.32573000 -0.58032000
 P 1.47678300 -4.27220600 -2.01978100
 O 1.87590700 -5.66224100 -1.71664600
 O 0.29035100 -4.19164300 -3.11006700
 O 2.64074400 -3.29231400 -2.60952600
 C -0.14828600 -2.94360100 -3.68398700
 H -0.40286300 -2.21492500 -2.90756000
 H 0.62599200 -2.52457300 -4.33294100
 H -1.03633500 -3.17679100 -4.27261000
 C 3.44329700 -3.80823200 -3.69839000
 H 4.20928100 -3.05726700 -3.89469000
 H 3.90429200 -4.75562300 -3.40952700
 H 2.82780700 -3.95234600 -4.59172900
 H 0.47048000 -0.57973800 0.65815000
 C -0.75908400 0.40620300 5.76031800
 C -0.83844500 0.69536600 4.39698700
 C -0.51298400 -0.27659500 3.45109400
 C -0.09646100 -1.55339300 3.87302300
 C 0.00006100 -1.82805700 5.25171100
 C -0.33562400 -0.85743800 6.18734900
 H -1.02601500 1.16461500 6.49116100

H -1.15632700 1.67669100 4.05915600
 H -0.56707200 0.00443800 2.40515800
 H 0.33098300 -2.81314100 5.56290900
 H -0.27188500 -1.08266700 7.24804000
 C 0.26490600 -2.65726200 2.95032800
 O 0.85445300 -3.65593000 3.31919300
 C -0.11483300 -2.55517800 1.41228000
 C 0.22371100 -3.89433600 0.64593300
 C -0.91374800 -4.87893500 0.46287200
 C -1.04988600 -5.93096700 1.37925500
 C -1.85335300 -4.75148400 -0.56914700
 C -2.10485800 -6.83614800 1.26738300
 H -0.32610700 -6.03465800 2.18296600
 C -2.90595800 -5.66042000 -0.68425000
 H -1.76496700 -3.94564900 -1.29131700
 C -3.03549200 -6.70304400 0.23485700
 H -2.19641400 -7.64748100 1.98400500
 H -3.62260200 -5.55302900 -1.49352600
 H -3.85562000 -7.40974200 0.14450500
 C -1.53308500 -2.18100000 1.27053300
 N -2.64360800 -1.86816100 1.19401700
 H 0.99151000 -4.37884000 1.26325500
 C -6.51756500 0.69974900 1.89118100
 O -5.48908200 1.20836600 2.37685900
 O -7.71677100 1.33467900 2.02849000
 H -7.51506300 2.14074700 2.53234900
 O -6.58960600 -0.40481300 1.23975100
 Ag -4.56997600 -1.06741000 1.25929100

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C 3.60506500 -5.40526800 -0.35935800
 C 3.22756800 -4.21167200 0.27547900
 C 2.00965600 -3.61565500 -0.05346800
 C 1.09922000 -4.26863500 -0.90830300
 C 1.48895600 -5.48711600 -1.48848800
 C 2.74300100 -6.04709300 -1.24266400
 C 5.00922800 -5.80054000 0.04457400
 C 5.54406800 -4.50744000 0.69778500
 C 4.27878800 -3.81530400 1.30774800
 H 0.79219500 -5.99255800 -2.15211300
 H 3.03536400 -6.97134300 -1.73468700
 H 4.99595600 -6.63450300 0.76085100
 H 5.96506400 -3.85170700 -0.07282700
 H 6.32275400 -4.68722500 1.44582300
 H 5.61568000 -6.12746300 -0.80796500
 C 3.96240700 -4.43377100 2.71152400
 H 4.09319000 -5.52072800 2.72954200
 H 2.91737000 -4.21852000 2.96211400
 C 4.89610400 -3.68537200 3.68874600
 C 5.03499200 -2.32787000 3.03273600
 C 4.57546700 -2.37397500 1.70759000
 C 5.50887500 -1.13855000 3.57753400
 H 5.86490700 -1.09944800 4.60418500
 C 5.52456100 0.01045800 2.78511400
 H 5.91735400 0.94030800 3.18724500
 C 5.02439200 0.01263400 1.47244800
 C 4.51149000 -1.19662400 0.96489100
 H 5.86980700 -4.18870300 3.77465300
 H 4.48379700 -3.62385600 4.70254600
 O 1.70325700 -2.36156200 0.44755500

O	3.90832100	-1.21922900	-0.28902700	P	-2.69323100	1.91805100	-3.24316600
P	2.27662200	-1.02189500	-0.36532400	O	-4.14972200	1.72351200	-3.40956300
O	1.96153700	-1.14209900	-1.84510900	O	-2.23269800	3.39751600	-3.70400200
O	1.79581400	0.14672200	0.44854800	O	-1.72831100	0.88478500	-4.04752700
C	-0.25733800	-3.73231600	-1.23115000	C	-0.84198700	3.77747800	-3.77246300
C	-0.56208200	-3.41009500	-2.57133500	H	-0.35816900	3.69194200	-2.79397500
C	-1.29455000	-3.65385900	-0.27487700	H	-0.30692900	3.15621300	-4.49622200
C	-1.87412700	-3.07947900	-2.96950700	H	-0.83132200	4.81825300	-4.09887000
C	-2.59476900	-3.33854200	-0.70136400	C	-2.07347400	0.56349900	-5.41577700
C	-2.92998400	-3.08230100	-2.04010100	H	-1.41236300	-0.25183200	-5.71101200
H	-2.06538100	-2.91284000	-4.02415700	H	-3.11821700	0.25180600	-5.48135000
H	-3.37205500	-3.30989100	0.05770200	H	-1.90326600	1.43111300	-6.06054300
C	5.02983900	1.27917300	0.68483700	H	0.30790600	0.79648700	0.22000600
C	4.34993400	2.39274200	1.18918800	C	-0.72827300	6.69923900	3.50187900
C	5.75029700	1.41967500	-0.52305700	C	0.48430800	6.47633100	2.84107300
C	4.35372000	3.61796200	0.52348800	C	0.59943500	5.42786900	1.93512600
H	3.78630600	2.28589400	2.11161800	C	-0.49261700	4.57448800	1.69455200
C	5.73776300	2.65878700	-1.17020200	C	-1.70948100	4.80756500	2.35819900
C	5.04366600	3.77746900	-0.68286700	C	-1.82438000	5.87090000	3.25315000
H	3.80657800	4.44624800	0.96005700	H	-0.81877400	7.51990400	4.20805300
H	6.30483600	2.74665400	-2.09416900	H	1.33667300	7.12142000	3.03312500
C	6.54214300	0.27908500	-1.11990300	H	1.52915700	5.24164600	1.40818900
H	7.13741300	-0.23931300	-0.35946300	H	-2.58177300	4.19031200	2.16804500
H	5.87846100	-0.46559300	-1.57368000	H	-2.77040100	6.05030500	3.75525000
H	7.22478700	0.64252800	-1.89507300	C	-0.29184200	3.48197800	0.70526500
C	-4.40417400	-2.91476900	-2.45250200	O	0.59921000	3.49774700	-0.12006200
C	-5.13890000	-4.24786500	-2.16253500	C	-1.29263500	2.26948100	0.63635500
H	-6.19272600	-4.17041600	-2.45652500	C	-2.46449800	2.65198600	-0.39962500
H	-4.68994000	-5.07804600	-2.72066800	C	-1.78443800	1.80946000	1.94210000
H	-5.10407300	-4.50080000	-1.09780300	N	-2.15659600	1.31398700	2.92183100
C	-5.07546800	-1.78224200	-1.64433400	C	-4.88485800	-2.48571100	3.18588100
H	-6.14017400	-1.72309600	-1.90261600	O	-4.54385300	-2.19770700	2.02047300
H	-5.00168900	-1.94857100	-0.56533700	O	-5.70118000	-3.55581700	3.40404600
H	-4.62981800	-0.81047600	-1.88237500	H	-5.87733900	-3.92385500	2.52240400
C	-4.56252600	-2.59408700	-3.95092400	O	-4.55357100	-1.87592300	4.26473500
H	-4.06415900	-1.65476000	-4.21645200	Ag	-3.31647900	-0.26530700	3.70871200
H	-4.16870100	-3.39295200	-4.59072300	H	-2.35998300	3.70910500	-0.66613200
H	-5.62516800	-2.47659100	-4.18966600	C	-3.88623800	2.42447400	0.08183400
C	5.07372400	5.10221000	-1.46618200	C	-4.74784700	3.51857800	0.23628900
C	4.53015700	4.87073900	-2.89654000	C	-4.34993100	1.14035000	0.40163100
H	4.54147600	5.80848600	-3.46665500	C	-6.04825800	3.33406700	0.71022000
H	5.12947800	4.13855300	-3.44684300	H	-4.40452100	4.51714500	-0.02504100
H	3.49894000	4.50044900	-2.86439700	C	-5.64481900	0.95641100	0.88624800
C	6.52887200	5.62110400	-1.54955900	H	-3.70723200	0.27314100	0.27994700
H	6.57096700	6.56105300	-2.11458500	C	-6.49599600	2.05411100	1.04149200
H	6.93558000	5.80656200	-0.54866500	H	-6.70862400	4.19005500	0.81780300
H	7.18652500	4.90122800	-2.04785100	H	-5.96843000	-0.04638000	1.14680700
C	4.21028300	6.19278300	-0.80346700	H	-7.50608400	1.91056000	1.41506700
H	3.15984300	5.88674100	-0.73255600	AgHCO₃			
H	4.56688600	6.43956000	0.20340300	C	1.51751000	-0.04117100	0.00037500
H	4.25042400	7.11115000	-1.40090900	O	0.95867300	1.10432500	0.00063500
H	0.21459800	-3.52553500	-3.32454500	O	2.86914400	-0.08508800	-0.00066700
C	-1.04796300	-3.95132200	1.18559300	H	3.16722000	0.84041300	-0.00093400
H	-0.61893400	-4.95157300	1.32179700	O	0.90744200	-1.14821300	0.00055900
H	-0.33809700	-3.23526200	1.61406600	Ag	-1.06711400	0.00932800	-0.00011800
H	-1.98011600	-3.89113700	1.75421600	7-ts-RR-an			
Ag	-0.23915100	-0.93996200	-2.33627800	C	2.90778200	-4.74163400	-2.08357500
N	-1.07125400	0.96630800	-1.26779500	C	3.08076600	-3.81786800	-1.04026500
N	-0.68301200	1.09335100	0.01693600	C	1.97703700	-3.43939100	-0.28216300
C	-2.03226900	1.77211700	-1.57375200	C	0.72607700	-4.06186200	-0.44465800

C	0.60523100	-5.02554400	-1.45962800	H	-3.69946300	-1.24003200	3.53555800
C	1.67393400	-5.34661000	-2.29789100	C	-5.35271400	-2.69746700	1.87270000
C	4.19263800	-4.89900700	-2.86831100	H	-5.16277700	-1.69859400	1.46626600
C	5.03341600	-3.69724500	-2.38083200	H	-5.59242600	-3.36910500	1.04064100
C	4.55412700	-3.45120400	-0.91129500	H	-6.24433800	-2.62770000	2.50561000
H	-0.35619200	-5.51187600	-1.59804200	C	3.65021200	5.95368600	-0.17389000
H	1.53715400	-6.06031900	-3.10614200	C	3.35378400	6.48520900	-1.58909000
H	4.68592800	-5.85349200	-2.63698000	H	3.10285400	7.55087700	-1.53841000
H	4.79786000	-2.81195300	-2.98225600	H	4.21862200	6.38240400	-2.25421200
H	6.11280200	-3.86691000	-2.44427300	H	2.50648700	5.96478200	-2.05012200
H	4.02545400	-4.88570100	-3.95116400	C	4.85795500	6.73975900	0.39179600
C	5.28776500	-4.44168300	0.05685900	H	4.64240000	7.81550700	0.40611100
H	5.39369600	-5.44249900	-0.37313700	H	5.09696600	6.43244000	1.41548800
H	4.69983300	-4.53456000	0.97729000	H	5.75176600	6.57999700	-0.22219500
C	6.63581800	-3.75884400	0.36854000	C	2.40982400	6.22178600	0.71092500
C	6.28240400	-2.29060000	0.28127500	H	1.53309200	5.68163700	0.33732200
C	5.04751600	-2.11639500	-0.36354600	H	2.57788900	5.91552700	1.74908000
C	6.99299800	-1.19627400	0.76238800	H	2.17314800	7.29325100	0.71707100
H	7.94921500	-1.33022600	1.26183900	H	-1.63233900	-3.09193600	-1.29387400
C	6.46170300	0.08191700	0.59643500	C	0.70337700	-4.56579000	2.51712500
H	7.01515300	0.94832800	0.94638500	H	1.14653700	-5.41381700	1.98277300
C	5.20825100	0.29638100	-0.00370500	H	1.48635700	-3.80569300	2.61970000
C	4.50381300	-0.83623400	-0.45044800	H	0.42701600	-4.90413200	3.52060700
H	7.40100400	-4.02819000	-0.37329700	Ag	-1.51529300	-0.63927000	-0.03954300
H	7.03556100	-4.03940000	1.34955100	N	-3.51585200	1.16574100	1.37935500
O	2.09911000	-2.36733700	0.62090100	N	-4.63886600	1.03073400	1.53985700
O	3.21291000	-0.68018400	-0.98342100	C	-2.31877000	1.32712700	0.87229100
P	1.91385100	-0.88624900	-0.03743600	P	-1.07949100	1.95655300	1.97557300
O	0.68973500	-0.71675400	-0.87258000	O	0.31498700	1.91410700	1.41261700
O	2.06109600	0.01323500	1.24372700	O	-1.57672100	3.42188500	2.38847700
C	-0.46284000	-3.74295800	0.39894600	O	-1.22143000	1.17253700	3.38987800
C	-1.62920600	-3.25402000	-0.21829700	C	-0.70172200	4.31828500	3.10166000
C	-0.49914600	-4.01814100	1.78318100	H	-0.57925700	3.98004900	4.13521800
C	-2.81535000	-3.04802500	0.50812400	H	0.26937900	4.37737400	2.60373000
C	-1.69824800	-3.81464900	2.47920000	H	-1.19109200	5.29255900	3.08143100
C	-2.87665300	-3.34360600	1.88055800	C	-0.49231500	-0.04088300	3.65019000
H	-3.69182800	-2.70822100	-0.03176700	H	-0.70299200	-0.30206700	4.68862400
H	-1.70859300	-4.06627200	3.53690700	H	-0.83532800	-0.85013400	2.99607000
C	4.69993200	1.69533300	-0.10737400	H	0.58063700	0.11334400	3.51260100
C	4.57404200	2.44543800	1.07259200	H	1.40201700	0.79215000	1.26967800
C	4.45138300	2.33191300	-1.34018800	C	-7.54594400	-1.51230700	-3.55047100
C	4.22240000	3.78944300	1.04729500	C	-7.67778300	-0.65050500	-2.46079400
H	4.75377000	1.95551900	2.02570700	C	-6.55557900	-0.02286700	-1.91756100
C	4.09935500	3.69041600	-1.33703500	C	-5.28162000	-0.26170700	-2.45546600
C	3.98302400	4.45079200	-0.16741200	C	-5.15623100	-1.15127100	-3.53638000
H	4.14470400	4.32617100	1.98863400	C	-6.27993400	-1.76041400	-4.08872100
H	3.93218700	4.16052800	-2.30064600	H	-8.42377400	-1.99105500	-3.97687100
C	4.59016400	1.60933300	-2.66095300	H	-8.65706300	-0.46183100	-2.02931500
H	5.50177000	1.00171700	-2.69405400	H	-6.67521800	0.64177200	-1.07025100
H	3.74573200	0.93297300	-2.83674700	H	-4.16668600	-1.34954800	-3.93537900
H	4.62845400	2.32122900	-3.49148900	H	-6.16940900	-2.43151500	-4.93663500
C	-4.16872700	-3.21877500	2.70888200	C	-4.01906600	0.32174200	-1.89064600
C	-4.54843200	-4.61415700	3.26311600	O	-3.00547600	-0.43312900	-1.88485600
H	-5.46573800	-4.54577700	3.86014200	C	-3.94504700	1.67639200	-1.40317800
H	-4.72626300	-5.32510700	2.44811300	C	-2.66814700	2.15688500	-0.93756900
H	-3.76330700	-5.02874200	3.90442100	C	-2.38015800	3.61181400	-0.79986500
C	-3.94414200	-2.24692900	3.89171800	C	-1.21355600	4.10974200	-1.40353600
H	-4.85430000	-2.17457400	4.49901400	C	-3.22446000	4.51131900	-0.12657600
H	-3.13362700	-2.58111200	4.54874300	C	-0.91695700	5.47248700	-1.37104800

H	-0.54342500	3.42334700	-1.91496200
C	-2.91895900	5.86970700	-0.08119800
H	-4.12388200	4.15294600	0.36009900
C	-1.76952900	6.35738600	-0.70849500
H	-0.02348300	5.84181500	-1.86678700
H	-3.58813200	6.55083400	0.43746800
H	-1.54143300	7.41974900	-0.68234800
C	-5.06668700	2.54868600	-1.47862800
N	-5.97435800	3.27966300	-1.55153200
H	-1.84272000	1.61786400	-1.39241100

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C	4.03070600	-4.05405200	-2.10067700
C	3.91761500	-3.20611300	-0.98750200
C	2.67728900	-3.05424000	-0.37666300
C	1.56254700	-3.81568300	-0.77059100
C	1.72580500	-4.69075300	-1.85744600
C	2.93910100	-4.79576000	-2.54001700
C	5.42342600	-3.97117700	-2.68732300
C	5.99280600	-2.69969600	-2.01881200
C	5.28062500	-2.62959300	-0.62564500
H	0.87376800	-5.28533600	-2.17456600
H	3.02250400	-5.44955200	-3.40428700
H	6.01665400	-4.85946400	-2.42827000
H	5.71120900	-1.81705100	-2.60413800
H	7.08349900	-2.70640100	-1.92854600
H	5.41526400	-3.90587100	-3.78105900
C	6.03013200	-3.54623800	0.39949300
H	6.35791800	-4.48981500	-0.04797100
H	5.34762700	-3.78642400	1.22281500
C	7.19345500	-2.67726100	0.92496000
C	6.62359900	-1.27831200	0.83290500
C	5.46876200	-1.26781900	0.03493300
C	7.08301500	-0.10959400	1.43142500
H	7.97724100	-0.11632700	2.04954200
C	6.38241100	1.07888500	1.22624500
H	6.74534700	2.00433400	1.66375100
C	5.19511300	1.12220400	0.47454900
C	4.73955200	-0.08644300	-0.08176700
H	8.08830100	-2.78415300	0.29571500
H	7.49252400	-2.94408900	1.94490500
O	2.52186400	-2.06608600	0.61285800
O	3.50556400	-0.10943200	-0.75449800
P	2.17270900	-0.58297900	0.03391700
O	1.02455700	-0.54032900	-0.91836400
O	2.04854700	0.22217000	1.37889600
C	0.23676800	-3.75162100	-0.08591500
C	-0.90284100	-3.34791100	-0.81023500
C	0.06299600	-4.21231400	1.23612800
C	-2.19730700	-3.43568300	-0.26377300
C	-1.23743500	-4.30369800	1.75055400
C	-2.38889300	-3.95520400	1.03023800
H	-3.04082900	-3.14927100	-0.88398200
H	-1.34776300	-4.70922800	2.75309500
C	4.48136600	2.42353700	0.32263600
C	4.08259100	3.10885100	1.48113600
C	4.27751200	3.04042800	-0.92861400
C	3.49751300	4.36800300	1.41757500
H	4.23011900	2.63357400	2.44716100
C	3.68805400	4.31329300	-0.96361000
C	3.28917200	5.00671200	0.18476900

H	3.20702900	4.85539300	2.34409400
H	3.55917100	4.77248300	-1.93830200
C	4.69819600	2.39063000	-2.22715300
H	5.67799100	1.90818300	-2.13944700
H	3.98357300	1.61805100	-2.53423400
H	4.75712700	3.13173800	-3.03068700
C	-3.78089000	-4.22906300	1.62960300
C	-3.91925900	-5.75369700	1.87095500
H	-4.90986300	-5.98031900	2.28306700
H	-3.80733300	-6.31075100	0.93372200
H	-3.16994600	-6.12874000	2.57670200
C	-3.93951100	-3.49044400	2.97946700
H	-4.91336600	-3.72690700	3.42406700
H	-3.16733800	-3.78062300	3.70093300
H	-3.89233500	-2.40511100	2.84384000
C	-4.92058400	-3.78986200	0.69105500
H	-4.88804200	-2.72080900	0.46251100
H	-4.89984700	-4.33637500	-0.25832800
H	-5.88519100	-3.99662400	1.16811100
C	2.66828000	6.41479900	0.13842400
C	2.49046400	6.93632700	-1.29996600
H	2.04051600	7.93532600	-1.27698900
H	3.44824300	7.01759000	-1.82606100
H	1.83007800	6.29070500	-1.89046900
C	3.58621900	7.40304200	0.89772800
H	3.15348600	8.41115400	0.88948700
H	3.72503500	7.10729600	1.94297400
H	4.57651800	7.45434800	0.43087900
C	1.27724700	6.38895700	0.81510800
H	0.60674400	5.68864000	0.30367200
H	1.34415000	6.08364900	1.86492600
H	0.81873300	7.38518200	0.78618900
H	-0.78377400	-3.04778600	-1.84967800
C	1.23133400	-4.66249200	2.08303600
H	1.87590200	-5.36165300	1.53827700
H	1.85697700	-3.81298300	2.38082300
H	0.88324300	-5.16086600	2.99301200
Ag	-1.18243600	-0.79863700	-0.21260500
N	-3.52235500	0.24189400	1.40329000
N	-4.58633800	-0.14730400	1.53425100
C	-2.47172400	0.77481900	0.78700300
P	-1.42472400	1.71283100	1.90510100
O	0.01726400	1.82230200	1.49696400
O	-2.16556300	3.12583800	2.04006600
O	-1.61094500	1.09463000	3.39157400
C	-1.58570800	4.18606500	2.82852100
H	-1.57453700	3.90339000	3.88502000
H	-0.57214600	4.40501000	2.48255500
H	-2.23006300	5.05350200	2.68268500
C	-0.78121800	0.01236000	3.85498800
H	-0.92009300	-0.03637900	4.93626100
H	-1.10126800	-0.93258900	3.40297800
H	0.27010100	0.19838900	3.62040300
H	1.28263300	0.89302100	1.38390800
C	-9.71993900	0.50279400	-1.58249700
C	-8.68112000	0.27682600	-2.48632900
C	-7.37434300	0.64940800	-2.16443600
C	-7.09308700	1.25867300	-0.93317700
C	-8.14999000	1.50513100	-0.04236300
C	-9.45036300	1.12009800	-0.35726300

H	-10.73545000	0.20619000	-1.83309500	C	-0.40296800	-4.09359400	-0.89117300
H	-8.88535200	-0.18756400	-3.44758100	C	0.51985400	-4.38742500	1.32557700
H	-6.58243700	0.47798000	-2.88483700	C	-1.69861500	-4.26267800	-0.39921000
H	-7.92542300	2.00812400	0.89241300	C	-0.79002700	-4.55001000	1.79222000
H	-10.25639700	1.30593800	0.34824200	C	-1.92211100	-4.50199000	0.96248500
C	-5.72554100	1.74455100	-0.52676200	H	-2.52945300	-4.20110000	-1.09127700
O	-5.64918400	2.72657900	0.22445600	H	-0.92078600	-4.74885900	2.85328700
C	-4.51369900	1.07930300	-1.01935100	C	3.93216400	2.69667100	0.03161900
C	-3.25165300	1.70251500	-0.68247600	C	3.54364800	3.46603700	1.14255900
C	-2.11981300	1.85693300	-1.66269100	C	3.54143200	3.13209800	-1.25210600
C	-1.33811900	3.02017600	-1.57088400	C	2.79627700	4.62900700	1.00227400
C	-1.81135200	0.93013400	-2.67663900	H	3.84272700	3.13809500	2.13477400
C	-0.28141200	3.25254600	-2.45103000	C	2.77232100	4.30175000	-1.36202800
H	-1.57076200	3.75387300	-0.80364600	C	2.38525600	5.07724100	-0.26406000
C	-0.75284200	1.16491400	-3.55608300	H	2.54496600	5.19957700	1.89208100
H	-2.41967700	0.04313000	-2.81174100	H	2.49314100	4.61622800	-2.36208600
C	0.01898200	2.32255000	-3.44654800	C	3.95628100	2.41896400	-2.51944200
H	0.30653000	4.16167400	-2.35678100	H	4.97183500	2.01582600	-2.44283800
H	-0.53718400	0.43754800	-4.33429300	H	3.29184900	1.57662600	-2.74252200
H	0.84182800	2.50006900	-4.13371700	H	3.92756700	3.10388600	-3.37291600
C	-4.52068700	-0.18484600	-1.64902200	C	-3.32827100	-4.71719300	1.55097100
N	-4.42891400	-1.25369800	-2.12413000	C	-3.37576400	-6.06358700	2.31195000
H	-3.46996800	2.64473500	-0.17939400	H	-4.37768400	-6.22568900	2.72728900
8-RR-an				H	-3.14747900	-6.90084700	1.64221500
C	4.59403300	-3.95412300	-1.92552300	H	-2.66382500	-6.09678500	3.14378400
C	4.29437900	-3.05343300	-0.89059100	C	-3.65356800	-3.56207900	2.52726400
C	3.02278000	-3.07730600	-0.32547500	H	-4.64713300	-3.70397400	2.96980200
C	2.07603700	-4.05940300	-0.66842800	H	-2.92802900	-3.50670000	3.34737200
C	2.43701600	-4.97976000	-1.66786600	H	-3.65296100	-2.60317000	1.99668900
C	3.67037300	-4.91761900	-2.31667600	C	-4.41700700	-4.74192300	0.46126800
C	5.96784800	-3.67164900	-2.49379900	H	-4.47054100	-3.79574200	-0.08578400
C	6.28604400	-2.27462200	-1.91755600	H	-4.24945400	-5.55124800	-0.25944600
C	5.53066400	-2.23060100	-0.54629400	H	-5.39590600	-4.91088200	0.92403100
H	1.71749400	-5.74484800	-1.94409300	C	1.59887500	6.39326400	-0.40405900
H	3.90137500	-5.61629600	-3.11669000	C	1.11870900	6.64040600	-1.84684700
H	6.69950400	-4.41991800	-2.15834300	H	0.55262200	7.57781500	-1.88919800
H	5.87198700	-1.50040900	-2.57351800	H	1.95647800	6.73347800	-2.54728800
H	7.35766500	-2.08137400	-1.80852600	H	0.45833000	5.83952500	-2.19683000
H	5.97969200	-3.68934000	-3.58933800	C	2.51987600	7.56697400	0.01099000
C	6.39266600	-2.94047800	0.55275300	H	1.98337200	8.52064800	-0.06871900
H	6.87295800	-3.85096000	0.18123500	H	2.86658500	7.46229300	1.04504300
H	5.73910000	-3.22400200	1.38565200	H	3.40438000	7.61944500	-0.63441300
C	7.39474200	-1.86287400	1.01904600	C	0.35648000	6.37224300	0.51680900
C	6.61550400	-0.58227000	0.81432300	H	-0.31617500	5.54687000	0.26206300
C	5.48398100	-0.81342700	0.01622100	H	0.63249900	6.27436500	1.57233500
C	6.88244100	0.68754000	1.31499100	H	-0.20472700	7.30840100	0.41118900
H	7.76134900	0.86941500	1.92829200	H	-0.25529200	-3.91740600	-1.95399700
C	6.01071600	1.73254900	1.01388900	C	1.67482000	-4.51884600	2.29312600
H	6.22662100	2.73541000	1.36981900	H	2.45285700	-5.18371800	1.90017600
C	4.83493700	1.53352400	0.26709200	H	2.14915200	-3.55077500	2.48968300
C	4.58096500	0.22713500	-0.19053400	H	1.33459600	-4.92804700	3.24964400
H	8.30859000	-1.87477600	0.40855400	Ag	-1.15353000	-0.87087200	-0.83358000
H	7.71003600	-2.00077700	2.05949700	N	-4.03020400	1.63063900	2.12975000
O	2.66135500	-2.06190900	0.58386800	N	-4.96715000	1.49841600	2.76386300
O	3.37138400	-0.04287300	-0.85779000	C	-2.97239700	1.74704800	1.37038500
P	2.12689100	-0.66955400	-0.04311400	P	-1.40975200	1.85099800	2.18245500
O	0.99789500	-0.79663400	-1.02227600	O	-0.28907400	1.52191200	1.23198700
O	1.87461700	0.14863700	1.27026600	O	-1.34533900	3.31095400	2.83858100
C	0.72019600	-4.15109100	-0.05337800	O	-1.44486100	0.93115900	3.50857700

C	-0.16934200	3.72364300	3.56891500
H	-0.04737700	3.10905800	4.46525000
H	0.71496500	3.65172400	2.93010000
H	-0.34171500	4.76294700	3.85061900
C	-1.22935500	-0.49317900	3.40781500
H	-1.39198000	-0.89362600	4.40923000
H	-1.94056300	-0.94730700	2.71164500
H	-0.20585000	-0.69934100	3.08374500
H	1.04975100	0.74936600	1.24924900
C	-7.68038600	-2.65100800	-2.24160900
C	-7.84243300	-1.74205600	-1.19520700
C	-6.76283400	-0.97563700	-0.75314600
C	-5.50182500	-1.11291300	-1.35031000
C	-5.34356700	-2.04662700	-2.38805000
C	-6.42571100	-2.79993500	-2.83894800
H	-8.52442600	-3.24161200	-2.58841700
H	-8.81210700	-1.62588600	-0.71847900
H	-6.90190700	-0.27304300	0.06099200
H	-4.36382300	-2.16949000	-2.83944400
H	-6.29018600	-3.50572400	-3.65468700
C	-4.29621000	-0.34851800	-0.88343000
O	-3.23975000	-1.09635000	-0.74031400
C	-4.35257300	1.01987700	-0.64091900
C	-3.12931500	1.79254200	-0.16327500
C	-3.04797600	3.20329400	-0.74826300
C	-2.59619300	3.34993600	-2.06777600
C	-3.44242600	4.34491900	-0.04393100
C	-2.54674400	4.60523700	-2.67145400
H	-2.29507600	2.46776900	-2.62903300
C	-3.39498900	5.60477900	-0.64645600
H	-3.79345100	4.25608300	0.97952600
C	-2.94904200	5.73981100	-1.96100500
H	-2.19985500	4.69748100	-3.69746700
H	-3.71479500	6.47925100	-0.08601200
H	-2.91671900	6.71925600	-2.43065900
C	-5.54327900	1.76891300	-0.83779200
N	-6.49373800	2.43707000	-0.96246900
H	-2.24644500	1.25480400	-0.53346700

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C	3.91921400	-4.24145200	-2.05039600
C	3.87207500	-3.29983300	-1.00949100
C	2.68634400	-3.14058300	-0.29840400
C	1.58058700	-3.98483000	-0.50658300
C	1.68709100	-4.95364100	-1.51852300
C	2.83140700	-5.06849400	-2.30895900
C	5.24036300	-4.15474900	-2.78377300
C	5.81380400	-2.81066900	-2.28192900
C	5.24105400	-2.65256300	-0.83324700
H	0.84052800	-5.61165800	-1.69217900
H	2.86572700	-5.79634300	-3.11550600
H	5.89828700	-4.99459500	-2.51980800
H	5.43473200	-1.99134200	-2.90315600
H	6.90721900	-2.76864200	-2.30439800
H	5.11745700	-4.18144900	-3.87227100
C	6.12316400	-3.46718400	0.17400700
H	6.43361900	-4.43471500	-0.23254700
H	5.53849200	-3.65850700	1.08110800
C	7.30428400	-2.53046500	0.50465200
C	6.67702100	-1.15967000	0.37731400
C	5.44731800	-1.24001700	-0.29556400

C	7.15101400	0.06086900	0.84628900
H	8.10370800	0.12414700	1.36600400
C	6.38721700	1.20940500	0.64193200
H	6.75566800	2.17257600	0.98242700
C	5.12853000	1.16554700	0.01657300
C	4.66913600	-0.09119200	-0.41765800
H	8.12845600	-2.65871500	-0.21115600
H	7.72188300	-2.71180100	1.50146600
O	2.57241400	-2.07007500	0.61076100
O	3.38052300	-0.19781400	-0.97182300
P	2.13900300	-0.64427300	-0.03815400
O	0.91853900	-0.68681700	-0.90032800
O	2.09581800	0.25633600	1.24679400
C	0.31358000	-3.89521300	0.27876800
C	-0.88808900	-3.61847200	-0.39140000
C	0.26097400	-4.18840600	1.65962700
C	-2.12410400	-3.63704700	0.26926900
C	-0.98735700	-4.21268900	2.29328500
C	-2.20047800	-3.95572200	1.63299600
H	-3.01621600	-3.41953700	-0.30632600
H	-1.00583900	-4.47373400	3.34868500
C	4.34807200	2.42954400	-0.11958400
C	4.07220900	3.16839900	1.04225700
C	3.96149000	2.96499700	-1.36523300
C	3.43247700	4.40081700	0.98751400
H	4.36284400	2.75697200	2.00519000
C	3.31346900	4.20963700	-1.39085400
C	3.03568300	4.95562400	-0.23962100
H	3.24860500	4.93542600	1.91525600
H	3.03750700	4.60330200	-2.36342000
C	4.25389000	2.26304300	-2.67206400
H	5.26965500	1.85185300	-2.69058900
H	3.56490300	1.42754500	-2.84011400
H	4.15412500	2.95506000	-3.51420700
C	-3.53484900	-4.07865200	2.39245800
C	-3.67990500	-5.52681000	2.92128500
H	-4.62944300	-5.63940200	3.45837800
H	-3.66912500	-6.24862100	2.09658000
H	-2.87278000	-5.79456500	3.61173000
C	-3.55621900	-3.09804800	3.58868500
H	-4.49630300	-3.20051300	4.14367600
H	-2.73579700	-3.28916100	4.28947700
H	-3.47953600	-2.05895200	3.24984400
C	-4.74913400	-3.77275300	1.49454200
H	-4.72762400	-2.75104200	1.10144700
H	-4.81481500	-4.46497500	0.64747800
H	-5.67074000	-3.88021000	2.07764700
C	2.36390400	6.34015200	-0.27942400
C	1.92736000	6.74206700	-1.70110200
H	1.44072000	7.72372200	-1.67389300
H	2.77972700	6.81805500	-2.38576900
H	1.21150400	6.02728000	-2.12278700
C	3.36654300	7.40034100	0.23774100
H	2.90828600	8.39717300	0.22954200
H	3.68669800	7.18733700	1.26346300
H	4.26317800	7.43297500	-0.39193500
C	1.10945800	6.34136200	0.62570400
H	0.37433400	5.60412000	0.28558500
H	1.36030500	6.11471300	1.66765700
H	0.63132900	7.32852800	0.60934800

H	-0.86075200	-3.42011800	-1.46048700	C	5.56013900	-3.13964400	-2.27421400
C	1.50675200	-4.51996600	2.44941300	C	5.00943300	-2.92544600	-0.82451600
H	2.10200800	-5.29411000	1.95131000	H	0.40020100	-5.56466100	-1.63930000
H	2.15245200	-3.64176400	2.56366100	H	2.40493400	-5.91898800	-3.05988400
H	1.24948900	-4.88286600	3.44941500	H	5.49112400	-5.32686200	-2.48512600
Ag	-1.27468200	-0.74186200	-0.40601800	H	5.23436900	-2.30327100	-2.90290000
N	-3.67940700	0.51567800	1.48154400	H	6.65370400	-3.17344100	-2.30328300
N	-4.74890200	0.12915800	1.25623300	H	4.76103900	-4.47803800	-3.84394200
C	-2.63544700	1.12571800	0.91934700	C	5.83717300	-3.79040800	0.18683800
P	-1.33692500	1.67746800	1.99026000	H	6.07685300	-4.78162300	-0.21083700
O	0.01252800	1.76337700	1.32426000	H	5.24478800	-3.93032900	1.09834700
O	-1.81774700	3.07204400	2.61625800	C	7.08296500	-2.93599900	0.50325500
O	-1.37068600	0.71990200	3.29103600	C	6.55218600	-1.52585200	0.36601500
C	-0.89554600	3.89406500	3.35847600	C	5.31726800	-1.52572300	-0.30171200
H	-0.70128600	3.44826100	4.33910400	C	7.11202000	-0.33776300	0.82365600
H	0.03863200	4.01399800	2.80397700	H	8.06899100	-0.33704600	1.33943900
H	-1.38528800	4.86109800	3.47921200	C	6.42760900	0.85904600	0.61484700
C	-0.59558400	-0.49136400	3.37094200	H	6.86141200	1.79677100	0.94948200
H	-0.76025700	-0.88646300	4.37450800	C	5.16624400	0.89734700	-0.00511600
H	-0.93862900	-1.22707500	2.63650700	C	4.61927100	-0.32684100	-0.43124700
H	0.46651000	-0.28367200	3.22069400	H	7.89240300	-3.12842700	-0.21508800
H	1.30711900	0.90685500	1.25888200	H	7.49174700	-3.13759200	1.49986000
C	-7.59225400	-2.20784800	-3.36236400	O	2.39631000	-2.13972400	0.62313400
C	-7.81501900	-1.39972100	-2.24636300	O	3.32761900	-0.34908800	-0.98251200
C	-6.75653800	-0.71509000	-1.64817600	P	2.05299800	-0.68681300	-0.04130400
C	-5.45596400	-0.83907700	-2.15913400	O	0.82690700	-0.66726200	-0.89373700
C	-5.23700100	-1.67380200	-3.26770600	O	2.08831600	0.22495200	1.23177100
C	-6.29839300	-2.34248300	-3.87288000	C	0.00745900	-3.78194000	0.30754800
H	-8.42115100	-2.73281500	-3.83024900	C	-1.16090900	-3.37973500	-0.36612800
H	-8.81626300	-1.29978400	-1.83615800	C	-0.08106000	-4.08114400	1.68333000
H	-6.94303800	-0.09671800	-0.77823600	C	-2.39742100	-3.28264900	0.29754000
H	-4.22659200	-1.78346600	-3.64815100	C	-1.32839200	-3.98474700	2.31721100
H	-6.11659000	-2.97108400	-4.74083800	C	-2.50794600	-3.59972900	1.66326800
C	-4.26133400	-0.17391900	-1.54147400	H	-3.27469000	-3.01887000	-0.28215500
O	-3.19475600	-0.86943500	-1.53755100	H	-1.37293200	-4.24410300	3.37199100
C	-4.31800500	1.15165100	-1.01560200	C	4.46753400	2.20874500	-0.13625200
C	-3.05305700	1.79341000	-0.48469300	C	4.23187300	2.95336800	1.03038900
C	-3.08607600	3.31395700	-0.41755900	C	4.11257300	2.77217800	-1.37847700
C	-2.27919900	4.05169100	-1.29245500	C	3.65614300	4.21678500	0.98367600
C	-3.91147200	4.00532100	0.47986800	H	4.49615000	2.51904700	1.99071600
C	-2.30130000	5.44823300	-1.28206900	C	3.53080300	4.04911600	-1.39649300
H	-1.63284600	3.52844900	-1.99378200	C	3.28864900	4.79892300	-0.23958500
C	-3.93400200	5.39861800	0.49426000	H	3.49417600	4.75167800	1.91515400
H	-4.54406000	3.45407500	1.16876800	H	3.27590300	4.46299100	-2.36653000
C	-3.13000800	6.12570100	-0.38720000	C	4.36711100	2.06088700	-2.68821600
H	-1.67474300	6.00270100	-1.97575100	H	5.36324500	1.60417300	-2.71205000
H	-4.58778600	5.91719900	1.19034300	H	3.64024300	1.25768600	-2.85442100
H	-3.15318400	7.21226200	-0.37819800	H	4.29516800	2.75851300	-3.52870300
C	-5.46728600	1.96217800	-1.21694700	C	-3.84536500	-3.56654600	2.42539600
N	-6.40313400	2.64297700	-1.37293800	C	-4.12914100	-4.97250500	3.00862700
H	-2.24027900	1.51796100	-1.16694300	H	-5.08282400	-4.96904500	3.54967300
10-RR-an				H	-4.19321400	-5.72457400	2.21345400
C	3.57165400	-4.43162500	-2.01610300	H	-3.35142100	-5.29223500	3.71049900
C	3.59697800	-3.47676700	-0.98635200	C	-3.76169900	-2.53751900	3.57868800
C	2.42917300	-3.22049800	-0.27329900	H	-4.70163400	-2.53254000	4.14401300
C	1.26393200	-3.98339300	-0.47443100	H	-2.95568400	-2.78093100	4.28054100
C	1.29431300	-4.97039200	-1.47304800	H	-3.59432100	-1.52553900	3.19446600
C	2.42613000	-5.18087000	-2.26226300	C	-5.02786200	-3.17677500	1.51686300
C	4.89193200	-4.44637800	-2.75646500	H	-4.91977100	-2.16761500	1.10624600

H	-5.15549500	-3.88230500	0.68707700
H	-5.95395200	-3.19095000	2.10250400
C	2.67765600	6.21143600	-0.26683900
C	2.27528100	6.65098200	-1.68729600
H	1.83296000	7.65324000	-1.65216700
H	3.13781000	6.69659600	-2.36208400
H	1.53263100	5.97456500	-2.12551100
C	3.71708600	7.22213600	0.27579100
H	3.29937200	8.23674200	0.27838600
H	4.01770800	6.98130000	1.30118300
H	4.62071100	7.22791200	-0.34481800
C	1.41436500	6.25005400	0.62551200
H	0.65666000	5.54408700	0.26985300
H	1.64547000	5.99972700	1.66649400
H	0.97392000	7.25487500	0.61665100
H	-1.11504100	-3.19896600	-1.43761500
C	1.12593000	-4.53208100	2.47326000
H	1.65483500	-5.34702600	1.96592100
H	1.84345900	-3.71327200	2.60090500
H	0.83343700	-4.88388300	3.46745000
Ag	-1.32817200	-0.78698500	0.02192200
N	-3.64562800	0.62667300	1.23858200
N	-4.62850700	0.65413300	0.44697000
C	-2.44546100	1.12693400	0.73781700
P	-1.29293000	1.69905700	1.97402000
O	0.13552200	1.84653000	1.50052500
O	-1.88470200	3.07683100	2.55589800
O	-1.42905100	0.73717200	3.26865800
C	-1.10962100	3.86983000	3.47145000
H	-1.04390200	3.36888200	4.44278100
H	-0.10780000	4.04766800	3.07077000
H	-1.64131500	4.81671900	3.57812300
C	-0.52867600	-0.35400200	3.50720200
H	-0.75398500	-0.71872900	4.51114200
H	-0.69698200	-1.16211400	2.78682500
H	0.51204200	-0.02400600	3.45367000
H	1.31679000	0.90742800	1.29522000
C	-7.37504300	-2.21848600	-3.29510100
C	-7.56079800	-1.33653900	-2.22850100
C	-6.48552000	-0.61029200	-1.71901500
C	-5.20316400	-0.77570500	-2.27114700
C	-5.02205600	-1.67812800	-3.33595400
C	-6.10245300	-2.38793400	-3.84956200
H	-8.21989600	-2.77330100	-3.69460400
H	-8.54667700	-1.21078700	-1.79035600
H	-6.63379200	0.05243800	-0.87544200
H	-4.02837200	-1.79828000	-3.75491800
H	-5.95560200	-3.07113200	-4.68149400
C	-3.99802900	-0.05388000	-1.77862500
O	-2.87137100	-0.49936100	-2.00249900
C	-4.13841800	1.22713000	-0.91488100
C	-2.75139900	1.88170200	-0.59623600
C	-2.75930700	3.40143900	-0.54567800
C	-1.92428000	4.11479000	-1.41506200
C	-3.59997500	4.12095600	0.31693600
C	-1.92759200	5.51143100	-1.42950900
H	-1.26824000	3.57031500	-2.09060900
C	-3.60755300	5.51436500	0.30270900
H	-4.25299500	3.59065900	1.00338800
C	-2.77190700	6.21539400	-0.57049800

H	-1.27669700	6.04550300	-2.11673600
H	-4.27305400	6.05389100	0.97142300
H	-2.78290800	7.30211900	-0.58324200
C	-5.13895200	2.13424900	-1.47256000
N	-5.94839500	2.82974700	-1.93112200
H	-2.05198400	1.57761600	-1.37647400

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C	4.26056400	-3.64060700	-2.48195500
C	4.13856500	-2.85183200	-1.32658500
C	2.93585800	-2.86171100	-0.62694500
C	1.88282800	-3.72399000	-0.98236500
C	2.06043900	-4.53655700	-2.11374100
C	3.22738500	-4.48329400	-2.87846500
C	5.58652700	-3.37698400	-3.16290200
C	6.05571500	-2.07074800	-2.48463300
C	5.45307300	-2.13378300	-1.04033900
H	1.25456400	-5.20560300	-2.40210600
H	3.31885000	-5.09106600	-3.77493400
H	6.29505400	-4.19798800	-2.98380100
H	5.62791400	-1.20833500	-3.00824700
H	7.14351100	-1.95033200	-2.47646700
H	5.48779700	-3.27756600	-4.24963200
C	6.38367300	-2.99096300	-0.11668500
H	6.77649300	-3.87577800	-0.62750100
H	5.80348900	-3.33401700	0.74770500
C	7.48143800	-2.01043200	0.35004700
C	6.74904900	-0.68608200	0.36926600
C	5.53864700	-0.78339100	-0.33522100
C	7.11633100	0.50484600	0.98756900
H	8.05336900	0.58088200	1.53351700
C	6.26481300	1.60680700	0.90126300
H	6.54866500	2.54904300	1.36096700
C	5.02238300	1.53558800	0.24833600
C	4.67098600	0.30582700	-0.33679500
H	8.32414900	-1.98892700	-0.35536500
H	7.89691300	-2.27677700	1.32853600
O	2.74683200	-1.94384900	0.41928900
O	3.39869500	0.16260900	-0.91568200
P	2.19524000	-0.47847200	-0.04165300
O	0.97361600	-0.52472700	-0.90045700
O	2.11370500	0.24331000	1.34472900
C	0.60253300	-3.80579400	-0.21703800
C	-0.60610500	-3.45562300	-0.84911800
C	0.54802000	-4.32609500	1.09268300
C	-1.84852200	-3.63243000	-0.21236100
C	-0.70449700	-4.50220300	1.69889300
C	-1.92193800	-4.18484200	1.08041500
H	-2.74974100	-3.39826500	-0.76794500
H	-0.71913800	-4.93602100	2.69563300
C	4.12784300	2.72936000	0.23559400
C	3.71734400	3.27345800	1.46239800
C	3.73011500	3.37222500	-0.95407700
C	2.92223300	4.41174700	1.52265100
H	4.01590300	2.77728400	2.38188600
C	2.92912900	4.52022100	-0.86421700
C	2.50312500	5.06460900	0.35280900
H	2.62453000	4.78932900	2.49682300
H	2.64160600	4.99905800	-1.79422000
C	4.15946600	2.87772200	-2.31707900
H	5.22146200	2.60710700	-2.33278600

H	3.59496000	1.98616000	-2.61422700	H	-7.78722200	2.50385700	-1.79906700
H	3.99627700	3.64729200	-3.07824500	H	-9.74955000	1.40747100	-2.87722300
C	-3.25345100	-4.48802100	1.79169000	C	-5.66851700	1.38866000	-0.70514600
C	-3.32700200	-6.00649900	2.08731800	O	-5.78434200	2.55404600	-0.36408500
H	-4.27096800	-6.24535500	2.59151200	C	-4.32130200	0.66324500	-0.44608100
H	-3.28027100	-6.59124700	1.16103300	C	-3.19359800	1.58542200	0.10338500
H	-2.51024000	-6.34029700	2.73621100	C	-2.44123300	2.43641300	-0.90753600
C	-3.32956300	-3.69888600	3.12101400	C	-2.94659900	3.71691700	-1.19412700
H	-4.26272000	-3.93913800	3.64524800	C	-1.28977300	2.01625800	-1.58617700
H	-2.50062300	-3.95297400	3.79179500	C	-2.33604300	4.53592800	-2.14336700
H	-3.31172800	-2.61914800	2.93886700	H	-3.83873100	4.05857900	-0.67961900
C	-4.47618800	-4.10821600	0.93392200	C	-0.67539800	2.83531200	-2.53548300
H	-4.51491700	-3.03389300	0.72763400	H	-0.83904800	1.05472200	-1.37101300
H	-4.49204200	-4.65399100	-0.01735400	C	-1.19853700	4.09568600	-2.82440400
H	-5.39243000	-4.36957400	1.47545100	H	-2.75160900	5.51878700	-2.35066300
C	1.62815100	6.32772600	0.44539500	H	0.21741100	2.48025500	-3.04268300
C	1.26463300	6.89643400	-0.93947800	H	-0.72441300	4.72991500	-3.56925500
H	0.64379800	7.79154000	-0.81676800	C	-3.85179000	-0.13169000	-1.59134900
H	2.15521800	7.18841200	-1.50806800	N	-3.42277200	-0.81494800	-2.43010700
H	0.69278700	6.17615700	-1.53459100	H	-3.72231000	2.27785000	0.77037100
C	2.39133900	7.42097300	1.23122600	13			
H	1.78095500	8.32897300	1.31334800	C	3.00373900	4.46103900	-1.18601200
H	2.64106500	7.09410500	2.24626500	C	2.18264900	3.76954000	-0.28176700
H	3.32751800	7.68563100	0.72595700	C	2.40377100	2.41253600	-0.05595100
C	0.31093200	5.98993300	1.18413900	C	3.52059100	1.76192900	-0.61877800
H	-0.25909300	5.22723100	0.64277700	C	4.35389800	2.49646900	-1.47735200
H	0.49976700	5.61470100	2.19585500	C	4.09003900	3.83203200	-1.78627700
H	-0.31491900	6.88700400	1.27269300	C	2.49871300	5.87439100	-1.38395800
H	-0.58074200	-3.10312100	-1.87790800	C	1.07970500	5.80982200	-0.77609800
C	1.79949400	-4.73163400	1.83678800	C	1.17792900	4.72623200	0.35053000
H	2.44450000	-5.36720100	1.21962900	H	5.21482100	1.99961900	-1.91686400
H	2.39128500	-3.85436700	2.12334000	H	4.72678000	4.36700900	-2.48646300
H	1.55068600	-5.28355600	2.74846500	H	3.12905800	6.60058200	-0.85102000
Ag	-1.16965200	-1.00128200	-0.04695700	H	0.36819500	5.46380900	-1.53437100
N	-3.49330800	-0.33602500	1.43263800	H	0.72381600	6.77390600	-0.39884100
N	-4.52655300	-0.34501900	0.71057400	H	2.49471700	6.17532700	-2.43792000
C	-2.47837300	0.54766800	1.00770100	C	1.75683900	5.37378700	1.65417300
P	-1.41866500	1.13472200	2.32263100	H	2.57234600	6.07436700	1.44669100
O	-0.01256900	1.52135700	1.93007000	H	2.15426100	4.57772400	2.29418300
O	-2.23150800	2.37598100	2.94968200	C	0.53927000	6.03178900	2.33879300
O	-1.44651100	0.05644500	3.52519900	C	-0.60123000	5.13610200	1.90569000
C	-1.61280500	3.22324900	3.93457700	C	-0.20408600	4.30757400	0.84530100
H	-1.44656200	2.66516500	4.86149800	C	-1.88715500	5.05113000	2.42970500
H	-0.66523500	3.61643500	3.55657300	H	-2.19798400	5.69354300	3.25001100
H	-2.31227900	4.04048500	4.11708400	C	-2.78004600	4.13028200	1.88264100
C	-0.40440000	-0.91780400	3.69907400	H	-3.79735400	4.07511200	2.25971600
H	-0.53168200	-1.32265100	4.70493000	C	-2.40315900	3.24684900	0.85551200
H	-0.51128700	-1.72541400	2.96771700	C	-1.08001800	3.32749100	0.37613900
H	0.58263200	-0.45795900	3.60345900	H	0.39249300	7.06330500	1.98772500
H	1.25856500	0.79207100	1.51878700	H	0.64390400	6.08306900	3.42881400
C	-9.01354000	-0.59085200	-2.51890500	O	1.49890600	1.68796500	0.70302400
C	-7.98369300	-1.36284400	-1.97839900	O	-0.62856200	2.41774700	-0.57226700
C	-6.87779800	-0.74797700	-1.39175900	P	0.16300400	1.06128600	-0.07133600
C	-6.80216500	0.65309600	-1.33473000	O	0.61469800	0.45960400	-1.41049900
C	-7.85331200	1.42289300	-1.86385700	O	-0.56131500	0.23402300	0.93289900
C	-8.94733400	0.80514200	-2.45989700	C	3.83213500	0.32751500	-0.34914300
H	-9.86909700	-1.07484000	-2.98270200	C	3.86750300	-0.58182200	-1.41938700
H	-8.04034600	-2.44717300	-2.01108400	C	4.17364600	-0.14451600	0.93854600
H	-6.09759100	-1.35533100	-0.94910600	C	4.23850300	-1.92340500	-1.24019900

C	4.54723000	-1.48605700	1.08883300
C	4.59978100	-2.40356000	0.02801600
H	4.27878600	-2.56939900	-2.11083000
H	4.83302200	-1.81372800	2.08528000
C	-3.40579800	2.26613500	0.34777000
C	-4.05139700	1.43280700	1.26956600
C	-3.80576900	2.20230800	-1.00770600
C	-5.05802500	0.54657500	0.88546600
H	-3.74679000	1.47343600	2.31168000
C	-4.80755600	1.29513600	-1.36841100
C	-5.45502500	0.45012400	-0.45364300
H	-5.52790700	-0.06562000	1.64798800
H	-5.10010500	1.26587600	-2.41532200
C	-3.21184900	3.10090900	-2.06796300
H	-3.10992900	4.13130900	-1.70860400
H	-2.21172400	2.76222600	-2.35884000
H	-3.84284500	3.11467900	-2.96266900
C	5.09405700	-3.84155300	0.27380600
C	6.57088700	-3.79139300	0.73666000
H	6.94964700	-4.80473200	0.91835400
H	7.20365700	-3.32334600	-0.02586500
H	6.68488700	-3.21864800	1.66285900
C	4.24390400	-4.51790200	1.37486300
H	4.61172900	-5.53220900	1.57107200
H	4.27421200	-3.96432000	2.31849600
H	3.19443900	-4.59496100	1.06570400
C	5.01697200	-4.71361900	-0.99432800
H	3.99248300	-4.79141300	-1.37740400
H	5.65311900	-4.32526800	-1.79749000
H	5.36282000	-5.72793100	-0.76526800
C	-6.54620700	-0.52095700	-0.93968900
C	-5.92936300	-1.51994200	-1.94833600
H	-6.69382400	-2.21735500	-2.31414500
H	-5.50084000	-1.00716900	-2.81570300
H	-5.12874200	-2.10425300	-1.47902900
C	-7.68068400	0.27105900	-1.63288000
H	-8.46191500	-0.41221400	-1.98903700
H	-8.14184600	0.98225400	-0.93792700
H	-7.31547700	0.83699900	-2.49598400
C	-7.16854600	-1.32788400	0.21604500
H	-6.42549200	-1.95046600	0.72791200
H	-7.63811500	-0.67595900	0.96156500
H	-7.94504500	-1.99598000	-0.17430700
H	3.63087500	-0.22081500	-2.41741500
C	4.17241900	0.76664400	2.14267400
H	4.69353300	1.70703300	1.93130600
H	3.14770700	1.02362700	2.43293100
H	4.66173500	0.28777300	2.99664500
Ag	1.20037100	-1.57715400	-1.19360600
N	0.43435400	-4.23986000	0.02701400
N	0.86997600	-3.72180200	-0.90893600
C	-0.11739500	-4.81550400	1.03019800
H	0.53080400	-5.25247400	1.78175800
P	-1.92227400	-4.84500900	1.19808500
O	-2.31564800	-5.22632700	2.57460100
O	-2.44045300	-3.43955600	0.63450700
O	-2.31294600	-5.82856600	-0.01270900
C	-2.60241900	-2.27702400	1.50606000
H	-1.75437600	-1.60227300	1.37362800
H	-3.51172900	-1.77636100	1.17444100

H	-2.70628900	-2.60061800	2.54440500
C	-3.70702500	-6.09338400	-0.28069000
H	-3.72504100	-6.84562300	-1.07016200
H	-4.20057200	-6.48178500	0.61477100
H	-4.20458600	-5.18119500	-0.62169700

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C	-5.77832700	-2.75186000	1.11247500
C	-5.07686500	-1.98326100	0.17034200
C	-3.74781500	-2.29454700	-0.11167000
C	-3.14211800	-3.43902600	0.44597200
C	-3.88816400	-4.21605500	1.34552500
C	-5.19302300	-3.86882700	1.70073400
C	-7.14583900	-2.15527000	1.36786700
C	-7.01122600	-0.74264500	0.75711300
C	-5.98977000	-0.91182000	-0.41862900
H	-3.42465300	-5.09708400	1.78187100
H	-5.73693200	-4.46290600	2.43089400
H	-7.93314500	-2.73473800	0.86477500
H	-6.58206000	-0.05938900	1.49883700
H	-7.96460100	-0.31914400	0.42507100
H	-7.40306600	-2.13379200	2.43314100
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H	-6.00403600	-1.87814100	-2.37361500
C	-7.33241000	-0.15682100	-2.34052100
C	-6.33374100	0.90979500	-1.94380100
C	-5.49312200	0.44010100	-0.92336900
C	-6.16843000	2.18875200	-2.46677500
H	-6.81879800	2.55497300	-3.25747400
C	-5.15261800	3.00179600	-1.96135300
H	-5.02753600	4.01169800	-2.34224100
C	-4.26015600	2.54634900	-0.97647300
C	-4.42912100	1.23306100	-0.49540500
H	-8.33209000	0.06333400	-1.93929600
H	-7.44309300	-0.24774300	-3.42732200
O	-3.00227800	-1.45200100	-0.91870200
O	-3.51367900	0.70583300	0.40688400
P	-2.23940400	-0.15961200	-0.18828700
O	-1.56360700	-0.64631300	1.09554200
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C	-1.73511100	-3.82673300	0.13019900
C	-0.77315100	-3.82660600	1.15621600
C	-1.33842700	-4.25491300	-1.15499700
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H	1.23508500	-4.27454100	1.77402400
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C	-2.24976600	3.94096900	-1.44002800
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C	-1.21968000	4.80685000	-1.07254300
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 P 3.53157200 1.58739800 -2.66922600
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 C 0.53462700 0.77383100 4.97694500
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C 3.17303800 1.28055800 1.62863700
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 H 5.00235500 1.64094900 -0.06086700
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 C 6.63806100 -1.41793500 -0.01360700
 C 8.61887200 0.29111200 -0.99500800
 H 7.14661300 1.84913800 -0.81073500
 C 7.89666000 -1.91811600 -0.34526000
 H 5.88329100 -2.09807400 0.36381100
 C 8.89224600 -1.06806900 -0.83225000
 H 9.38230900 0.96089700 -1.38074400
 H 8.09847500 -2.97844500 -0.22140500
 H 9.87116800 -1.46371900 -1.08818900
 C 4.32289400 -0.96370500 1.98130100
 N 4.41519500 -1.97063600 2.56384300
 H 4.64540600 -0.55492500 -2.07825000

14-ts-b

C -5.32546100 -4.36703400 1.19013300
 C -5.01879700 -3.34524700 0.27729700
 C -3.70293700 -3.18730200 -0.15455700
 C -2.70883900 -4.11590500 0.21593200
 C -3.05947500 -5.15762100 1.08840400
 C -4.35410300 -5.27633300 1.59750700
 C -6.77140600 -4.26768300 1.62779100
 C -7.16490400 -2.85013500 1.15683800
 C -6.28747800 -2.59435000 -0.11493900
 H -2.29522600 -5.87345900 1.37997400
 H -4.59306800 -6.06744700 2.30373500
 H -7.38786300 -5.03625500 1.14000200
 H -6.89278000 -2.11703900 1.92473300
 H -8.23494300 -2.73982600 0.95423600
 H -6.89422100 -4.40492600 2.70826100
 C -6.97348100 -3.23955500 -1.36643800
 H -7.40676100 -4.22089400 -1.14704400
 H -6.21868900 -3.37507500 -2.14961400
 C -8.01603700 -2.19519000 -1.82331000
 C -7.37405300 -0.88879600 -1.40734200
 C -6.31172500 -1.12371000 -0.52100600
 C -7.69286400 0.40569400 -1.80585900
 H -8.51590200 0.58975100 -2.49211600
 C -6.94097100 1.47185600 -1.30993000
 H -7.19511700 2.49031800 -1.59038600
 C -5.83783600 1.27003600 -0.46355200
 C -5.51481800 -0.05527400 -0.11235500
 H -8.98028000 -2.34608300 -1.31710000
 H -8.21639500 -2.24206600 -2.90000000
 O -3.36092400 -2.09589200 -0.93523500
 O -4.37207600 -0.31037400 0.63752300
 P -2.97688800 -0.66361900 -0.17019800
 O -2.01187700 -0.95500200 0.98216800
 O -2.61483600 0.29663800 -1.24896000
 C -1.30113500 -3.99815500 -0.26659800
 C -0.27723700 -3.73850200 0.66166400
 C -0.94391400 -4.17763700 -1.62002800
 C 1.07338600 -3.64815800 0.27072800
 C 0.40986400 -4.10525600 -1.98197300

C	1.44677600	-3.84877500	-1.07391900	H	1.75980900	6.29320000	-1.90684100
H	1.82728800	-3.51229700	1.03904400	H	0.41634700	5.69174000	-2.91347700
H	0.65559400	-4.27724400	-3.02666900	H	0.58820900	5.12666800	-1.21402400
C	-5.04491100	2.44346400	0.00512200	C	0.03566200	1.01970800	4.79113300
C	-4.46720200	3.29341900	-0.94419200	C	-0.73489600	1.19756500	3.63895100
C	-4.90777300	2.77232300	1.37340900	C	-0.15075400	1.71620000	2.48396400
C	-3.75618100	4.43515500	-0.57440400	C	1.22158900	2.01949200	2.46177500
H	-4.56462300	3.04108400	-1.99643800	C	1.98994100	1.83933700	3.62219200
C	-4.18547600	3.91884300	1.71778600	C	1.39270400	1.35363000	4.78561900
C	-3.59289600	4.77292100	0.77366900	H	-0.42139400	0.62526700	5.69468600
H	-3.32895200	5.05480300	-1.35542900	H	-1.78666300	0.92974200	3.62848500
H	-4.09816400	4.15701900	2.77536900	H	-0.74994000	1.87592000	1.59327400
C	-5.54092200	1.93920500	2.46443400	H	3.04294700	2.10381200	3.63237300
H	-6.58309200	1.69459300	2.22845700	H	1.98819300	1.23490300	5.68646600
H	-5.01067200	0.98936800	2.59600200	C	1.79094500	2.54320200	1.18349200
H	-5.52750300	2.47420700	3.41971800	O	1.17024300	3.35778400	0.50088700
C	2.91461300	-3.85335200	-1.53925500	C	3.08084500	2.00618600	0.65762800
C	3.27381400	-5.27117700	-2.04852900	C	3.59457200	2.58474100	-0.54410400
H	4.32015300	-5.30063000	-2.37414800	H	3.16505900	3.56701800	-0.72182800
H	3.14376900	-6.01663500	-1.25586100	C	5.00165000	2.43575300	-1.01259400
H	2.64798300	-5.56954100	-2.89658200	C	5.68705100	3.59477700	-1.41438100
C	3.11075500	-2.84051700	-2.69184200	C	5.66537100	1.19842000	-1.09296300
H	4.15336800	-2.85040900	-3.02864400	C	7.01356500	3.52202700	-1.83925300
H	2.47648200	-3.06721000	-3.55500600	H	5.17759100	4.55445000	-1.38622400
H	2.87351500	-1.82136900	-2.36323700	C	6.99073800	1.12361300	-1.51966600
C	3.89013000	-3.48904600	-0.40375600	H	5.15965200	0.27519500	-0.82943700
H	3.66161100	-2.50816100	0.03174000	C	7.66849500	2.28926800	-1.88814400
H	3.86945100	-4.23047200	0.40390500	H	7.53217500	4.42903300	-2.13718400
H	4.91586800	-3.43751200	-0.78142300	H	7.47438700	0.15148600	-1.54605400
C	-2.81998400	6.01879800	1.24311100	H	8.70129100	2.23480800	-2.22087300
C	-1.63125000	5.58784500	2.13545200	C	3.81819900	1.01910500	1.34645400
H	-1.08538100	6.47060800	2.49301200	N	4.47235100	0.20965000	1.87257100
H	-1.96856600	5.02815200	3.01416800	H	3.35374600	1.38158800	-2.71335600
H	-0.92951200	4.95164900	1.58427100	C	7.79518500	-2.64842600	0.42411100
C	-3.76412800	6.93779200	2.05513000	O	7.60445200	-2.57982300	1.70491700
H	-3.22844800	7.83369800	2.39346600	O	8.80858900	-3.47828000	0.04956100
H	-4.61671000	7.26062100	1.44637300	H	9.17555200	-3.84344700	0.87234700
H	-4.15989600	6.43210400	2.94192100	O	7.15841200	-2.05076500	-0.45232100
C	-2.26125900	6.83687500	0.06324700	Ag	6.00798900	-1.20996700	1.91362000
H	-1.56083800	6.24771700	-0.54002000	15			
H	-3.05761200	7.20068500	-0.59626400	C	-6.38633800	-1.55938000	1.80427700
H	-1.71958800	7.71102800	0.44296900	C	-5.63631500	-1.01100800	0.75229200
H	-0.53873200	-3.64038500	1.71245000	C	-4.45507300	-1.63542600	0.35678200
C	-1.98514200	-4.45895900	-2.67613800	C	-4.07207400	-2.87622600	0.90406900
H	-2.67440900	-5.24805300	-2.35595600	C	-4.87640400	-3.42460600	1.91583800
H	-2.58701600	-3.56388100	-2.87095900	C	-6.01295500	-2.76549000	2.38882200
H	-1.51819700	-4.76934900	-3.61594000	C	-7.54010500	-0.64603000	2.16187000
Ag	0.05592700	-1.14868100	0.32500400	C	-7.15634800	0.67008800	1.44874800
N	1.86615900	0.80015000	-1.48276000	C	-6.34452700	0.21676700	0.18924800
N	1.59420800	0.28425200	-0.48993400	H	-4.58474300	-4.37839500	2.34730500
C	2.55794000	1.78797600	-2.08648400	H	-6.59215900	-3.19200900	3.20426400
P	1.47968300	2.96569300	-3.07609000	H	-8.49449300	-1.04093300	1.78461800
O	1.64342000	2.69195800	-4.52133700	H	-6.49853100	1.26186700	2.09543200
O	0.03320100	2.79201200	-2.43736200	H	-8.01877100	1.29274200	1.18889000
O	2.01101900	4.37908800	-2.54223400	H	-7.65790800	-0.52118800	3.24459300
C	-1.11928200	2.31901600	-3.20567500	C	-7.33293200	-0.17470400	-0.96118700
H	-1.67345200	1.64646100	-2.55080300	H	-8.20456800	-0.72528500	-0.59267300
H	-1.72069400	3.19223100	-3.46861700	H	-6.80532000	-0.82103000	-1.67186000
H	-0.78276300	1.81483600	-4.11391100	C	-7.69276000	1.16312000	-1.64351000
C	1.11774100	5.43654600	-2.11495300	C	-6.43717700	1.98253800	-1.43542900

C	-5.61645000	1.38749200	-0.46480100	H	1.75368500	6.17753600	-2.02295500
C	-6.04317400	3.14998600	-2.08159900	H	3.15295400	6.09597400	-0.94717400
H	-6.67828800	3.61093400	-2.83431200	H	-1.95320200	-3.48003200	2.41919600
C	-4.81413300	3.72357600	-1.75321000	C	-3.71834600	-3.86428500	-1.91530200
H	-4.50031500	4.64577000	-2.23469000	H	-4.72242400	-4.09790800	-1.54313100
C	-3.94495400	3.12927600	-0.82350400	H	-3.73104500	-2.81971600	-2.24587100
C	-4.35658000	1.92945200	-0.21014400	H	-3.52246100	-4.49589600	-2.78789900
H	-8.56178800	1.63567500	-1.16324700	Ag	0.16000100	-0.94634800	0.74111700
H	-7.94656000	1.04255100	-2.70315800	N	2.35132400	-1.27916500	-1.22222100
O	-3.62768000	-1.00721000	-0.56518700	N	2.19771700	-1.14226000	-0.00275200
O	-3.49010900	1.26137300	0.64627400	C	3.68036500	-0.88136700	-1.68631600
P	-2.52022200	0.08305000	0.01140500	P	3.39867700	0.20384400	-3.18009800
O	-1.84770900	-0.49590600	1.26563400	O	3.14912300	-0.54837100	-4.43164000
O	-1.68142900	0.51794100	-1.14371100	O	2.27603000	1.24631500	-2.71365900
C	-2.83864000	-3.59557800	0.46890500	O	4.75514400	1.06949900	-3.08232200
C	-1.83192000	-3.85578000	1.40689800	C	0.89470300	1.18129200	-3.19475900
C	-2.67003100	-4.07886900	-0.84854600	H	0.23551400	0.94957900	-2.35672400
C	-0.67558200	-4.56480200	1.06991500	H	0.66101700	2.17007300	-3.59284400
C	-1.50640100	-4.78995700	-1.15992500	H	0.80941600	0.42969400	-3.98161500
C	-0.48705800	-5.05166400	-0.23045700	C	5.04911200	2.02464400	-4.12392600
H	0.06815900	-4.73972100	1.84022600	H	6.06485500	2.37522500	-3.93715100
H	-1.40652700	-5.16359200	-2.17615700	H	4.99235900	1.54652000	-5.10549300
C	-2.61904800	3.75790400	-0.55361600	H	4.34897100	2.86376400	-4.07178200
C	-1.72574400	3.92732500	-1.61648500	C	5.42862300	1.76846700	5.00581500
C	-2.24840000	4.24152900	0.72114800	C	4.15236900	2.29166900	4.77048000
C	-0.48275600	4.53476700	-1.44226300	C	3.41724900	1.86088000	3.67294900
H	-2.00454200	3.54846700	-2.59561700	C	3.94679100	0.88858000	2.80090800
C	-0.99827100	4.85036500	0.86915200	C	5.23052800	0.36902500	3.04340500
C	-0.08389200	5.00264000	-0.18519600	C	5.96617800	0.81363800	4.14060800
H	0.17233500	4.63025200	-2.30146700	H	6.00281900	2.10550400	5.86448000
H	-0.73737600	5.22483600	1.85650000	H	3.73402300	3.03404900	5.44364900
C	-3.16849200	4.13074200	1.91487300	H	2.42869900	2.25858800	3.47063500
H	-4.19195000	4.43134600	1.66269600	H	5.67026800	-0.36828600	2.38296600
H	-3.21609500	3.09817000	2.27889000	H	6.95807600	0.41001100	4.31984800
H	-2.82030100	4.76617500	2.73600800	C	3.10031000	0.49680200	1.65075600
C	0.74994900	-5.86441200	-0.65504700	O	2.08408500	1.10209100	1.34884900
C	0.30571400	-7.27972400	-1.09814900	C	3.48023600	-0.70125400	0.71862800
H	1.17385900	-7.87243200	-1.41302200	C	4.40440200	-0.23938900	-0.47063700
H	-0.18815200	-7.80994900	-0.27573800	H	4.27688800	0.84406900	-0.53838400
H	-0.39541200	-7.24070400	-1.93825800	C	5.88785200	-0.53710500	-0.37960400
C	1.45543500	-5.16105700	-1.83848900	C	6.79048200	0.52891700	-0.26244500
H	2.34092300	-5.73043600	-2.14856000	C	6.39322100	-1.84494000	-0.43428500
H	0.79874000	-5.06607700	-2.70894600	C	8.16458900	0.29683600	-0.19414700
H	1.77556500	-4.15067700	-1.55833500	H	6.41319900	1.54773600	-0.23263200
C	1.77070300	-6.02120700	0.48862600	C	7.76699300	-2.07770500	-0.36360100
H	2.14715800	-5.05426500	0.84186500	H	5.72045600	-2.69301700	-0.52483000
H	1.34462200	-6.55363400	1.34646300	C	8.65665700	-1.00826300	-0.24346300
H	2.63164000	-6.60177600	0.13692400	H	8.84840100	1.13651700	-0.10665000
C	1.27693700	5.67767400	0.06464300	H	8.13967100	-3.09705100	-0.40493400
C	2.01427300	4.96143900	1.22141700	H	9.72619000	-1.19160900	-0.19249300
H	2.99353000	5.42647200	1.39473600	C	3.90730500	-1.89751000	1.44759400
H	1.45088500	5.01866900	2.15867500	N	4.18018500	-2.87043800	2.02015500
H	2.16816900	3.90114400	0.99178900	H	4.17981800	-1.78112900	-2.06361300
C	1.05151000	7.16056000	0.44550700	16			
H	2.00934400	7.65947400	0.64199400	C	-5.40657100	-2.66271300	1.39766200
H	0.54657500	7.69970400	-0.36435400	C	-4.69241700	-1.85952800	0.49502000
H	0.43293300	7.25519200	1.34438800	C	-3.39671600	-2.22557500	0.13458000
C	2.18732300	5.63054400	-1.17803200	C	-2.84066100	-3.44760200	0.56222900
H	2.37853300	4.59981700	-1.49934800	C	-3.60604700	-4.25237000	1.42164300

C	-4.87123500	-3.86006500	1.86185000	H	3.50542500	-3.34563600	-0.72332800
C	-6.72384100	-2.01034600	1.75929800	H	3.52513100	-4.15801800	0.85094800
C	-6.52626400	-0.56273400	1.25764200	H	4.63838900	-4.68247100	-0.42568900
C	-5.56151500	-0.69427200	0.03094000	C	0.95666200	5.88262100	1.44645900
H	-3.18273400	-5.19416400	1.76032600	C	1.79099700	5.05432900	2.45284500
H	-5.42423000	-4.48291300	2.56077600	H	2.64713200	5.63845900	2.81350100
H	-7.56559900	-2.49914700	1.24795600	H	1.19926700	4.75570500	3.32417500
H	-6.02870400	0.03144900	2.03256900	H	2.17505100	4.14129700	1.98229600
H	-7.46370300	-0.05893000	1.00034600	C	0.44174000	7.16418100	2.14449700
H	-6.93704700	-2.06011400	2.83337600	H	1.28317100	7.76958100	2.50467700
C	-6.38417500	-1.06437700	-1.24914700	H	-0.14597200	7.77720800	1.45147500
H	-7.16902400	-1.79957800	-1.04348700	H	-0.19459400	6.93146700	3.00479600
H	-5.70386100	-1.49987000	-1.99000400	C	1.88510100	6.30680300	0.29238800
C	-6.92740100	0.28487700	-1.76988400	H	2.30224700	5.44033200	-0.23366100
C	-5.85296900	1.25885600	-1.33512800	H	1.36406600	6.93244800	-0.44125800
C	-5.00509900	0.66313400	-0.38847200	H	2.72440900	6.89066300	0.68791900
C	-5.62947900	2.56237200	-1.76765700	H	-0.78883300	-3.90535400	2.20673600
H	-6.28572000	3.02544600	-2.50069600	C	-2.08043100	-3.96248000	-2.30843300
C	-4.54688300	3.27337300	-1.24677100	H	-3.05698900	-4.40064700	-2.07281400
H	-4.37374300	4.30054800	-1.55611100	H	-2.24663700	-2.90051300	-2.52097600
C	-3.64737400	2.69129600	-0.33843000	H	-1.70504900	-4.43831100	-3.22031500
C	-3.87881300	1.35709100	0.05090100	Ag	1.03744000	-0.52312600	1.07861600
H	-7.89622200	0.52826800	-1.31062800	C	7.76130600	-1.72162100	2.58328500
H	-7.08467800	0.28708700	-2.85480400	C	6.71707400	-2.13327600	1.75316900
O	-2.63288700	-1.35724300	-0.63609500	C	6.21342300	-1.26820600	0.78158100
O	-2.95764400	0.70867800	0.86652400	C	6.76221000	0.01432700	0.62619900
P	-1.77151900	-0.17246000	0.12983000	C	7.83349100	0.40893400	1.44570100
O	-1.02746500	-0.78209500	1.33106700	C	8.31985500	-0.44878600	2.42731200
O	-1.00506300	0.56581000	-0.91618500	H	8.14470000	-2.39318900	3.34661400
C	-1.46888900	-3.88508200	0.16998300	H	6.29472000	-3.12851100	1.85665100
C	-0.51502600	-4.10770100	1.17510800	H	5.41829600	-1.61366500	0.12915600
C	-1.10535600	-4.14050600	-1.16758800	H	8.26682500	1.39279200	1.29854200
C	0.76892400	-4.55533700	0.87762700	H	9.13707400	-0.13015700	3.06816800
C	0.19490800	-4.59217200	-1.44219100	C	6.31386800	0.96924700	-0.42945400
C	1.15707900	-4.80850100	-0.44861600	O	7.09853900	1.76289500	-0.93041800
H	1.46777500	-4.71575900	1.69463000	C	4.86997500	0.98036900	-0.89051900
H	0.44130000	-4.79015000	-2.48034400	C	4.58675000	1.64796900	-2.05682100
C	-2.47735900	3.47765200	0.15063200	H	5.48604500	2.06134200	-2.51211400
C	-1.55798700	3.97447000	-0.77911300	C	3.36389500	1.90412300	-2.78478900
C	-2.28662500	3.78667700	1.51673300	C	3.49776400	2.59070000	-4.01649600
C	-0.45907300	4.74129700	-0.39130600	C	2.06482100	1.53183500	-2.36659800
H	-1.69588300	3.73199400	-1.82892100	C	2.38572300	2.88284200	-4.79597300
C	-1.17844200	4.55774400	1.88021500	H	4.48853700	2.88823800	-4.35055900
C	-0.23961100	5.04617400	0.95686300	C	0.95147800	1.82765900	-3.14449300
H	0.22610800	5.08836000	-1.15692900	H	1.89971500	1.01668900	-1.43137400
H	-1.05487000	4.79001800	2.93546300	C	1.11167100	2.50041200	-4.36128600
C	-3.25260300	3.32426700	2.58323600	H	2.50816400	3.40806200	-5.73877200
H	-4.29294300	3.50448600	2.28863600	H	-0.02466300	1.52697400	-2.77557200
H	-3.15067800	2.24886700	2.76698300	H	0.24163400	2.72950400	-4.97085500
H	-3.07157400	3.84969300	3.52664800	C	3.85831100	0.40047400	-0.08819300
C	2.57419600	-5.32737400	-0.75525800	N	3.00629800	-0.04750600	0.56628200
C	2.78484100	-6.68989300	-0.05183700	17-ts-1			
H	3.79211700	-7.07533800	-0.25408400	C	-5.85793300	-2.17379000	-1.16156000
H	2.66859500	-6.60861900	1.03406800	C	-4.69573100	-2.04649200	-0.38437700
H	2.05967600	-7.42941700	-0.40996900	C	-4.09189400	-0.79704600	-0.24961100
C	2.81848100	-5.52240300	-2.26364700	C	-4.70361200	0.35480200	-0.78529800
H	3.84127800	-5.87995400	-2.43038000	C	-5.88922200	0.19790700	-1.52058500
H	2.13596600	-6.26357700	-2.69421000	C	-6.45893600	-1.05784000	-1.73366800
H	2.69925600	-4.58546400	-2.81972700	C	-6.26713200	-3.62658000	-1.27139000
C	3.62215600	-4.31743700	-0.22839100	C	-4.99899300	-4.36445400	-0.79189200

C	-4.33268500	-3.38924600	0.23835700	H	-2.04213400	7.56685300	-1.36199600
H	-6.35926800	1.08392200	-1.93902900	C	4.64115700	-3.72639200	-2.55906700
H	-7.35698800	-1.15649400	-2.33838200	C	4.56488300	-2.58305700	-3.59899400
H	-7.12748900	-3.84693600	-0.62319900	H	5.51800200	-2.48830400	-4.13463000
H	-4.31310600	-4.50355600	-1.63520700	H	3.78029100	-2.76069500	-4.34186600
H	-5.20345200	-5.35013900	-0.36172900	H	4.34972200	-1.62498200	-3.11207200
H	-6.56081800	-3.90581800	-2.28985100	C	4.95441400	-5.05685300	-3.28444700
C	-4.99238900	-3.57566400	1.64492700	H	5.91050400	-4.98628800	-3.81834500
H	-6.08002300	-3.68798000	1.58610400	H	5.02374400	-5.88527300	-2.56995700
H	-4.77953000	-2.68851200	2.25240600	H	4.18167900	-5.31204400	-4.01693100
C	-4.27962600	-4.80636700	2.24976900	C	5.80516800	-3.42137300	-1.59654000
C	-2.90778300	-4.73890500	1.61162500	H	5.65340400	-2.47635000	-1.06255600
C	-2.90480300	-3.82622200	0.54621200	H	5.93671600	-4.21555400	-0.85241800
C	-1.74934100	-5.42796300	1.95693100	H	6.74081600	-3.33845300	-2.16175200
H	-1.74811900	-6.13957900	2.77916000	H	-3.75461600	1.97605000	-2.70284600
C	-0.58697900	-5.20609900	1.21820300	C	-4.60114500	1.65854900	1.90058600
H	0.31340600	-5.77067400	1.44380500	H	-5.58812500	1.20539300	1.75275500
C	-0.53202800	-4.25605600	0.18298700	H	-3.91615000	0.84797500	2.17562400
C	-1.70509000	-3.52796600	-0.10036400	H	-4.66963200	2.35294700	2.74434200
H	-4.79825900	-5.73871000	1.98434900	Ag	-0.93049400	1.92013900	-1.53994800
H	-4.23588900	-4.77288500	3.34474200	C	5.08281900	4.80929700	-3.47317600
O	-2.87034400	-0.69722000	0.40312500	C	4.09392900	5.28756200	-2.61179800
O	-1.67242100	-2.49430200	-1.02859800	C	3.71685900	4.54164500	-1.49417500
P	-1.48505300	-0.94441800	-0.49037300	C	4.33342900	3.31073900	-1.22466100
O	-1.58294400	-0.13621400	-1.78227400	C	5.34655300	2.85166500	-2.08150600
O	-0.34092200	-0.76287000	0.45657700	C	5.71017200	3.58884600	-3.20491100
C	-4.14808400	1.72854500	-0.60525300	H	5.36937200	5.38820500	-4.34717200
C	-3.71680800	2.45371000	-1.72697400	H	3.61761500	6.24471500	-2.80535900
C	-4.12868200	2.36823400	0.65297500	H	2.96160200	4.93501500	-0.82206700
C	-3.27341500	3.78044900	-1.62128800	H	5.83642400	1.91191900	-1.84877300
C	-3.68811600	3.69521000	0.73077800	H	6.48489900	3.21663600	-3.86975300
C	-3.25575200	4.43548200	-0.38036900	C	4.01425600	2.48262500	-0.01747200
H	-2.97638000	4.30047200	-2.52570700	O	4.90402400	1.79469400	0.50208200
H	-3.70156000	4.17100700	1.70814600	C	2.66250300	2.47172500	0.56674700
C	0.74930200	-4.06587000	-0.55518900	C	2.52981200	1.87029000	1.86430000
C	1.91407800	-3.79885600	0.17512200	H	3.49644200	1.82826700	2.35896400
C	0.86048000	-4.24172200	-1.95479300	C	1.41621700	2.18003300	2.80866100
C	3.16245700	-3.68987500	-0.43887200	C	1.76852000	2.71763600	4.05820500
H	1.83786300	-3.65755300	1.24928300	C	0.05911200	1.97130400	2.51497800
C	2.12247000	-4.12127800	-2.54566600	C	0.78499900	3.08883300	4.97387300
C	3.29381100	-3.84279900	-1.82399300	H	2.81810200	2.83888700	4.30915600
H	4.02513400	-3.47487500	0.18192200	C	-0.92041700	2.33061400	3.44044300
H	2.18540200	-4.26703900	-3.62153100	H	-0.23467400	1.47745000	1.59401500
C	-0.32763700	-4.58681900	-2.82285800	C	-0.56330900	2.90040000	4.66488900
H	-0.95092400	-5.36056600	-2.35999100	H	1.07401800	3.51098100	5.93246200
H	-0.96700500	-3.71224200	-2.98361000	H	-1.96471100	2.15174100	3.20388700
H	0.00034000	-4.95540500	-3.80024800	H	-1.33122000	3.17804600	5.38219000
C	-2.82289500	5.90284100	-0.20989200	C	1.54188700	2.90465100	-0.15039200
C	-4.02490200	6.72742200	0.31145400	N	0.58635700	3.24618800	-0.74406200
H	-3.73838900	7.77862700	0.43909300	N	2.58839300	-0.34615300	0.36722400
H	-4.86466500	6.68713900	-0.39210700	N	2.74616500	-0.18300300	-0.73393200
H	-4.38167300	6.35933200	1.27922800	C	2.38917500	-0.12572000	1.68427400
C	-1.65916100	5.99193600	0.80600900	H	1.34847800	-0.37214600	1.91152100
H	-1.36075300	7.03837900	0.94620000	P	3.62984000	-0.86809400	2.82241900
H	-1.93851900	5.59214100	1.78635500	O	4.03788800	0.03020600	3.92984600
H	-0.78875500	5.42951600	0.45201300	O	2.83016700	-2.20213900	3.23246600
C	-2.34970900	6.52944000	-1.53569400	O	4.81849000	-1.40786200	1.88330900
H	-1.48925800	5.99460200	-1.95363100	C	3.33282100	-3.01518200	4.31519600
H	-3.14568300	6.54542100	-2.28938400	H	3.49244300	-2.40320200	5.20658900

H	2.56733900	-3.76766200	4.50619200
H	4.26664500	-3.50247400	4.01836100
C	6.13889700	-0.79651800	1.91204900
H	6.80997600	-1.53753100	1.47556400
H	6.12461100	0.11789800	1.31949500
H	6.43048600	-0.57833200	2.94123600

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C	-1.92477800	5.97062200	-0.28569900
C	-1.81441200	4.73129700	0.36257500
C	-0.61717700	4.01929400	0.29934700
C	0.52595700	4.59751900	-0.28991200
C	0.39276300	5.86251000	-0.88892000
C	-0.82524300	6.54088200	-0.91805900
C	-3.34041000	6.49707300	-0.18926200
C	-4.12754100	5.25255200	0.27598200
C	-3.10005500	4.42126600	1.11635700
H	1.27054200	6.31085900	-1.34636400
H	-0.90574600	7.50051300	-1.42253000
H	-3.41149300	7.31305600	0.54425900
H	-4.42885500	4.65928400	-0.59484100
H	-5.03193400	5.49536500	0.84303400
H	-3.70609300	6.89809000	-1.14166400
C	-3.04435800	4.97205800	2.58100900
H	-3.07327100	6.06596800	2.61802100
H	-2.10488000	4.64637700	3.04203500
C	-4.23634100	4.30107500	3.29700300
C	-4.36522300	2.98684500	2.55745000
C	-3.61696400	3.01027200	1.37086200
C	-5.08902600	1.85530200	2.91751000
H	-5.67002300	1.83334900	3.83640800
C	-5.07523800	0.75094600	2.06695300
H	-5.67238800	-0.12430100	2.30705300
C	-4.30063600	0.72122900	0.89324500
C	-3.52280700	1.85601800	0.59089600
H	-5.15120700	4.90295600	3.19972000
H	-4.06269200	4.16570100	4.37101600
O	-0.57175900	2.72653400	0.80363500
O	-2.64398500	1.83479300	-0.48892100
P	-1.05645900	1.48089900	-0.19387400
O	-0.39858200	1.67093200	-1.55852900
O	-0.86745600	0.22606100	0.59931700
C	1.87360400	3.95664800	-0.31034600
C	2.50707300	3.74404300	-1.55176700
C	2.60604500	3.68527500	0.86424200
C	3.83468200	3.31702700	-1.63613200
C	3.93935100	3.25711600	0.74908400
C	4.59261200	3.08040700	-0.47666300
H	4.28119100	3.19929800	-2.61941100
H	4.48213900	3.08530000	1.67269000
C	-4.38149200	-0.50202600	0.04185700
C	-4.06066200	-1.74216900	0.61431700
C	-4.91623000	-0.48504900	-1.26266600
C	-4.28217500	-2.94003100	-0.05781300
H	-3.62274600	-1.75645800	1.60806600
C	-5.13794600	-1.70746900	-1.91837800
C	-4.84754200	-2.95183200	-1.34318600
H	-4.00442000	-3.86985700	0.42820500
H	-5.57728900	-1.66481700	-2.91022600
C	-5.29274800	0.80497000	-1.95444700
H	-5.91066500	1.44086800	-1.30929100

H	-4.40184400	1.38580700	-2.21884900
H	-5.85514000	0.60626000	-2.87256800
C	6.08334700	2.71087200	-0.58620500
C	6.84892000	3.91771100	-1.18298500
H	7.91723600	3.68561700	-1.27540400
H	6.47566900	4.17856900	-2.17922600
H	6.74633100	4.80299100	-0.54483900
C	6.70640700	2.37797200	0.78329900
H	7.75749200	2.09714900	0.65017600
H	6.68157600	3.23392100	1.46717600
H	6.19420600	1.53943900	1.26985300
C	6.26958400	1.48539000	-1.51054100
H	5.73505600	0.61112400	-1.12559800
H	5.90229800	1.67707300	-2.52404600
H	7.33391100	1.23150500	-1.58933100
C	-5.16026700	-4.29419600	-2.03139200
C	-3.88014800	-5.15829000	-2.12501600
H	-4.11826100	-6.13843500	-2.55731100
H	-3.12936600	-4.68047300	-2.76347700
H	-3.41934900	-5.32472600	-1.14635100
C	-5.72187700	-4.11127400	-3.45421100
H	-5.91507500	-5.09241700	-3.90318600
H	-6.66780800	-3.55739900	-3.45480500
H	-5.01625500	-3.58297600	-4.10589200
C	-6.21931400	-5.04740800	-1.18946400
H	-5.85728000	-5.25014200	-0.17597900
H	-7.14260900	-4.46223100	-1.10517600
H	-6.46637400	-6.00914900	-1.65655000
H	1.95442700	3.96392200	-2.46213000
C	2.01063400	3.89215900	2.23714600
H	1.55337000	4.88447000	2.32708100
H	1.22303300	3.15772100	2.43787100
H	2.77644500	3.79784700	3.01354000
Ag	1.67490600	1.02141000	-1.55518200
C	7.74203800	-2.92084900	1.19441400
C	6.84346400	-1.85297400	1.18843900
C	5.48268700	-2.07907500	0.97425200
C	5.00621700	-3.38286300	0.77157700
C	5.91536700	-4.45333300	0.80553500
C	7.27399600	-4.22399000	1.00306400
H	8.80159100	-2.73979100	1.35467100
H	7.19878000	-0.84025600	1.35616900
H	4.79797000	-1.23885600	0.99842300
H	5.53282800	-5.46009000	0.67482400
H	7.96810400	-5.06001000	1.01313500
C	3.55986800	-3.73127900	0.57008600
O	3.15249400	-4.83191600	0.95924000
C	2.63808400	-2.83071500	-0.14393800
C	1.28202600	-3.24915200	-0.34221500
C	2.99377300	-1.58797200	-0.70305300
N	3.14329600	-0.53821800	-1.20284900
N	1.09911300	-1.92469600	1.96622000
N	2.12676500	-1.59970600	2.30606700
C	0.14965100	-2.47815800	1.18592000
H	-0.45647000	-1.65933900	0.76037400
P	-0.79705700	-3.80907800	2.02776200
O	-1.50945500	-4.69874600	1.07888300
O	0.25240300	-4.52092200	3.01313900
O	-1.67047600	-2.91924100	3.04238400
C	0.72746400	-5.87758100	2.79393500

H	0.00383000	-6.43872100	2.19892100	C	-1.66539200	4.94706000	-0.47363800
H	1.69050200	-5.82884300	2.28581300	H	-1.38541100	4.61558400	-2.59542200
H	0.83042900	-6.32509700	3.78421800	H	-2.29549900	5.03042100	1.58564300
C	-2.52699700	-3.56603500	4.00804500	C	-2.13674700	-3.98790200	0.31740100
H	-1.92411300	-4.12828500	4.72699100	C	-1.07880100	-3.97065100	1.23781600
H	-3.06379300	-2.76505900	4.51686400	C	-1.87138900	-4.40085700	-1.00387400
H	-3.23684500	-4.23052000	3.50732300	C	0.21225700	-4.33389000	0.87022400
H	1.14032800	-4.28126500	-0.02327600	H	-1.27551600	-3.63703200	2.25242600
C	0.56403500	-2.88305600	-1.61620000	C	-0.56067300	-4.76178900	-1.35029200
C	-0.81034000	-2.62124000	-1.70517300	C	0.50554700	-4.73357800	-0.44338300
C	1.31194500	-2.90129400	-2.81090400	H	0.99831800	-4.29423800	1.61980900
C	-1.40355500	-2.32897200	-2.93437600	H	-0.38817800	-5.08127400	-2.37308600
H	-1.44249300	-2.63702400	-0.82724100	C	-2.95852800	-4.47750000	-2.05144200
C	0.71374000	-2.63240200	-4.04067900	H	-3.86088400	-4.96172400	-1.66070100
H	2.36785700	-3.14835600	-2.77836100	H	-3.25007600	-3.47645600	-2.38918100
C	-0.64667400	-2.32923200	-4.10607100	H	-2.61925700	-5.04524300	-2.92422700
H	-2.46306600	-2.09659100	-2.96094000	C	-0.49481600	5.92510300	-0.26329800
H	1.31601900	-2.66015300	-4.94489100	C	-1.03777900	7.27894200	0.25448200
H	-1.11376600	-2.10256900	-5.06058200	H	-0.21378700	7.98534000	0.41667300
17-ts-3				H	-1.73082800	7.72470300	-0.46843000
C	-7.11512000	0.43847700	-1.50947000	H	-1.57257400	7.16640400	1.20326300
C	-6.14449100	0.08882100	-0.55753000	C	0.48972100	5.33900900	0.77675200
C	-5.06178800	0.94069800	-0.34296500	H	1.32030300	6.03524200	0.95073100
C	-4.98609400	2.19542000	-0.98087600	H	0.00371000	5.14972300	1.73906600
C	-6.00292100	2.53377800	-1.88812000	H	0.90838000	4.38856900	0.42579400
C	-7.05280700	1.65927700	-2.17400300	C	0.28623600	6.19130600	-1.56444100
C	-8.11663100	-0.68360300	-1.68081300	H	0.71826900	5.27144500	-1.97523900
C	-7.39754700	-1.87375900	-1.00901100	H	-0.34725700	6.64512200	-2.33524500
C	-6.52306900	-1.22654000	0.11827100	H	1.11179900	6.88470600	-1.36486400
H	-5.94861500	3.49699200	-2.38830900	C	1.94649200	-5.11290400	-0.83236200
H	-7.80460300	1.93028900	-2.91139800	C	2.87197100	-3.89271900	-0.60726800
H	-9.06547100	-0.45350300	-1.17491600	H	3.91050700	-4.13098700	-0.86959000
H	-6.73280700	-2.35871200	-1.73296200	H	2.54867600	-3.04657200	-1.22623800
H	-8.08224000	-2.63535600	-0.62172100	H	2.85418100	-3.56611300	0.43777700
H	-8.35945600	-0.87487600	-2.73259100	C	2.06976700	-5.53912000	-2.30752700
C	-7.40006800	-0.99437300	1.39436800	H	3.11169800	-5.79569200	-2.53162800
H	-8.40161900	-0.62424700	1.15171600	H	1.45595300	-6.41953400	-2.52935200
H	-6.91007700	-0.24434200	2.02569300	H	1.77206700	-4.73512000	-2.99030800
C	-7.40779400	-2.35985900	2.11833300	C	2.43042400	-6.28954000	0.04833700
C	-6.06274300	-2.94061000	1.73531900	H	2.40300300	-6.03843100	1.11383600
C	-5.50441500	-2.22089700	0.66783200	H	1.80008600	-7.17379200	-0.10128100
C	-5.37543400	-4.00493200	2.31104900	H	3.46316900	-6.55988100	-0.20563700
H	-5.80650100	-4.56283700	3.13897400	H	-3.25162600	3.04693700	-2.81850900
C	-4.11752900	-4.34943000	1.81233900	C	-4.41008700	3.41138300	1.71702700
H	-3.57808200	-5.19199900	2.23654000	H	-5.48047400	3.47839400	1.49057000
C	-3.50525300	-3.61680100	0.78271700	H	-4.22131200	2.39665700	2.08442900
C	-4.20970100	-2.52066200	0.24731700	H	-4.18957600	4.11522000	2.52646700
H	-8.23315000	-2.99418100	1.76399200	Ag	-0.25930000	0.79853100	-1.18299400
H	-7.53060000	-2.26213600	3.20335100	C	-0.15469300	2.04242800	4.23526900
O	-4.03446100	0.53645100	0.49791600	C	-0.04283200	1.10573200	3.20545700
O	-3.59308200	-1.70261800	-0.69120900	C	1.18088000	0.93776400	2.55595200
P	-2.79602700	-0.37088400	-0.12173000	C	2.29896400	1.70470200	2.92499000
O	-2.28619500	0.27864500	-1.41828000	C	2.18066800	2.62034800	3.98579100
O	-1.85025300	-0.64193800	0.99986900	C	0.95834900	2.79455000	4.62809600
C	-3.84739800	3.13469400	-0.76050600	H	-1.10849300	2.18319500	4.73697300
C	-3.04572400	3.49381200	-1.84995600	H	-0.89126800	0.51017800	2.87976800
C	-3.56752300	3.71146900	0.49875800	H	1.25019600	0.18143300	1.78326400
C	-1.97437900	4.37891300	-1.71581600	H	3.05460400	3.19013100	4.28474600
C	-2.48930700	4.59555300	0.60781900	H	0.87164700	3.51592200	5.43633100

C	3.63813400	1.57507700	2.28170700	C	-3.17944300	-3.37395600	0.10696500
O	4.67273400	1.75155700	2.93584100	C	-3.77058500	-2.11982500	-0.14772300
C	3.78586500	1.23463200	0.83590400	H	-7.60794900	-2.34193100	1.84698800
C	5.11998800	1.23179300	0.31747900	H	-6.63560800	-1.93035800	3.25569500
C	2.67460400	1.18623200	-0.02854200	O	-3.15708700	0.83675600	0.50615100
N	1.73582500	1.19558000	-0.72019400	O	-3.16062900	-1.23658800	-1.02983500
N	4.95476000	-1.12526400	1.53008900	P	-2.13545800	-0.10670500	-0.39787100
N	3.82756200	-1.24187300	1.63608100	O	-1.70841300	0.67153800	-1.64840300
C	6.02758900	-0.36609100	1.16519500	O	-1.11948400	-0.66015800	0.54628800
P	7.24181800	-1.31776600	0.15757000	C	-2.79183200	3.56909200	-0.42121200
O	6.62620800	-2.15843500	-0.88803400	C	-2.05795900	3.95899700	-1.54765300
O	8.20808500	-0.11111100	-0.28318100	C	-2.34306700	3.98816500	0.85076400
O	8.09233700	-2.17854500	1.22200700	C	-0.89967300	4.73290600	-1.44006400
C	8.82256600	-0.12038300	-1.59620200	C	-1.18321200	4.76616600	0.93268600
H	8.09496200	-0.42021700	-2.35189300	C	-0.43376200	5.15703700	-0.18876100
H	9.15634200	0.90087300	-1.77732600	H	-0.37464200	5.00737200	-2.34864300
H	9.67659600	-0.80334800	-1.60055600	H	-0.86374500	5.08779400	1.92094500
C	8.96923600	-1.58994700	2.19849500	C	-1.95508300	-3.85023000	-0.59983400
H	8.39226500	-1.10303000	2.99318500	C	-0.84010500	-4.22204100	0.16015600
H	9.54284700	-2.41293100	2.62630200	C	-1.89074500	-4.00691300	-2.00392700
H	9.64260800	-0.86596900	1.73256500	C	0.32438300	-4.71660000	-0.42654400
H	5.77200200	1.88165700	0.89751100	H	-0.88336900	-4.10475600	1.23894400
C	5.38303800	1.25166600	-1.14755100	C	-0.71113800	-4.50224400	-2.56851800
C	6.16654200	2.29588000	-1.66758800	C	0.41776200	-4.86230100	-1.81527700
C	4.84461900	0.30377700	-2.03222300	H	1.15615100	-4.98081200	0.21759500
C	6.38048900	2.40963300	-3.04053700	H	-0.68599100	-4.61908300	-3.64942500
H	6.59158400	3.03271900	-0.99038800	C	-3.05950200	-3.68102000	-2.90502300
C	5.07242400	0.40978400	-3.40429100	H	-4.00258400	-4.05662700	-2.49173000
H	4.26602700	-0.53200000	-1.65307600	H	-3.17068100	-2.59836900	-3.02930300
C	5.83263100	1.46545900	-3.91306100	H	-2.92203700	-4.12672900	-3.89563300
H	6.97205100	3.23450400	-3.42818600	C	0.81910600	6.03484800	-0.01122100
H	4.65431600	-0.33558800	-4.07431800	C	0.41454200	7.37835800	0.64219400
H	5.99995100	1.55004600	-4.98321800	H	1.29587000	8.01766600	0.77834500
H	6.43014500	0.11357600	2.06078200	H	-0.30397800	7.91909900	0.01530100
17-ts-4				H	-0.04561400	7.22942900	1.62458000
C	-6.43871700	1.38375000	-1.06810600	C	1.84047100	5.31042300	0.89713400
C	-5.41684300	0.79157300	-0.30908300	H	2.73086200	5.93562000	1.04197300
C	-4.21410000	1.47479200	-0.13202500	H	1.42577000	5.08531000	1.88478000
C	-4.05156200	2.79042000	-0.61037500	H	2.15645800	4.36234100	0.44778400
C	-5.11375500	3.36921100	-1.32320400	C	1.51006700	6.34420500	-1.35314600
C	-6.29568600	2.67114400	-1.57478000	H	1.84005100	5.42987700	-1.85984300
C	-7.59405100	0.42243100	-1.24513600	H	0.85238700	6.89544000	-2.03497900
C	-6.96505700	-0.92743800	-0.83871600	H	2.39632100	6.96484900	-1.17661000
C	-5.88205100	-0.55769000	0.23207500	C	1.67665700	-5.39484900	-2.52338900
H	-4.99165700	4.38149900	-1.69892500	C	2.22218000	-4.31392000	-3.48707700
H	-7.08679800	3.12862300	-2.16385900	H	3.11494200	-4.68044900	-4.00968500
H	-8.43595100	0.68499200	-0.58839300	H	1.48138900	-4.03577100	-4.24361500
H	-6.46305300	-1.37479300	-1.70414300	H	2.49685600	-3.40525900	-2.93881300
H	-7.69389000	-1.65323700	-0.46365300	C	1.32184800	-6.66659900	-3.33074000
H	-7.98419700	0.41652800	-2.26948600	H	2.21171800	-7.05678700	-3.84052300
C	-6.55760300	-0.42278600	1.63754300	H	0.93397200	-7.45288200	-2.67284300
H	-7.52165800	0.09420600	1.59089600	H	0.56251000	-6.46562000	-4.09358500
H	-5.89754300	0.15943800	2.29082900	C	2.79573600	-5.75934900	-1.52888200
C	-6.66455600	-1.87303500	2.16121900	H	3.11818800	-4.89040600	-0.94351600
C	-5.47275000	-2.54500100	1.51220100	H	2.48154800	-6.54324300	-0.83021100
C	-4.94909800	-1.73668600	0.49169700	H	3.66981400	-6.13260200	-2.07529400
C	-4.88533300	-3.76879900	1.81879600	H	-2.39599900	3.63461000	-2.52785900
H	-5.29121800	-4.39938400	2.60627500	C	-3.10014900	3.63731000	2.11096100
C	-3.76658100	-4.18348400	1.09451500	H	-4.16609000	3.87583300	2.01700500
H	-3.31757000	-5.15145200	1.29985900	H	-3.03107100	2.56541700	2.32910200

H	-2.70454900	4.18827300	2.97068300	H	8.54386700	-1.66350800	-1.31064400
Ag	0.29859400	1.32982500	-1.58077800	H	6.44109300	-3.12238700	0.37070600
C	7.08486900	1.85715600	-4.04293600	H	7.11810500	-3.65842700	-1.17317800
C	6.13802300	2.62609800	-3.36405500	H	8.53138100	-1.91105000	0.43336000
C	5.63307000	2.19381000	-2.13719100	C	5.84965600	-2.01484700	-2.86773600
C	6.07830700	0.98754100	-1.57538100	H	6.89298900	-1.80727500	-3.12701200
C	7.05170800	0.23492000	-2.25270600	H	5.23086400	-1.22844500	-3.31512100
C	7.54274300	0.66019400	-3.48359700	C	5.36340100	-3.40217700	-3.34857400
H	7.47071300	2.19235200	-5.00195100	C	4.28211900	-3.74133500	-2.34335700
H	5.79444100	3.56646300	-3.78577900	C	4.33181800	-2.86006600	-1.25299400
H	4.91477300	2.81371400	-1.61165400	C	3.32401000	-4.75039700	-2.39370000
H	7.41014100	-0.68095200	-1.79449300	H	3.28867000	-5.44355400	-3.23089300
H	8.28536800	0.06352700	-4.00614400	C	2.42066100	-4.88019700	-1.33673700
C	5.61829100	0.48554500	-0.24362100	H	1.70188300	-5.69493100	-1.33587500
O	6.37457700	-0.21462100	0.44547900	C	2.39776500	-3.97319600	-0.26192100
C	4.27128400	0.78288800	0.27593700	C	3.33825400	-2.92334100	-0.27617700
C	4.05256400	0.52998700	1.68470900	H	6.17641400	-4.14139700	-3.32548100
H	4.98252600	0.65357000	2.23819600	H	4.98818900	-3.38298600	-4.37853400
C	2.87404600	1.09648700	2.40614500	O	3.49526500	0.14638200	-0.85658600
C	3.11894100	1.90237000	3.53018900	O	3.27020800	-1.92404000	0.68767400
C	1.54553900	0.88139400	2.00509000	P	2.50670700	-0.51423600	0.30541900
C	2.06639600	2.50591900	4.21576400	O	2.64005300	0.28585500	1.59770200
H	4.14101700	2.05812600	3.86606100	O	1.17962800	-0.70280200	-0.36290700
C	0.49103600	1.47358500	2.69950400	C	4.27477000	2.79446000	0.07409800
H	1.30323900	0.22584800	1.17649600	C	3.94357000	3.26931200	1.35187600
C	0.74941700	2.29309500	3.80112800	C	3.75707000	3.47577400	-1.04831700
H	2.27530000	3.13028200	5.08004500	C	3.11617800	4.38880100	1.53138800
H	-0.52303000	1.27406900	2.36774600	C	2.94710900	4.60086500	-0.84416300
H	-0.07313800	2.75385100	4.34170800	C	2.60549700	5.09024100	0.42614700
C	3.22749400	1.26058700	-0.53068800	H	2.92157700	4.73189000	2.54195300
N	2.33058300	1.66123800	-1.16768800	H	2.58484300	5.12441200	-1.72540600
N	3.83250300	-1.90199200	0.71913100	C	1.39629100	-4.15181800	0.82944000
N	3.63714300	-1.81564800	-0.39229100	C	0.03984700	-4.25112700	0.49520900
C	4.10765100	-1.39623500	1.95744700	C	1.76584100	-4.31022900	2.18657200
H	5.17469200	-1.54044900	2.14076700	C	-0.94270300	-4.47557100	1.46013400
P	3.04843200	-2.09928900	3.30306500	H	-0.25909700	-4.13447400	-0.54176400
O	3.20399100	-1.36349000	4.57739000	C	0.75995000	-4.53105800	3.13255000
O	1.66488100	-2.15306000	2.52976400	C	-0.60406200	-4.61313200	2.81085100
O	3.46938500	-3.66062800	3.35244100	H	-1.97643800	-4.53948100	1.13750500
C	0.37030200	-2.11377500	3.19540200	H	1.06851600	-4.65702700	4.16779000
H	0.40302100	-1.40519300	4.02531300	C	3.20665300	-4.28078700	2.64207900
H	-0.33392100	-1.78447000	2.43129900	H	3.85493700	-4.84504800	1.96202900
H	0.13036200	-3.11675600	3.55746100	H	3.58985900	-3.25520900	2.67697200
C	4.47809400	-4.11148400	4.27905500	H	3.30539100	-4.71564400	3.64196300
H	4.34258100	-5.18958300	4.37647700	C	1.75061600	6.36350100	0.56280500
H	5.47809500	-3.90583000	3.88064100	C	2.51759800	7.55405400	-0.06292100
H	4.35737200	-3.62413000	5.249064001	H	1.92430900	8.47300300	0.01843900
17-ts-5				H	3.47314800	7.72008300	0.44793400
C	7.08176400	-0.44122100	-0.27816800	H	2.73019000	7.38683500	-1.12414600
C	5.75792600	-0.64223300	-0.70040600	C	0.40355300	6.17803200	-0.17502200
C	4.82650600	0.38330500	-0.54326700	H	-0.20028600	7.08990500	-0.09132700
C	5.22222100	1.64732400	-0.06181600	H	0.54221200	5.96961200	-1.24074500
C	6.56311900	1.82659100	0.31248300	H	-0.16687400	5.34833600	0.25607200
C	7.49148400	0.78822300	0.22700600	C	1.44581800	6.70600100	2.03390600
C	7.88673200	-1.71309600	-0.43057100	H	0.89203100	5.90164800	2.53200900
C	6.78649500	-2.77970500	-0.61123400	H	2.35831500	6.90390500	2.60812500
C	5.60825300	-2.02693900	-1.32216100	H	0.82860800	7.61026600	2.07985300
H	6.87047200	2.79860000	0.68910600	C	-1.64313200	-4.85650400	3.91997500
H	8.51594100	0.94153900	0.55669400	C	-1.56156100	-3.71556500	4.96199700

H -2.29392300 -3.87596600 5.76333100
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 H 5.15996700 2.88234800 -2.58726100
 H 3.60080500 2.06694300 -2.67939700
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 C -4.31167800 3.07921300 5.24594600
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 C -3.66195900 3.33736700 2.93028500
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 H -4.43172400 3.49824200 6.24121400
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 H -3.30664700 3.97197800 2.12486500
 H -4.78670700 0.18105700 3.52314300
 H -5.03599200 1.12492100 5.80769500
 C -3.89559000 1.38941500 1.31964200
 O -4.84163700 0.63340100 0.98086200
 C -2.75437100 1.68052300 0.46636500
 C -2.71027000 1.24591300 -0.89686000
 H -3.66272500 0.84571800 -1.23539100
 C -1.97747400 1.90467600 -2.00081000
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 C -0.62900900 2.30113700 -1.94186500
 C -2.12908200 2.83787500 -4.23819500
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 C -0.04523700 2.96160200 -3.01915900
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 C -0.79607100 3.24325900 -4.16476900
 H -2.71347900 3.03546000 -5.13219800
 H 1.00043400 3.24823700 -2.96360000
 H -0.33607800 3.76160900 -5.00207900
 C -1.62154000 2.30588300 1.02785100
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 C -1.73457800 -0.68119800 -0.89371400
 H -0.68100700 -0.41341900 -1.04612200
 P -2.43469300 -1.76630200 -2.19567400
 O -2.83296800 -1.00019900 -3.39834000
 O -1.33308600 -2.91720600 -2.44004400
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 C -0.13944900 -2.60959500 -3.20567000
 H 0.53910700 -2.00368300 -2.59778100
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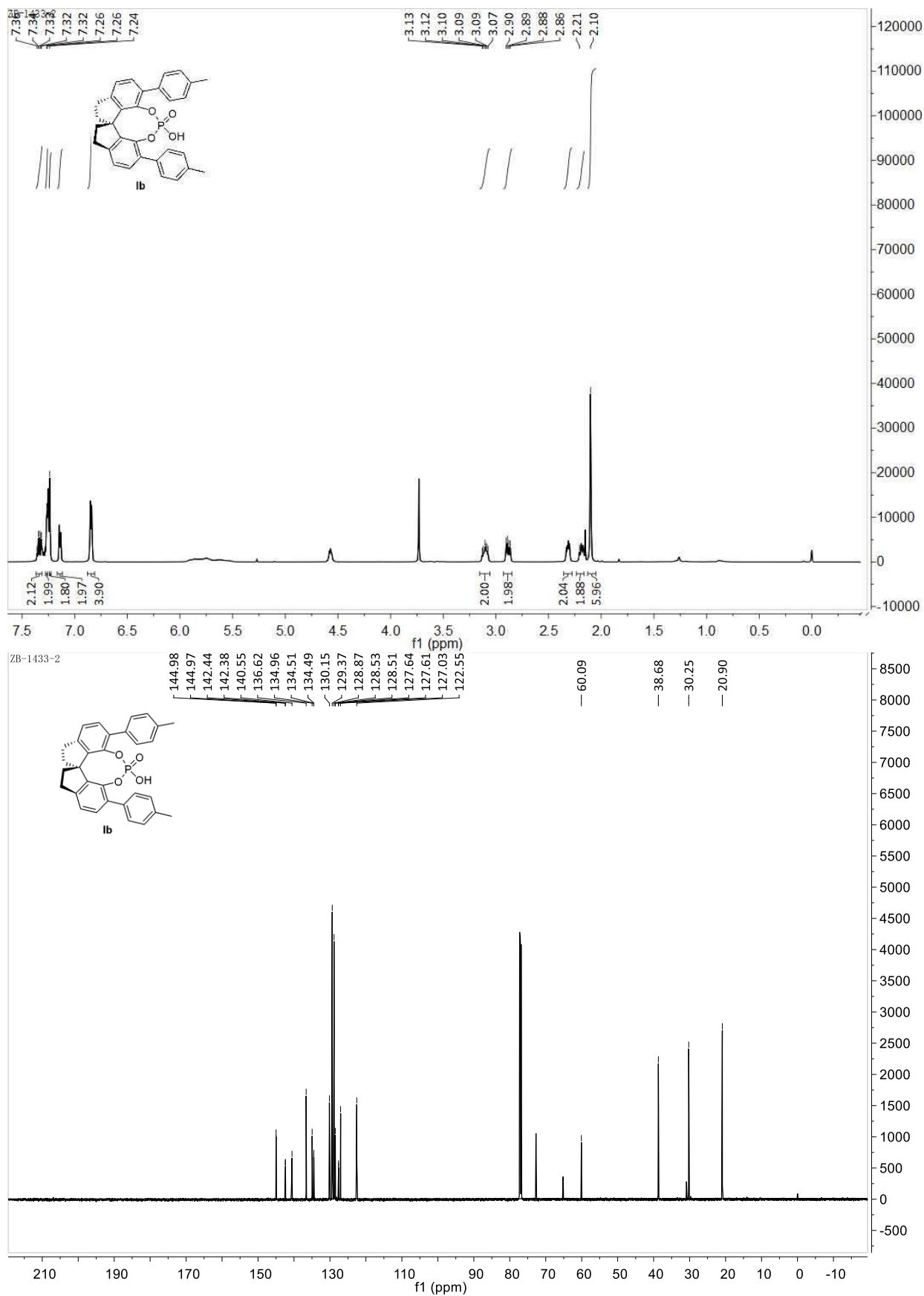
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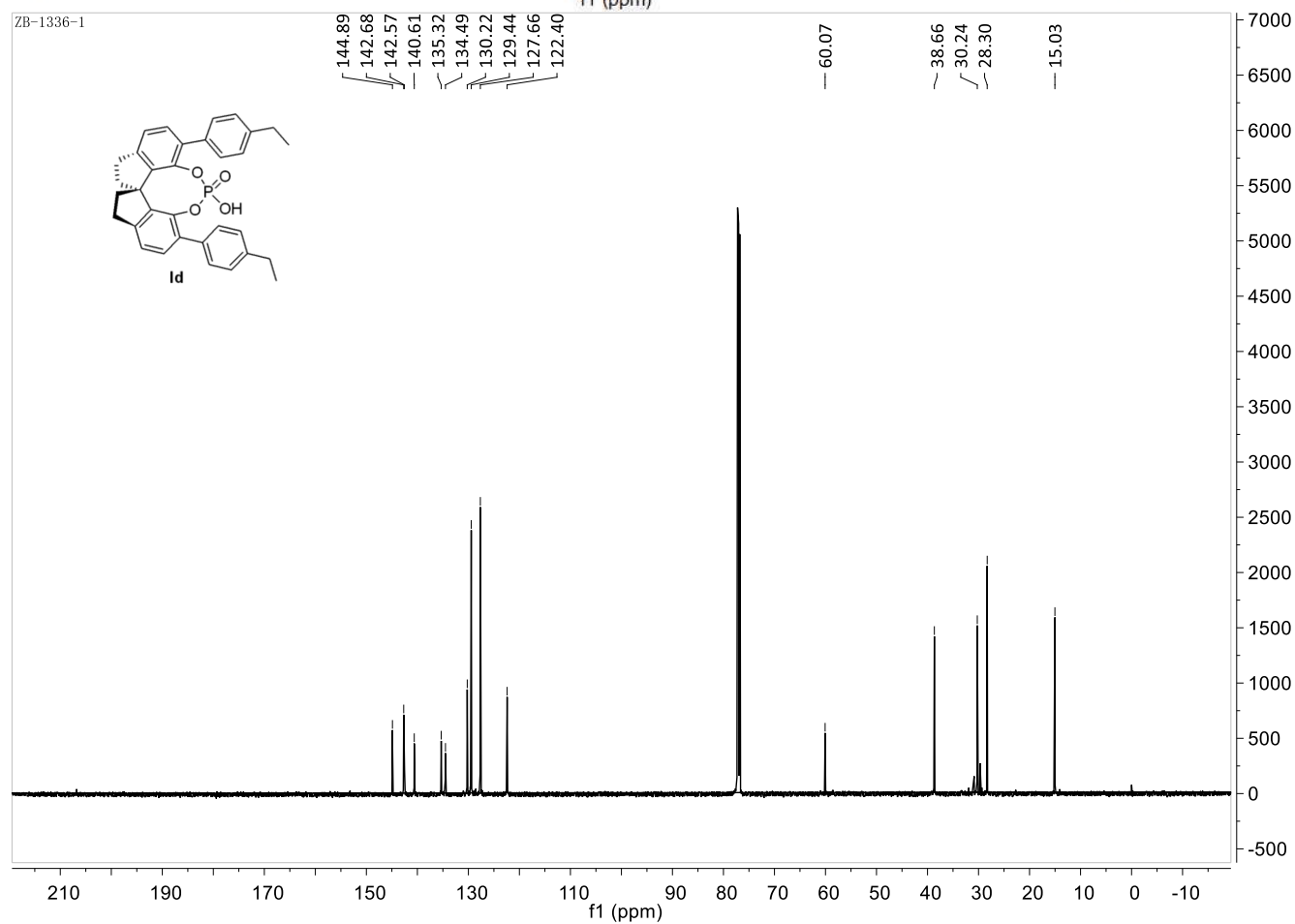
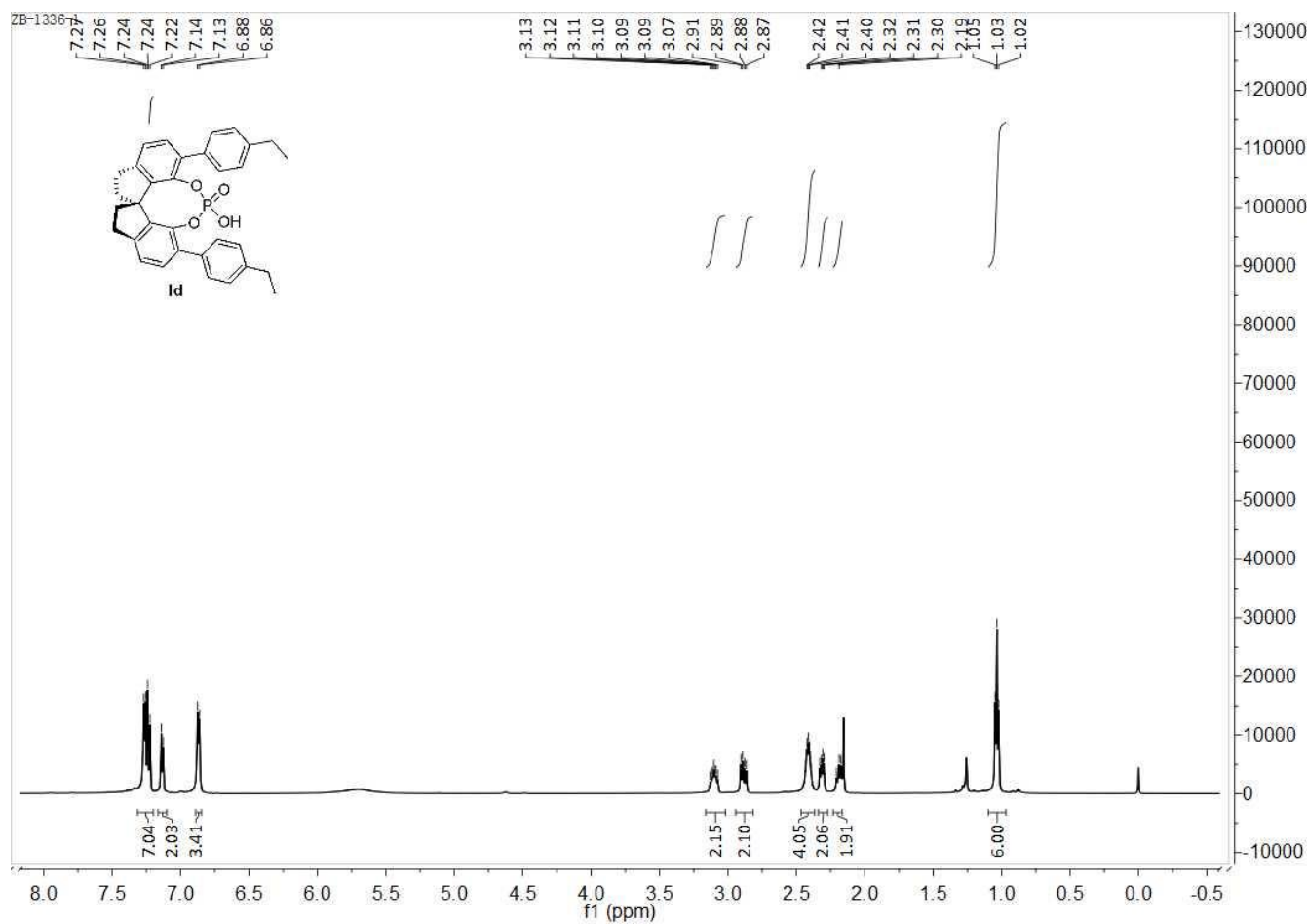
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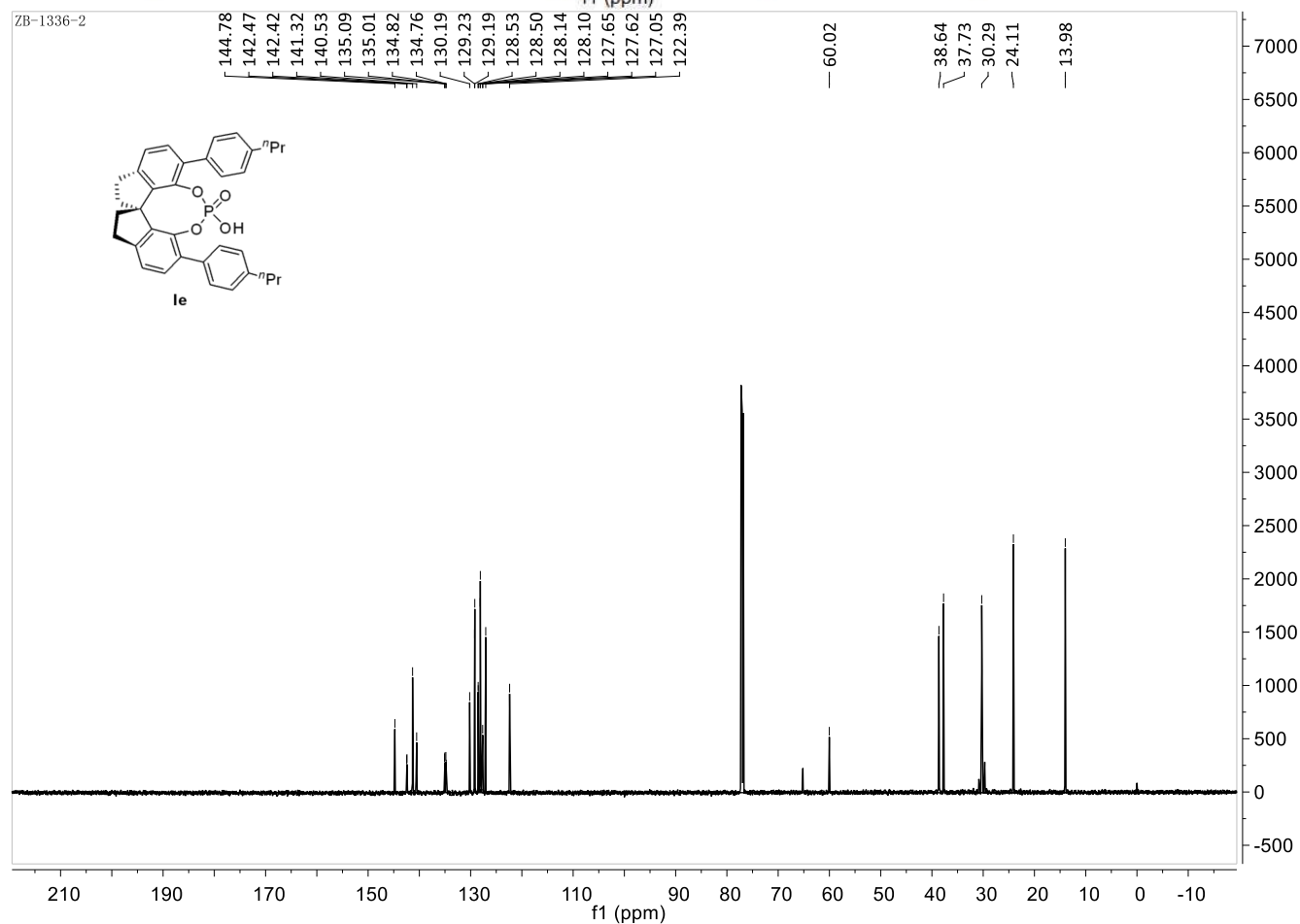
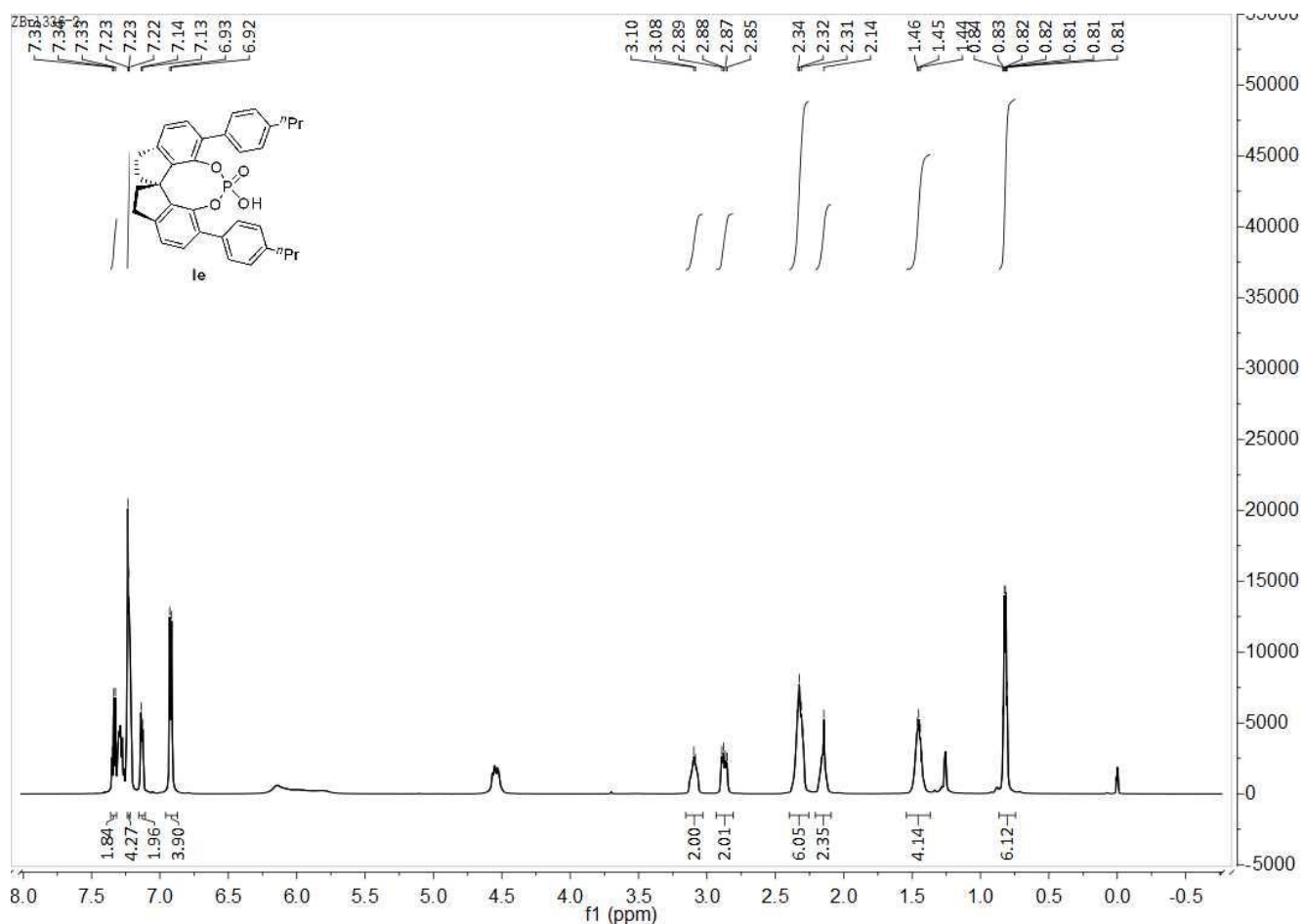
14. References

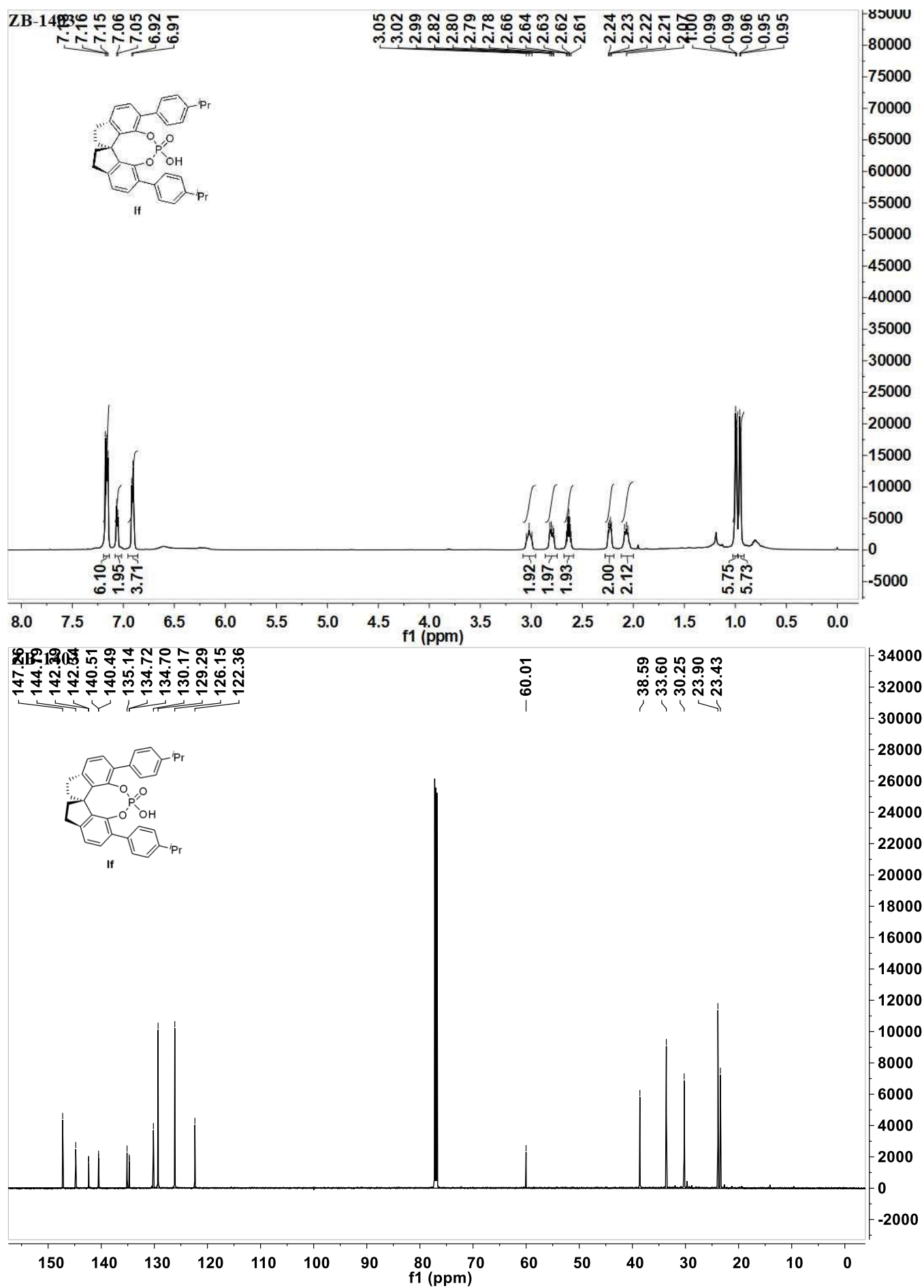
- [1] F. X. Xu, D. Huang, C. Han, W. Shen, X. F. Lin, Y. G. Wang, *J. Org. Chem.* **2010**, 75, 8677
- [2] P. S. Bhadury, Y. P. Zhang, S. Zhang, B. A. Song, S. Yang, D. Y. Hu, Z. Chen, W. Xue, L. H. Jin, *Chirality*, **2009**, 21, 547.
- [3] A. Henseler, M. Kato, K. Mori, T. Akiyama, *Angew. Chem. Int. Ed.* **2011**, 50, 8180.
- [4] a) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785.
- [5] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, 113, 6378.

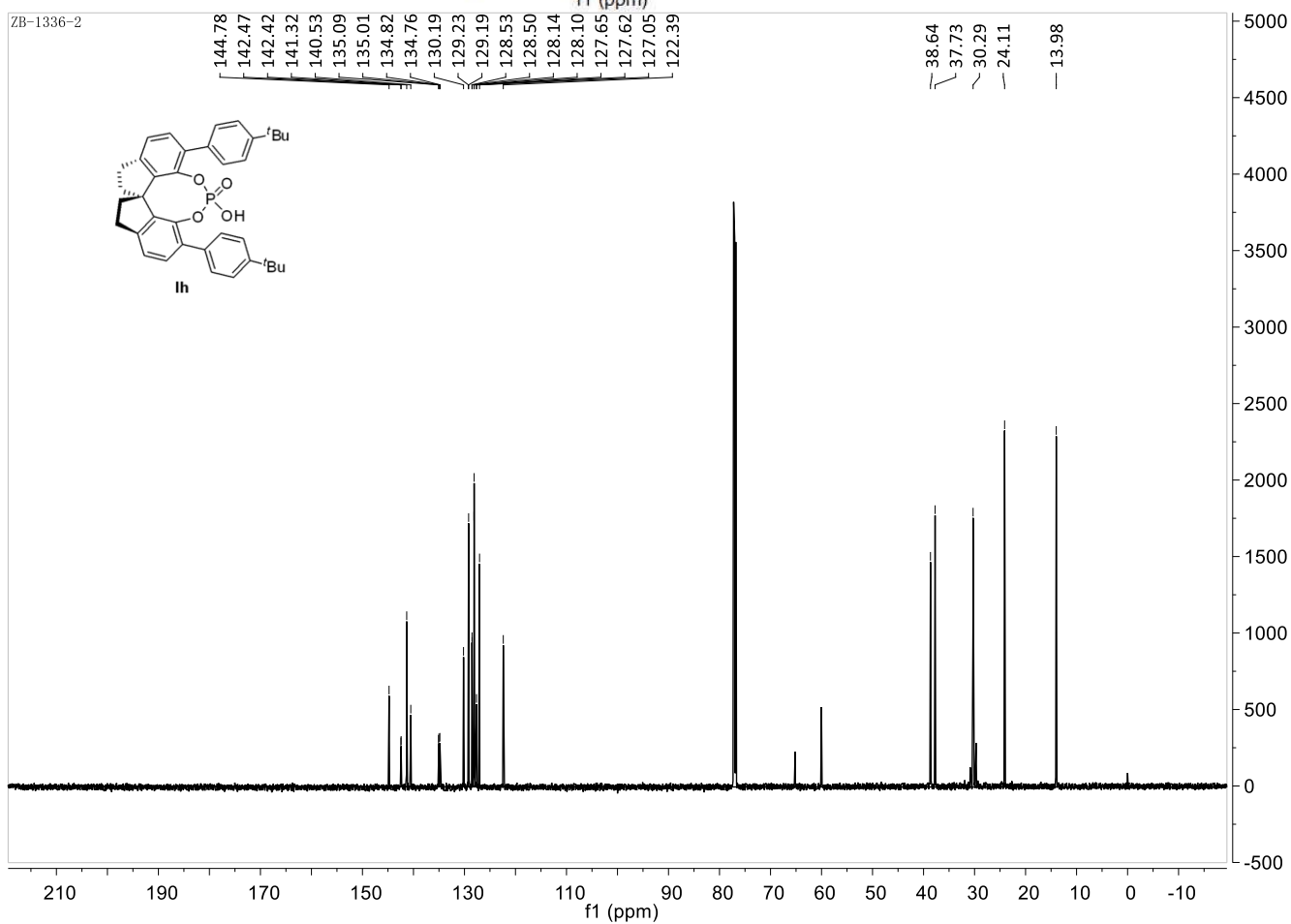
15. NMR spectra and HPLC for CPAs and asymmetric 1,3-dipolar cycloaddition reaction products

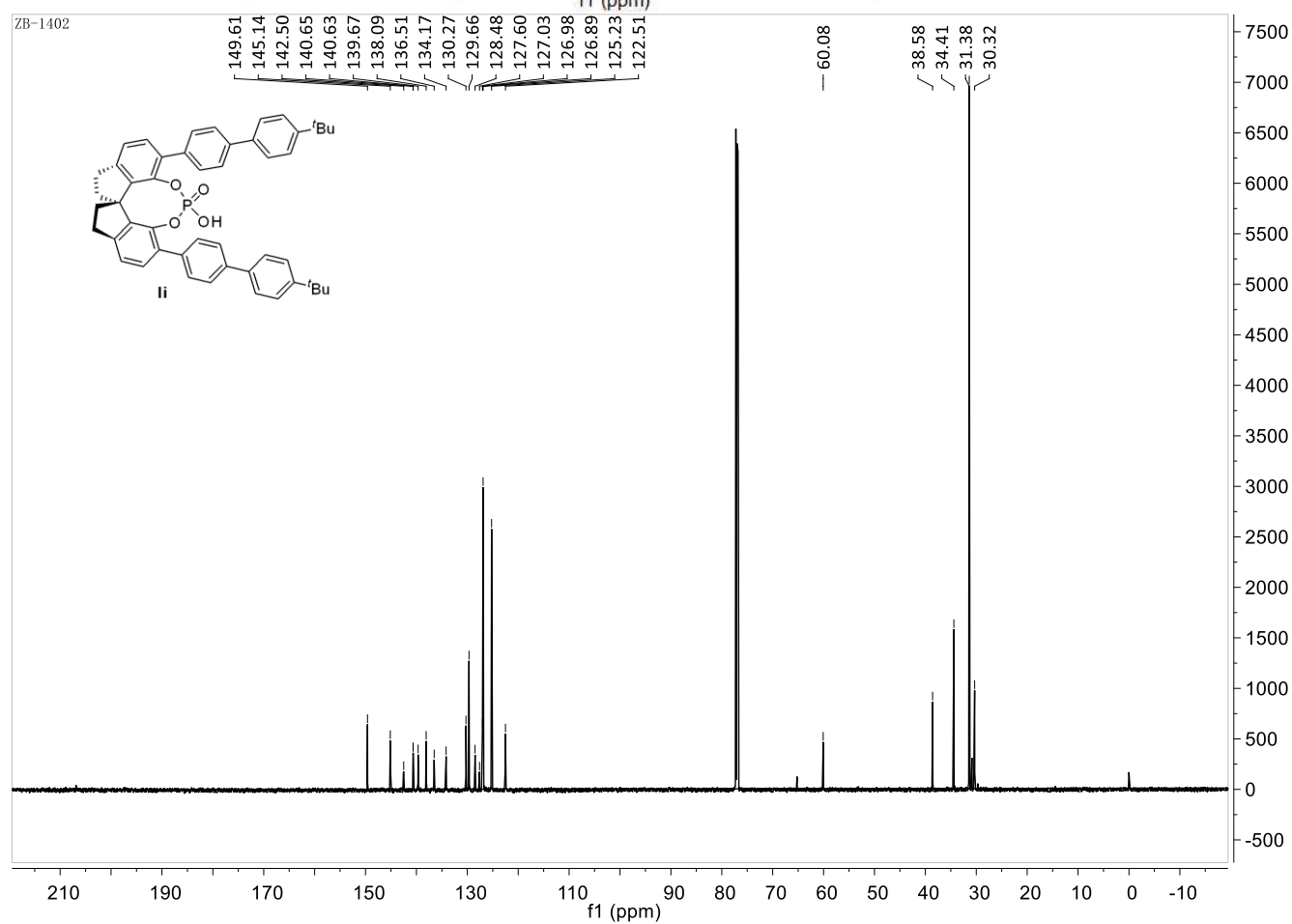
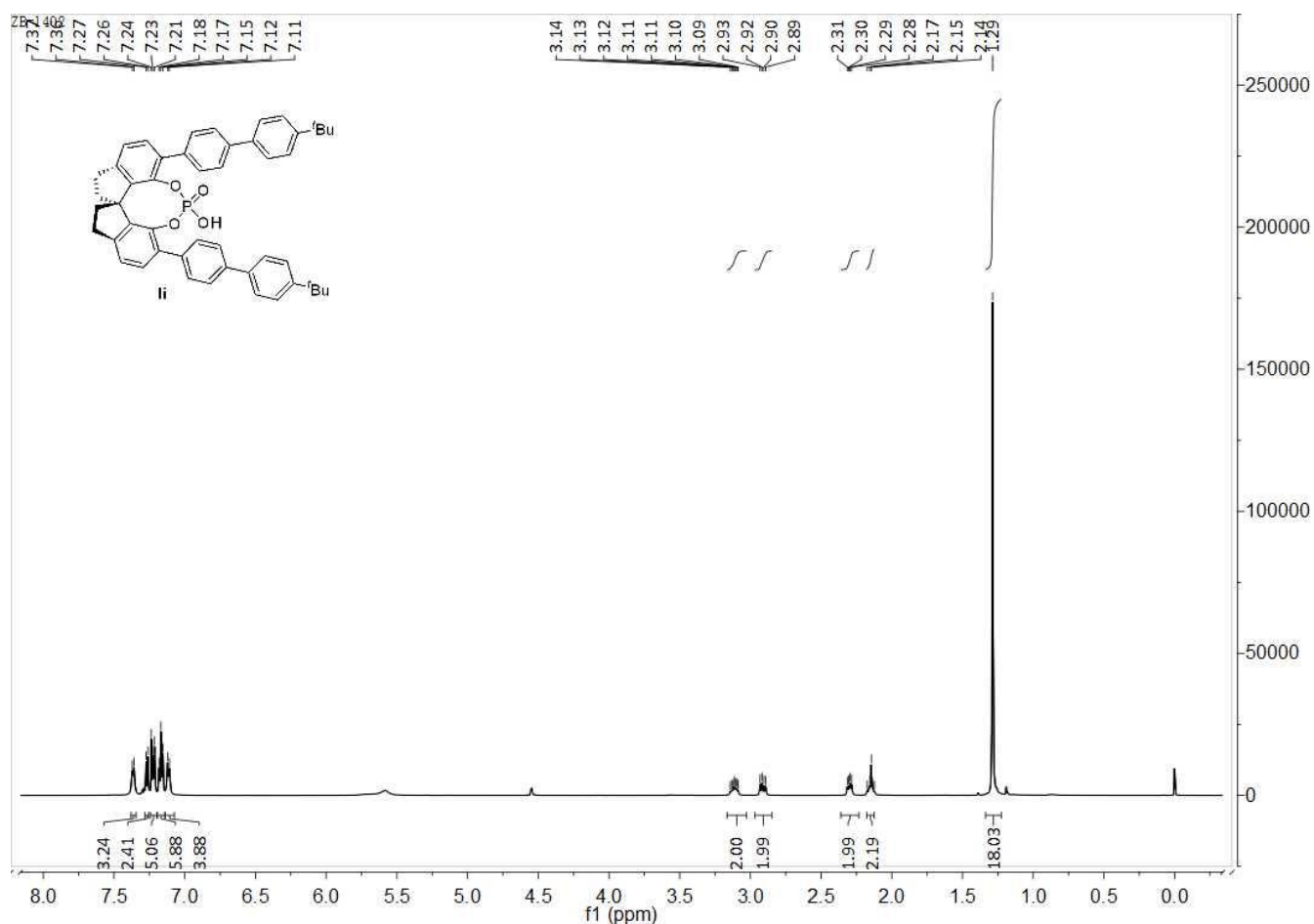


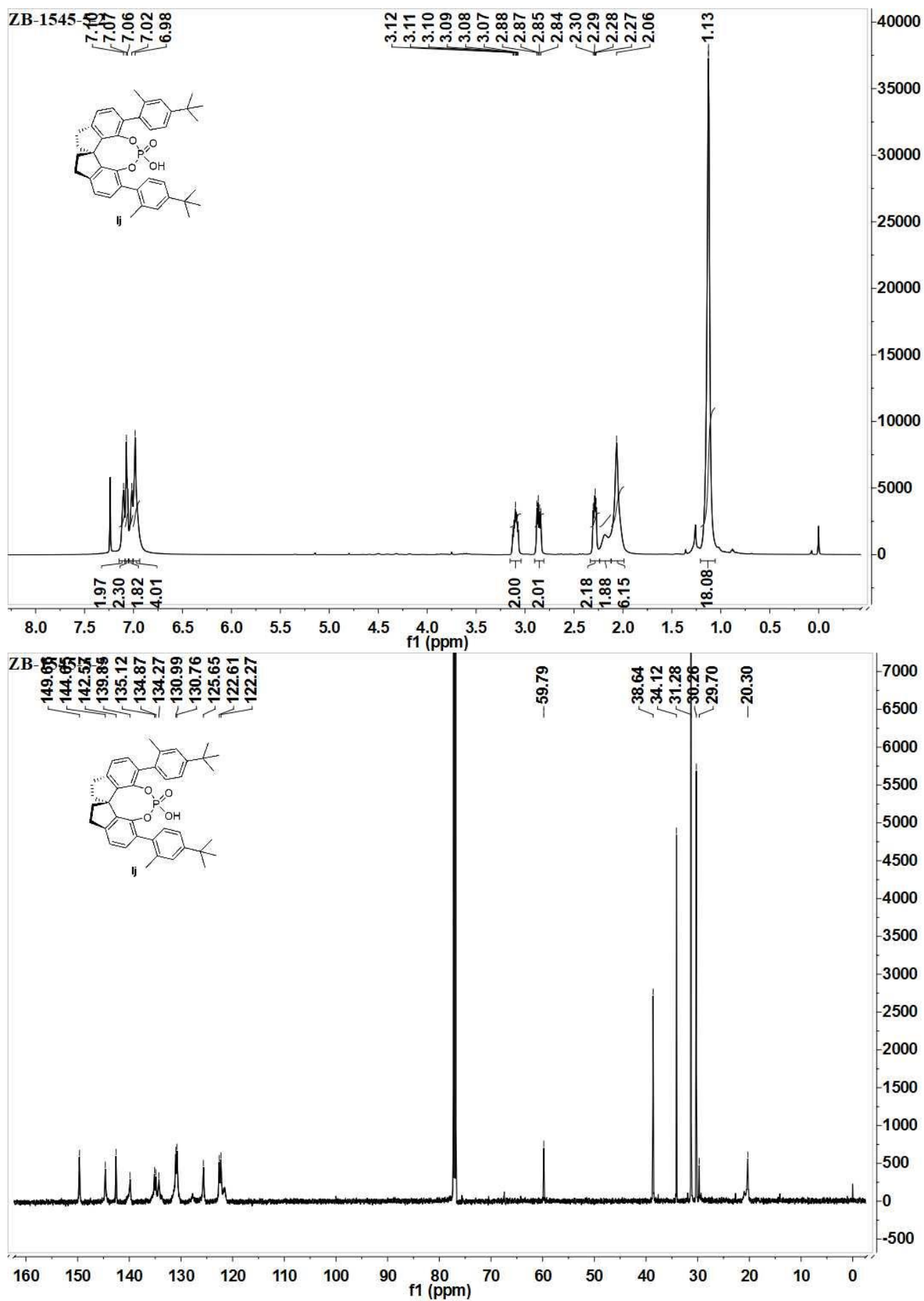


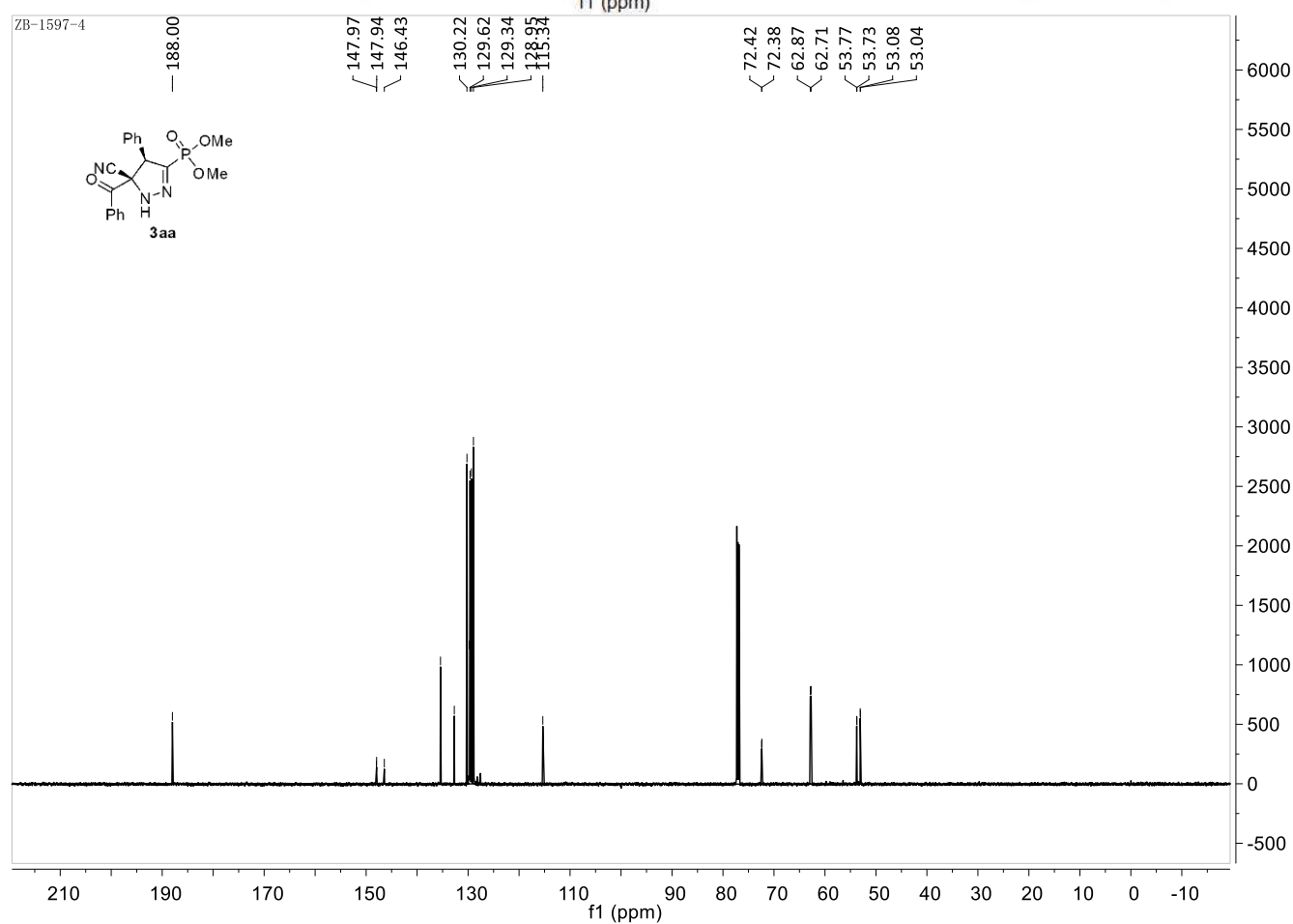
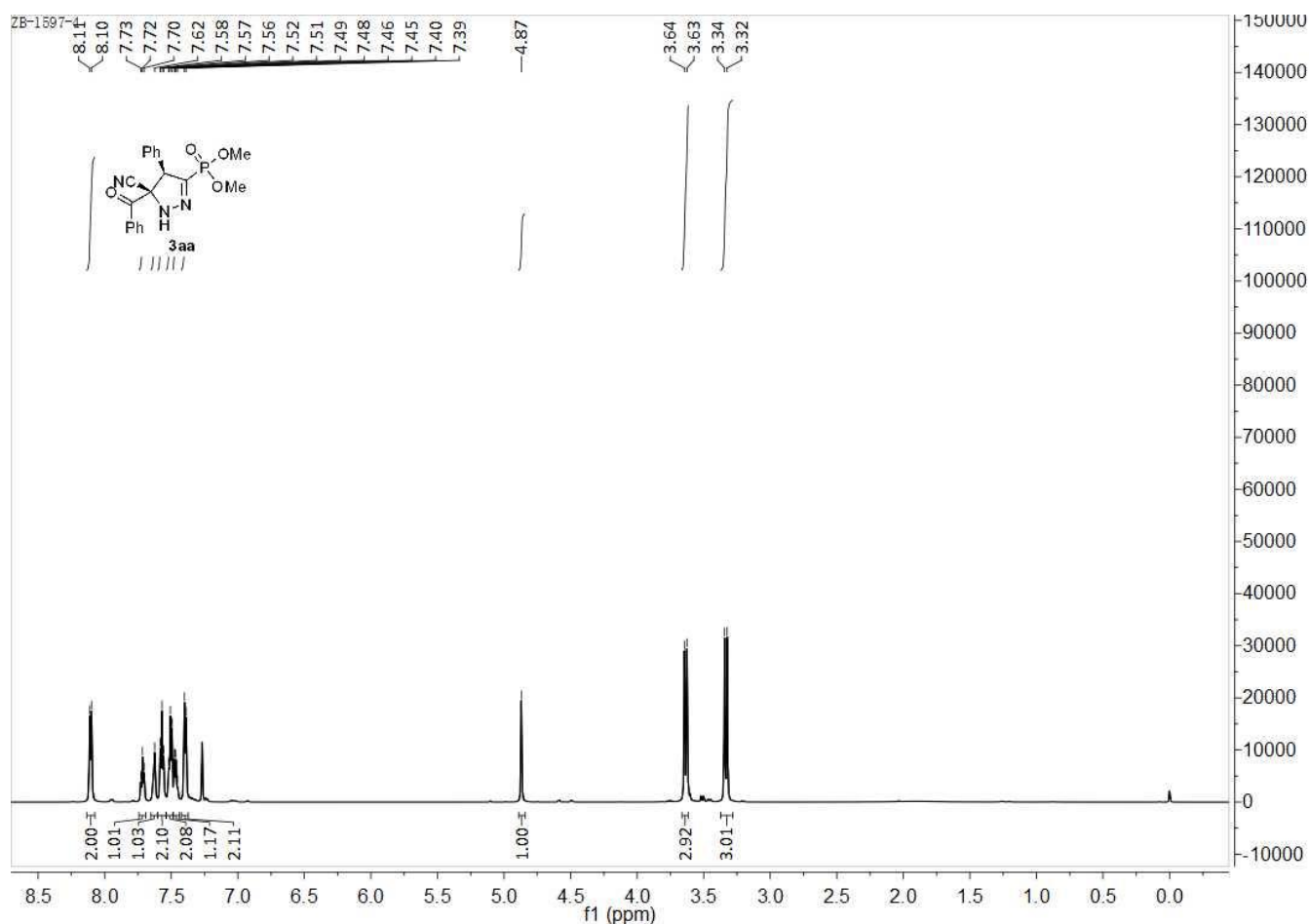


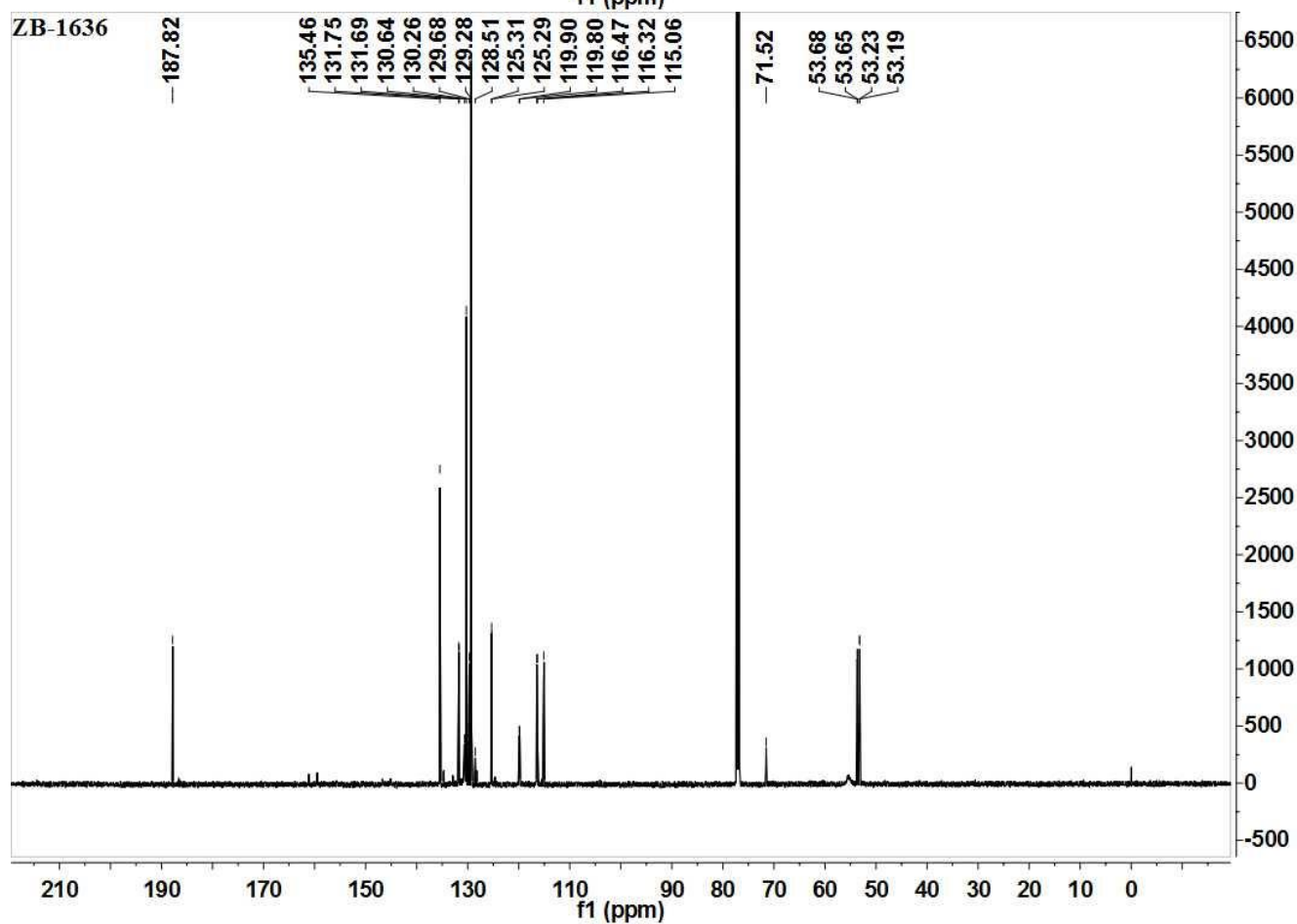
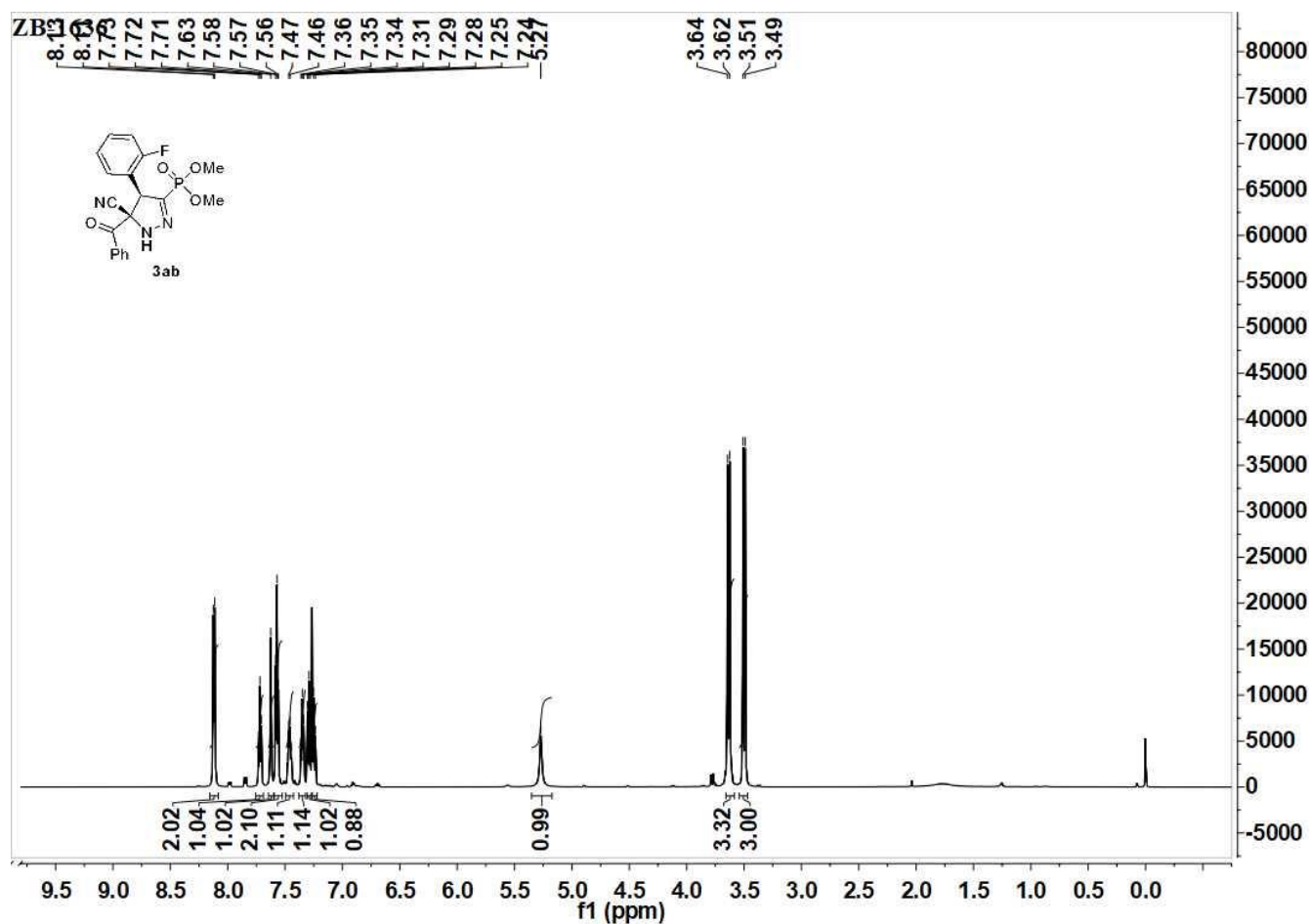


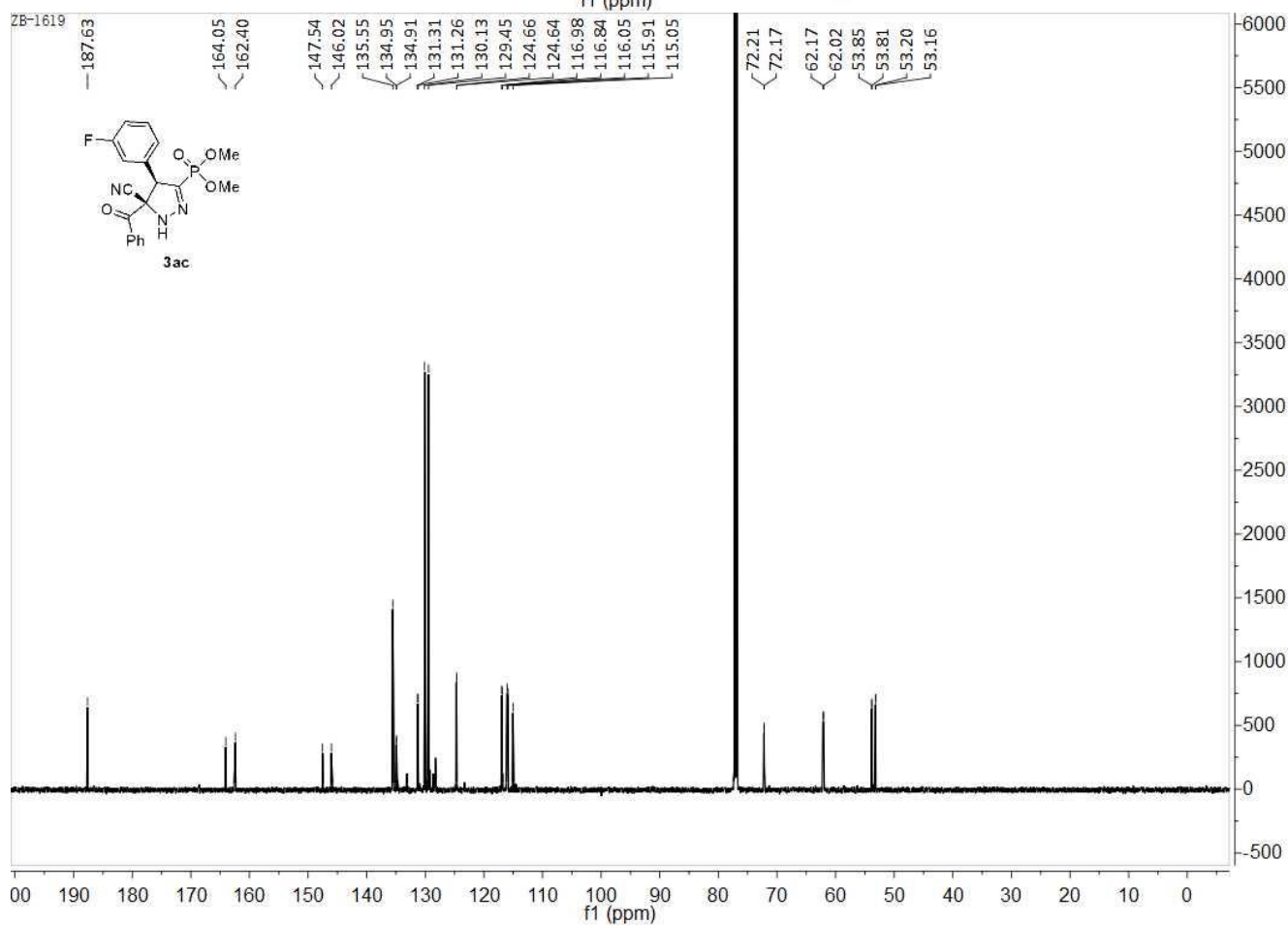
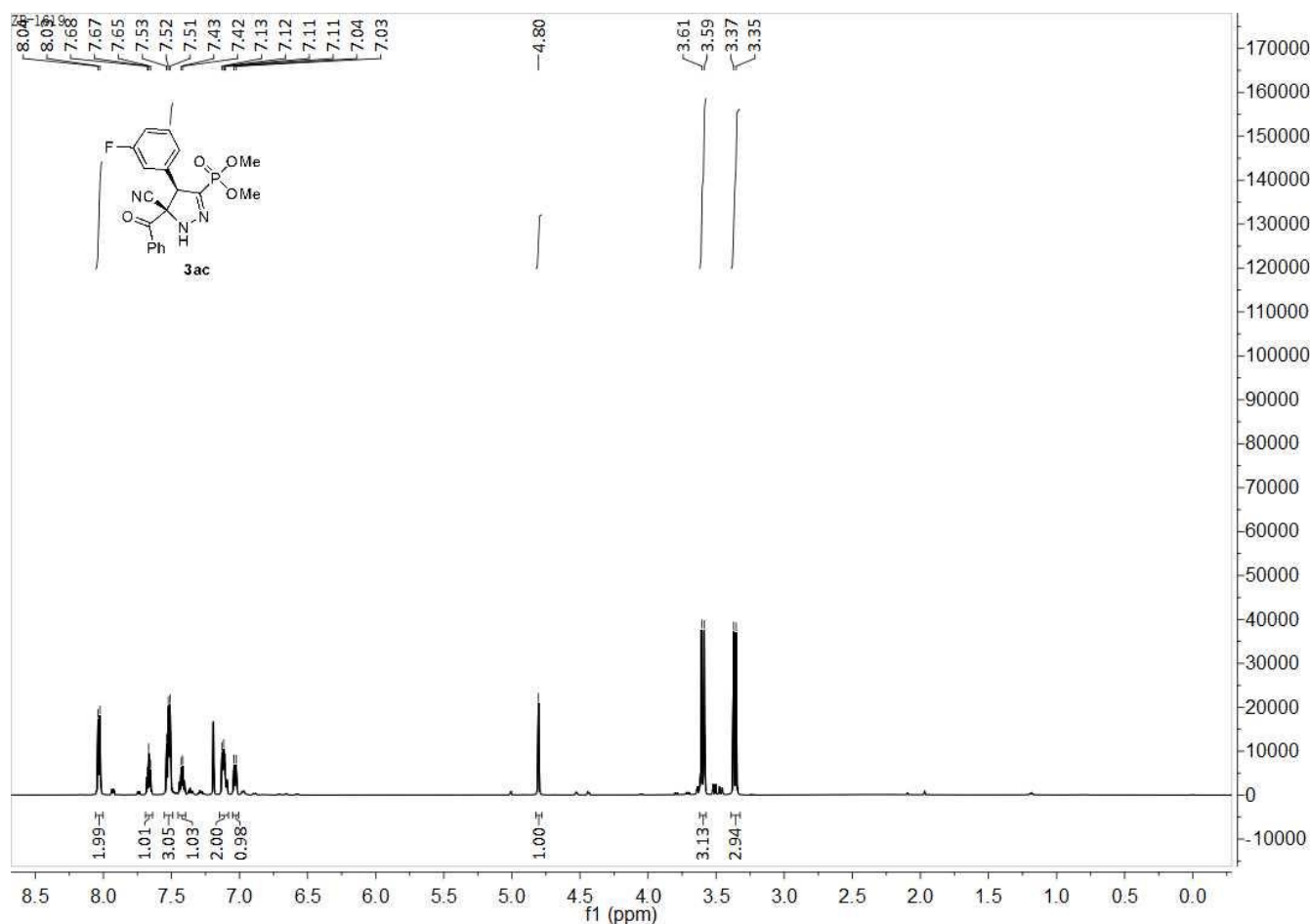


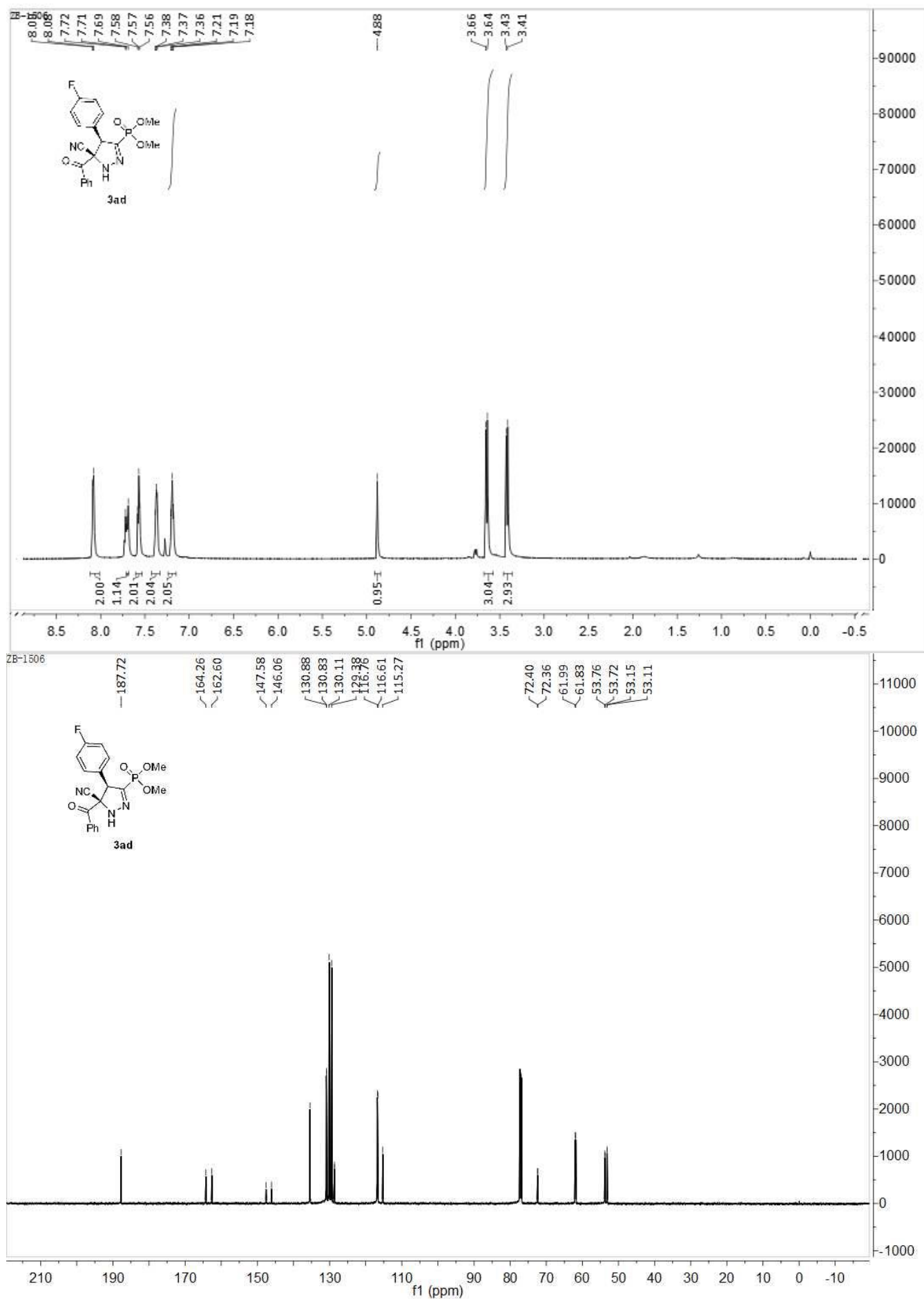


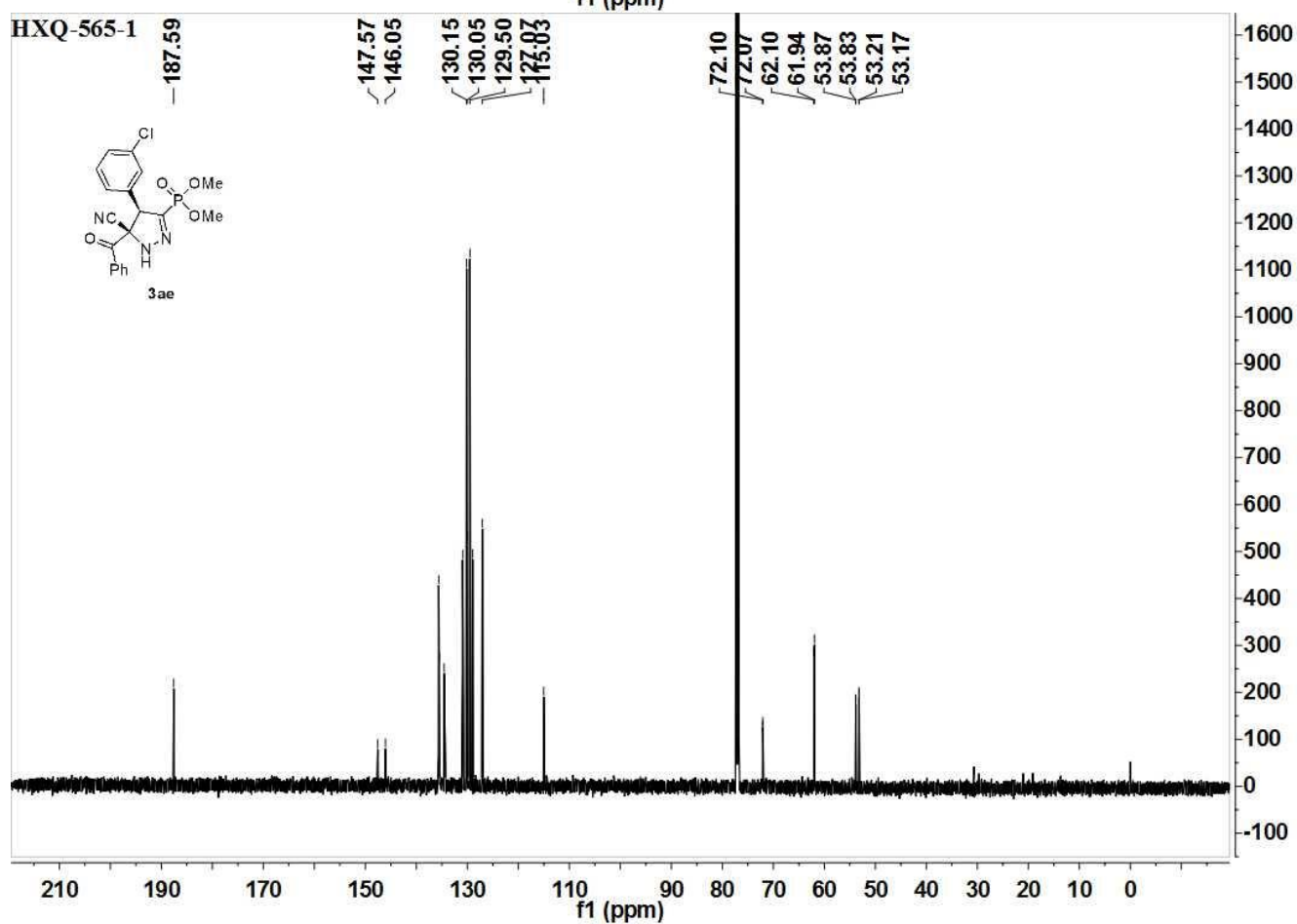
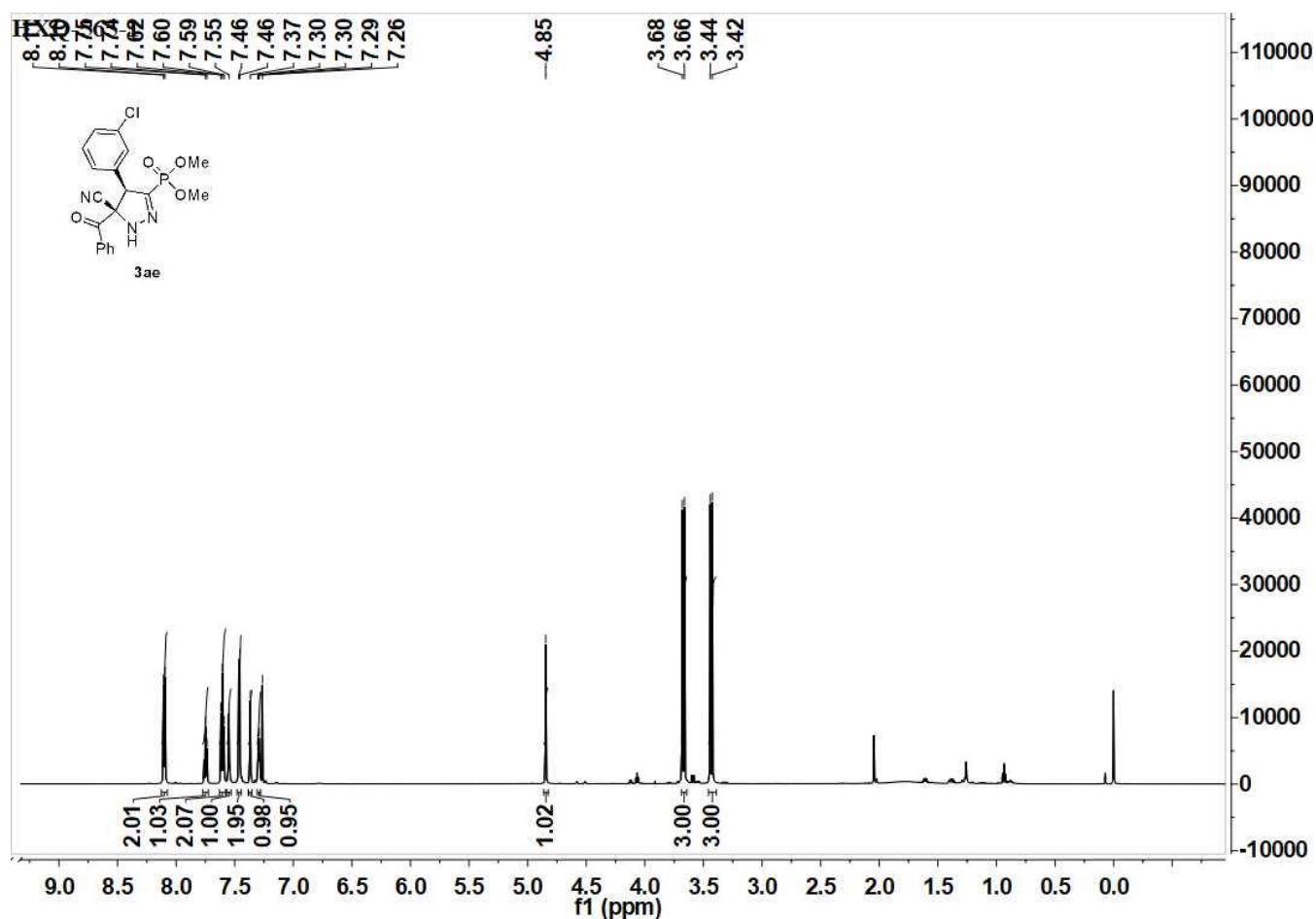


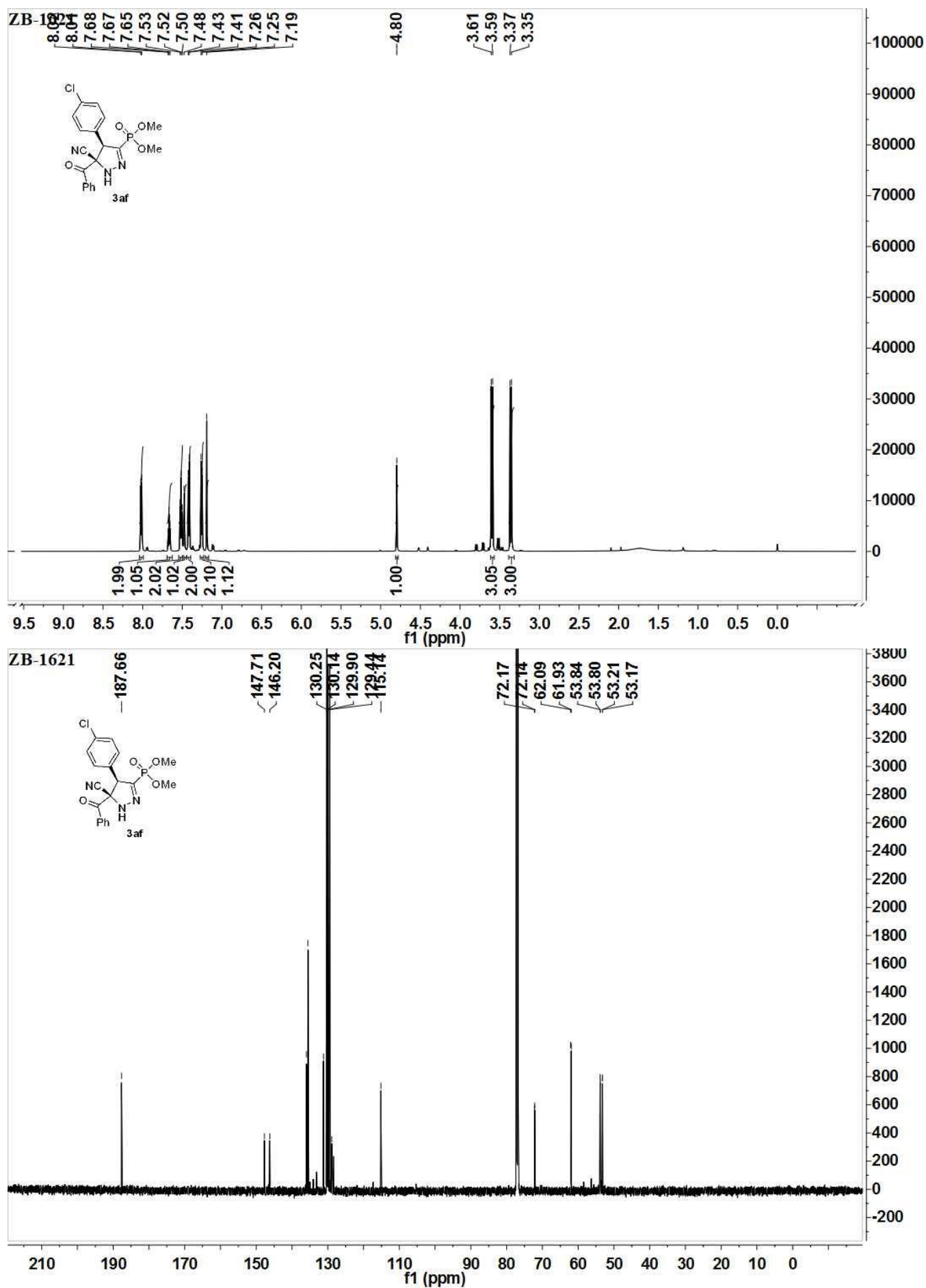


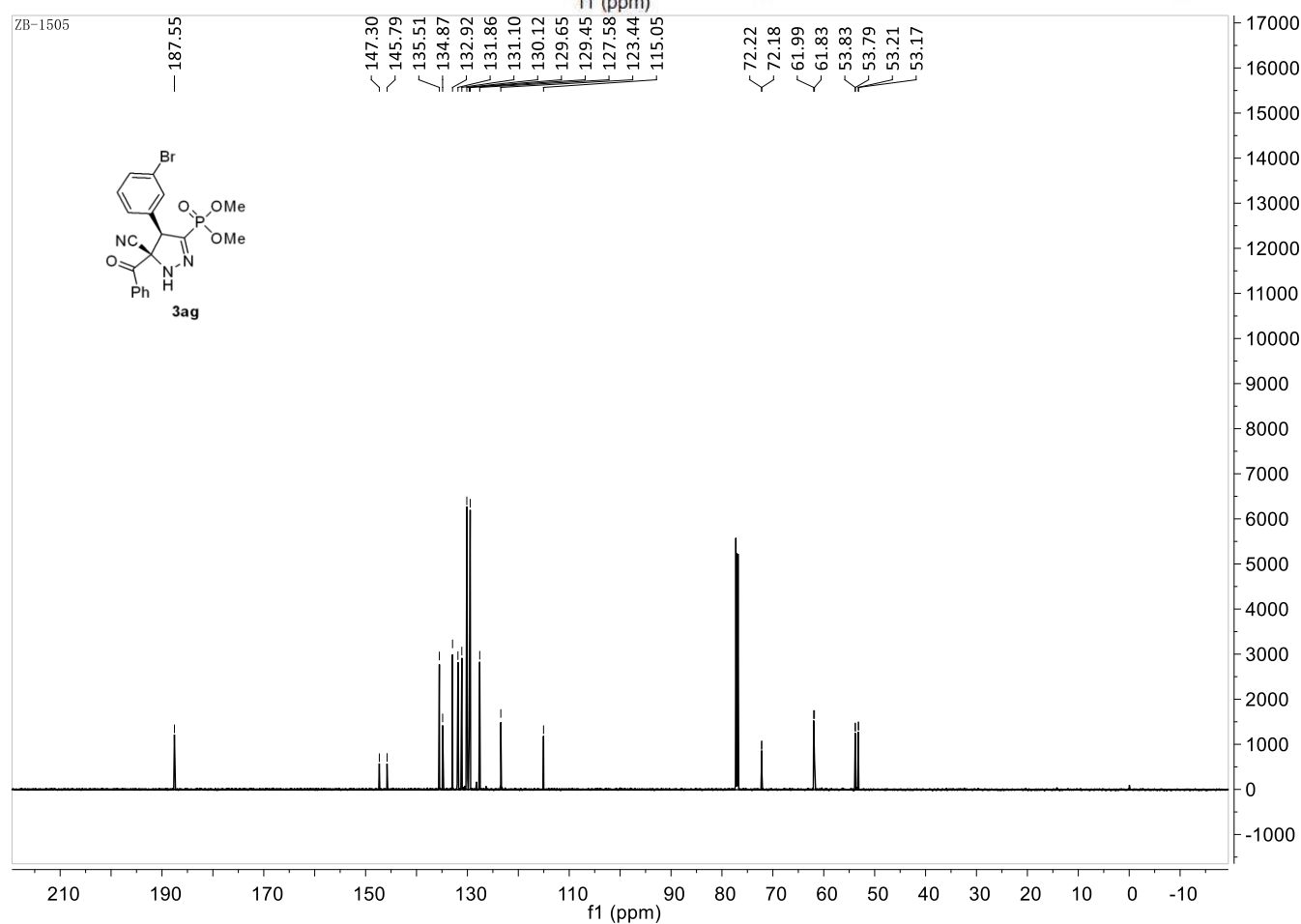
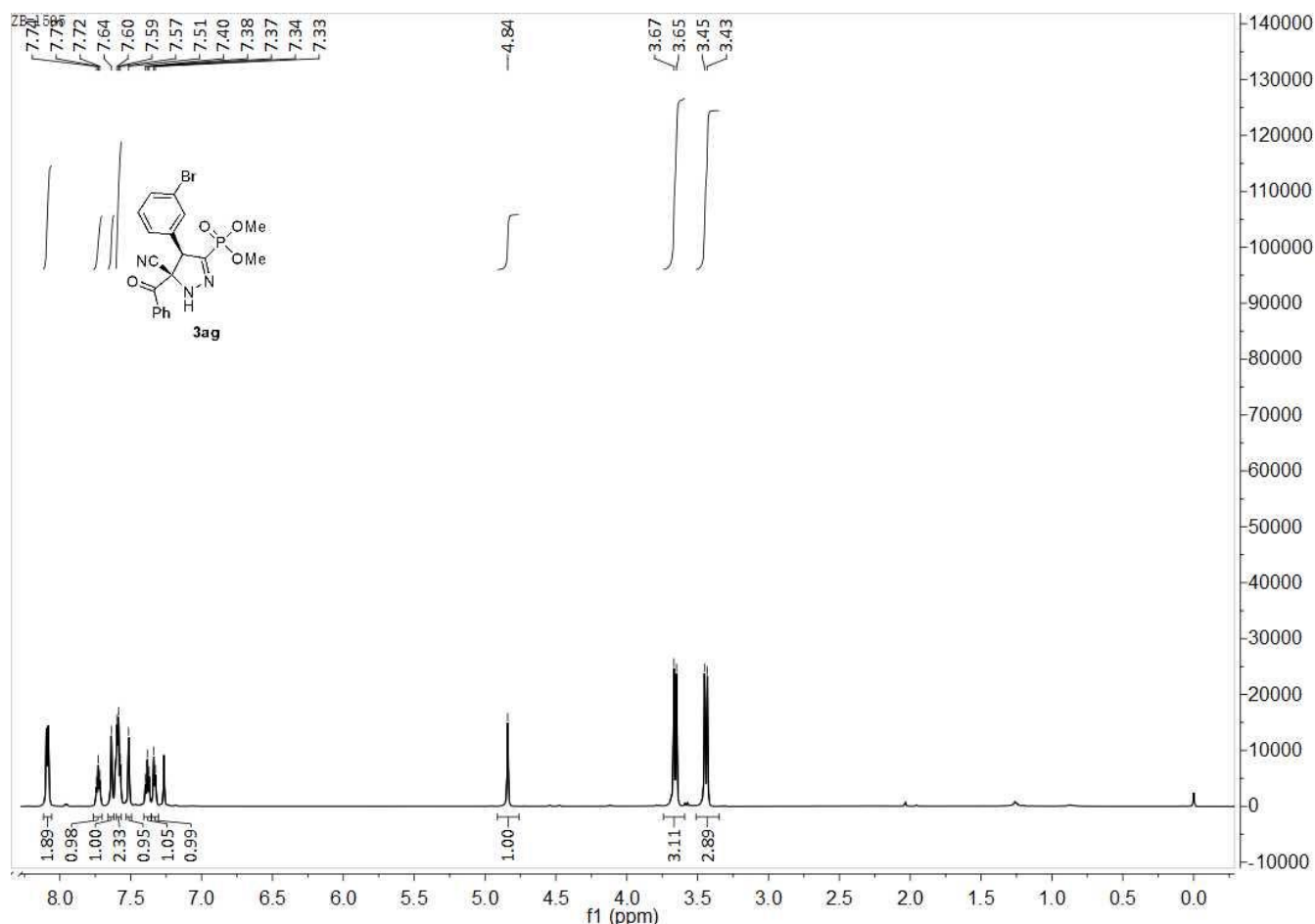


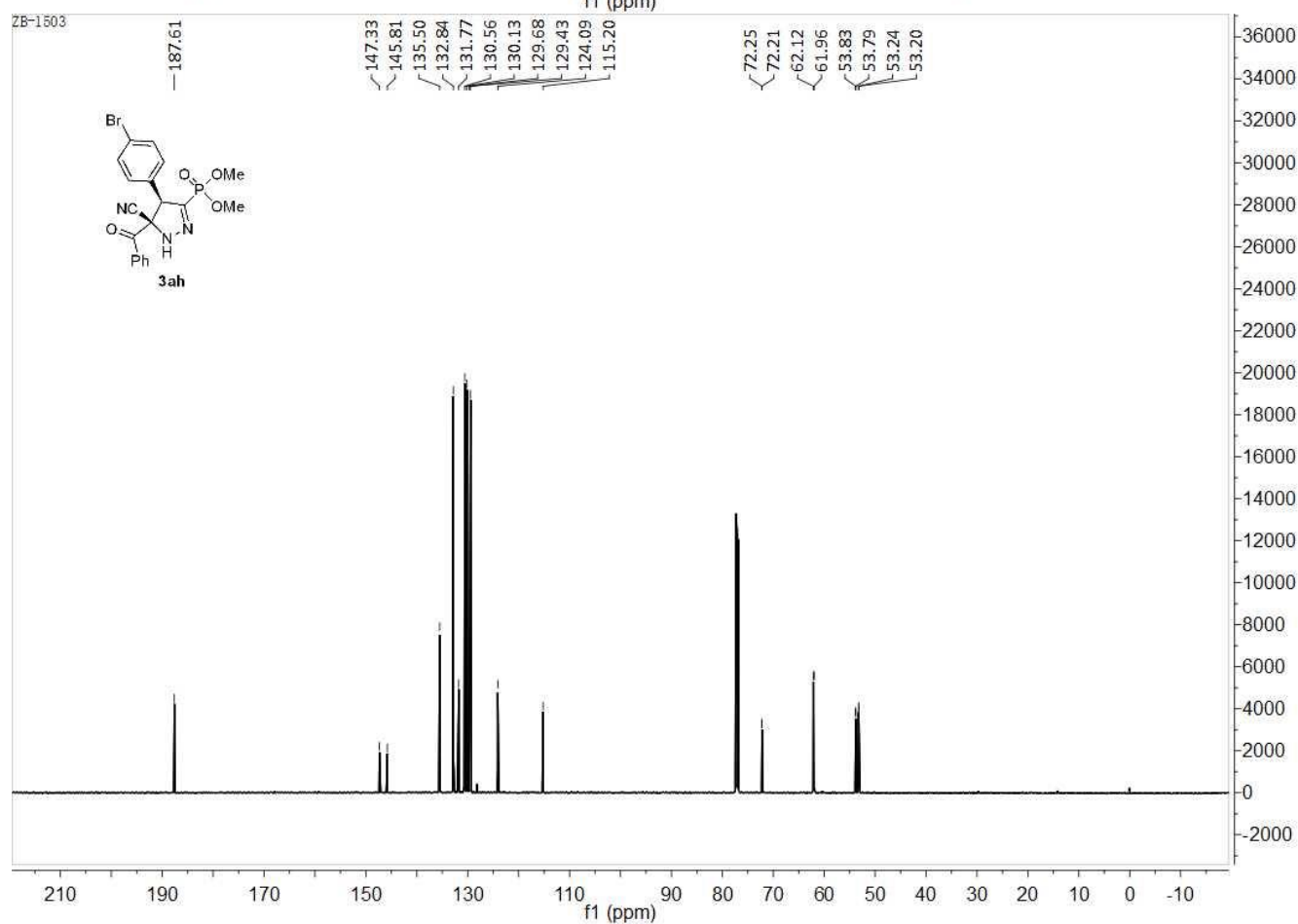
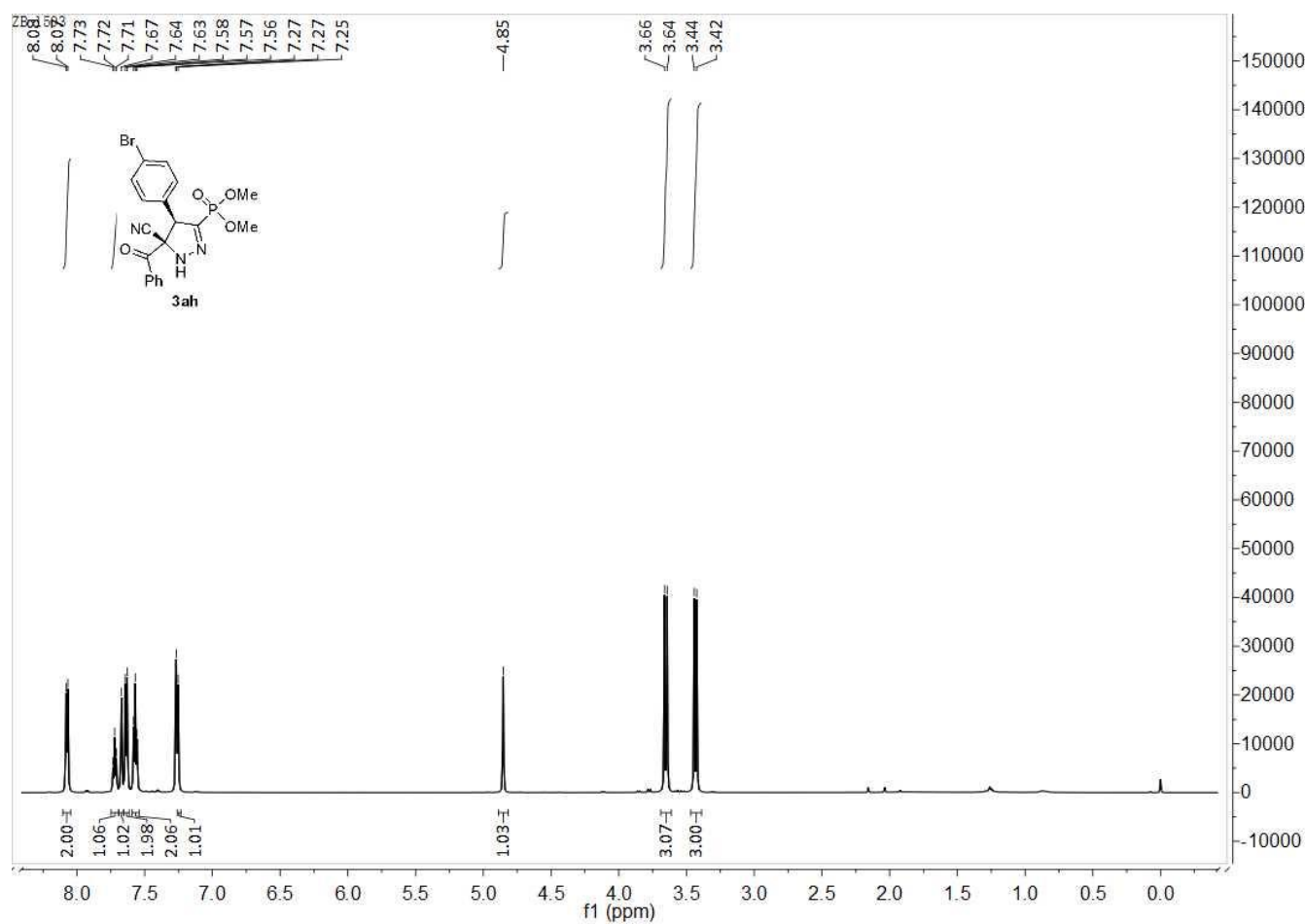


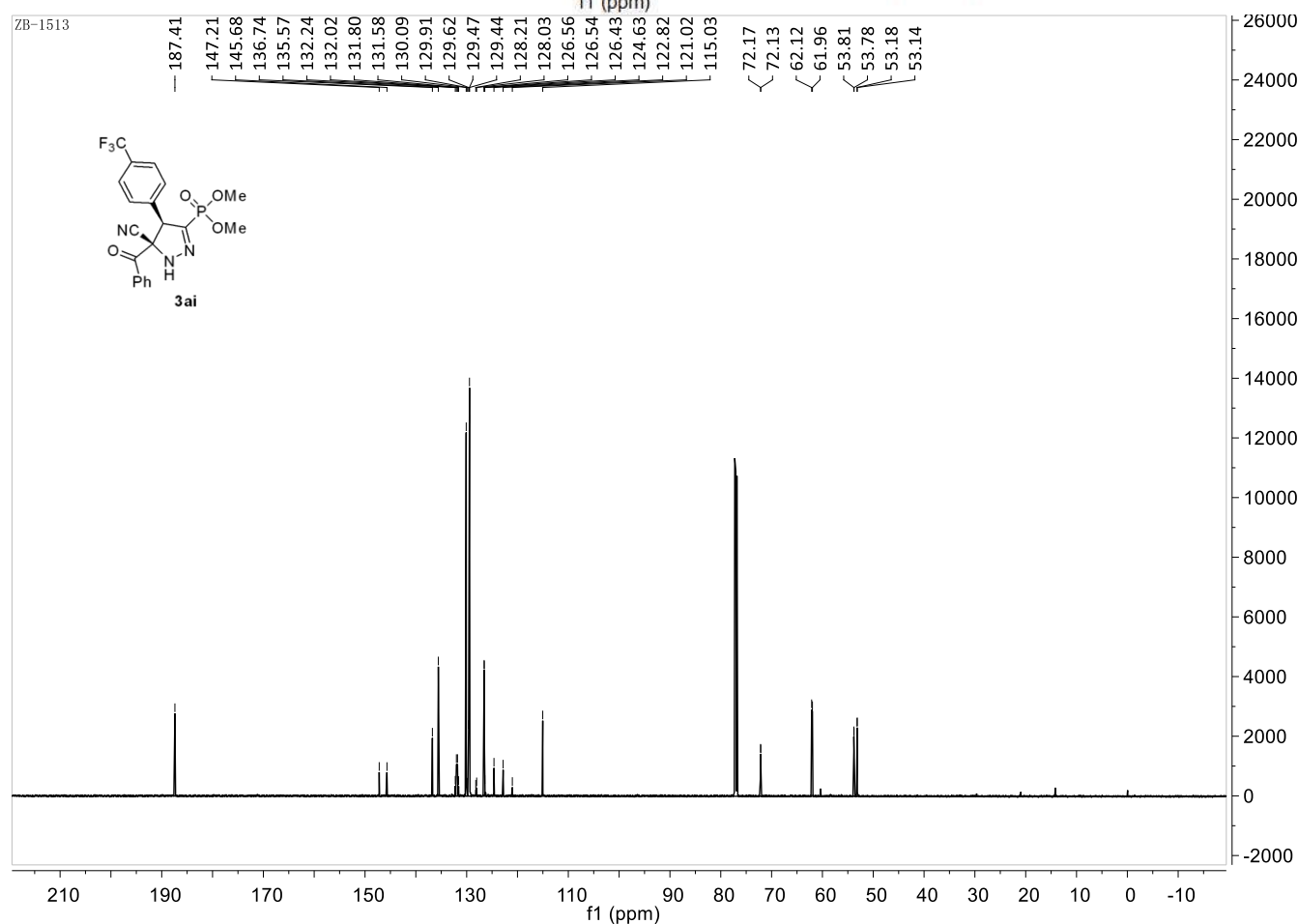
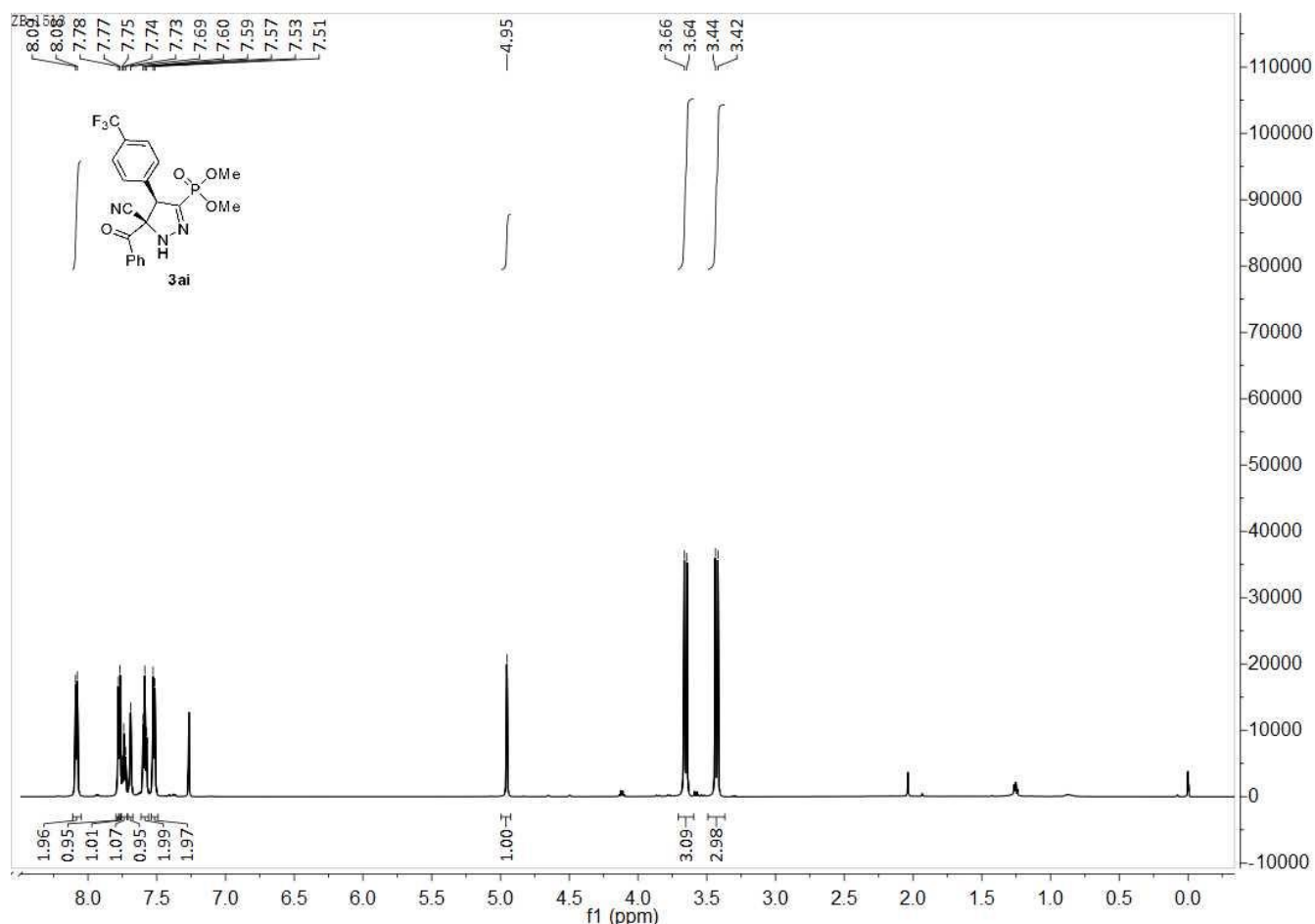


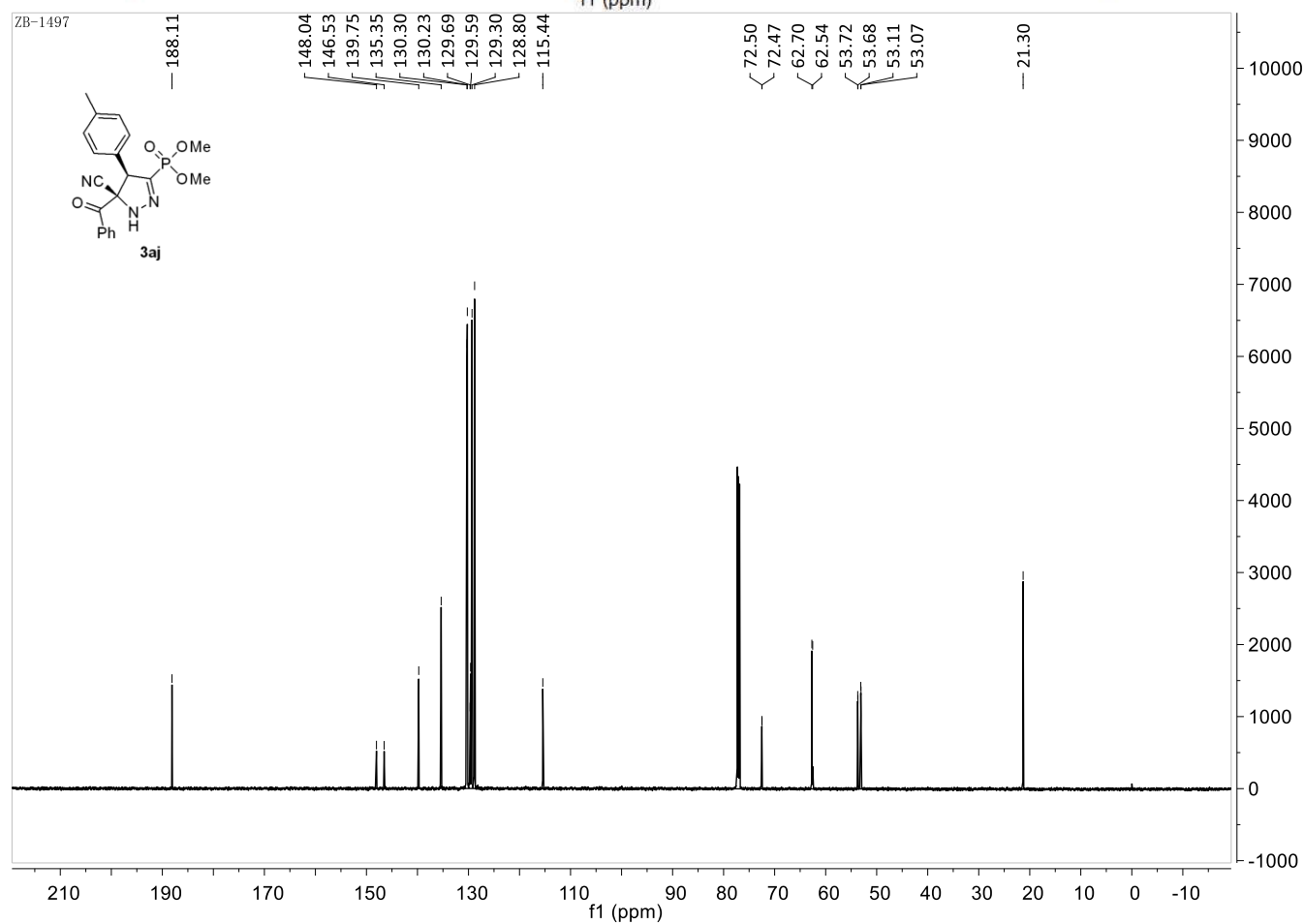
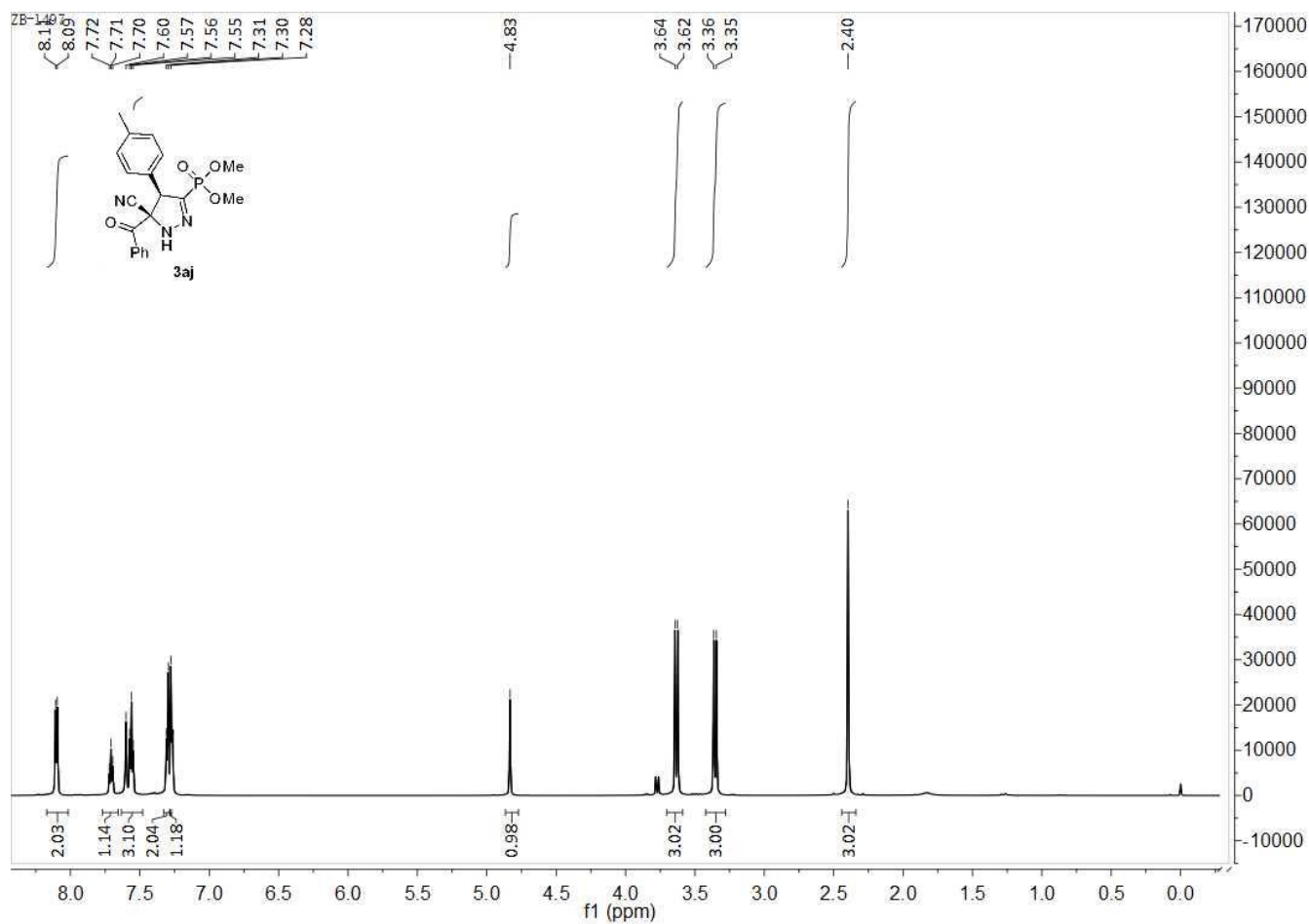


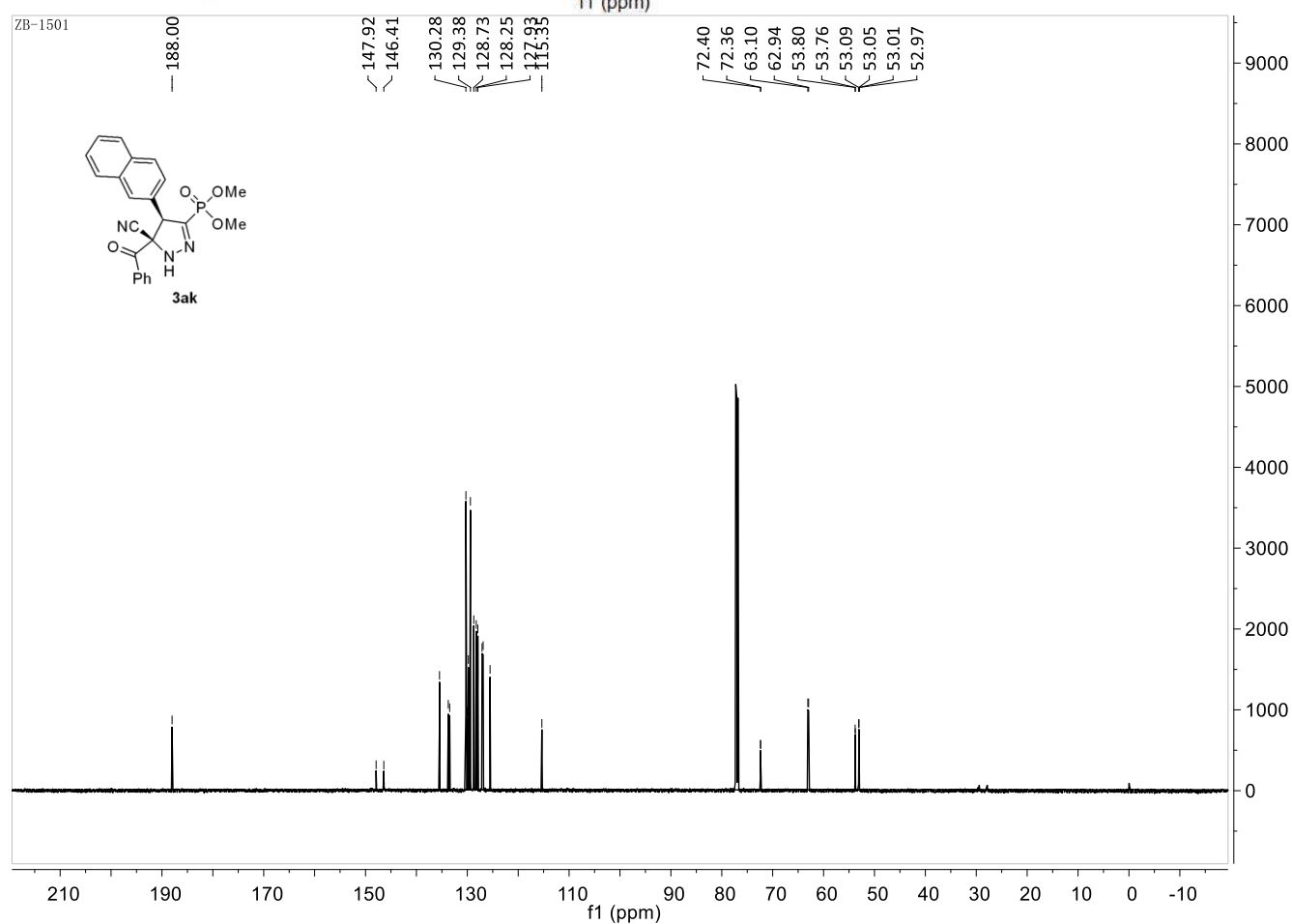
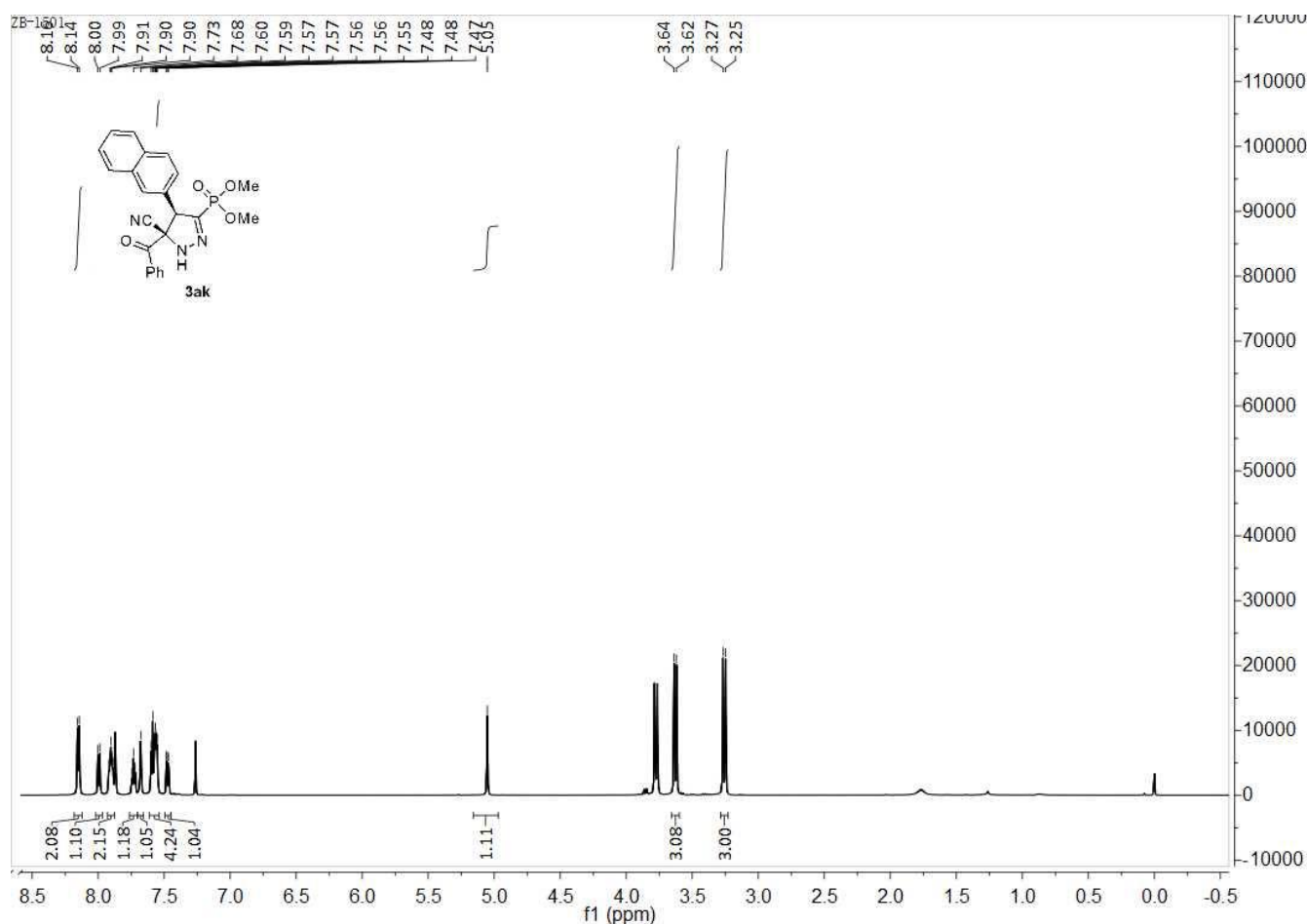


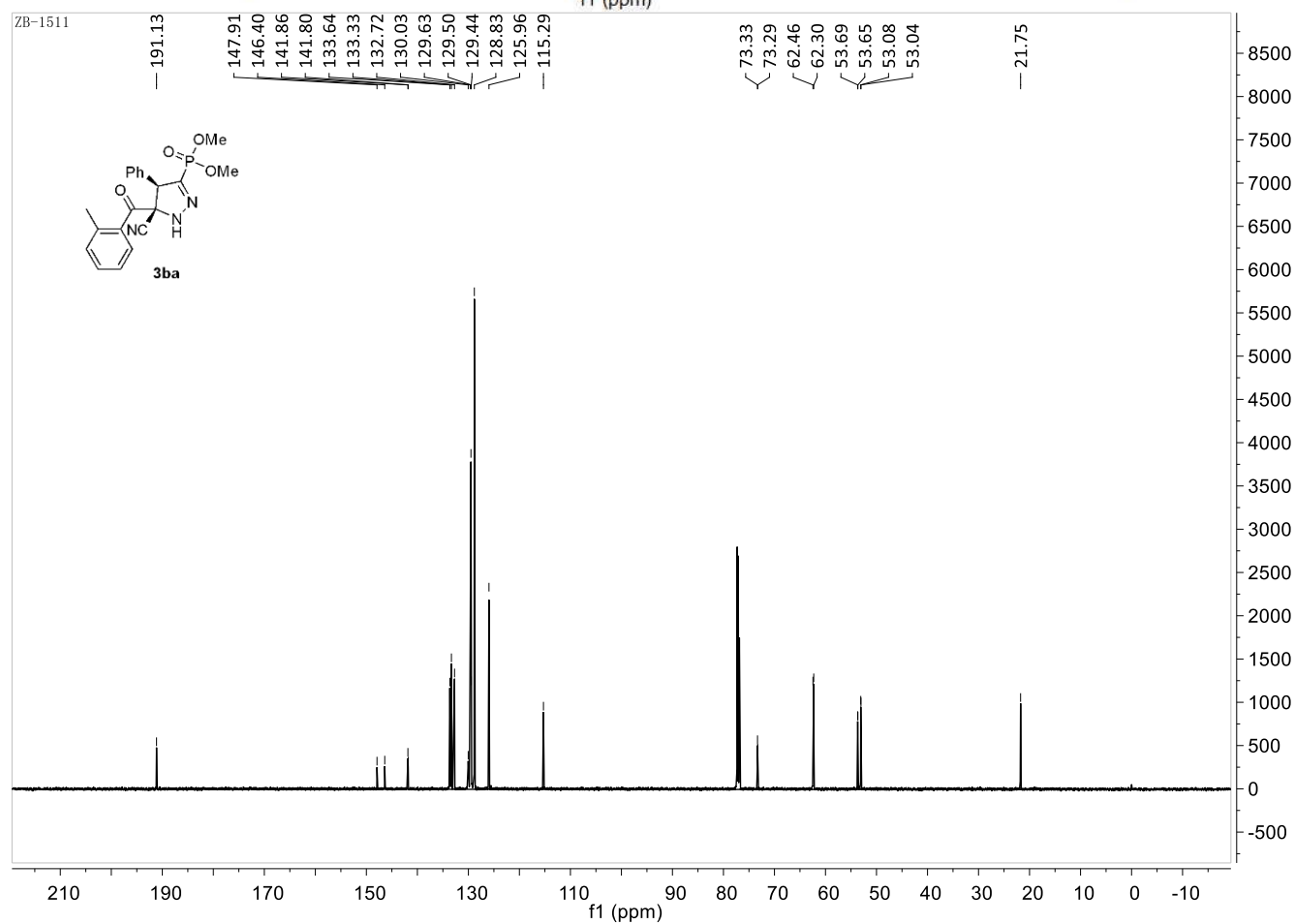
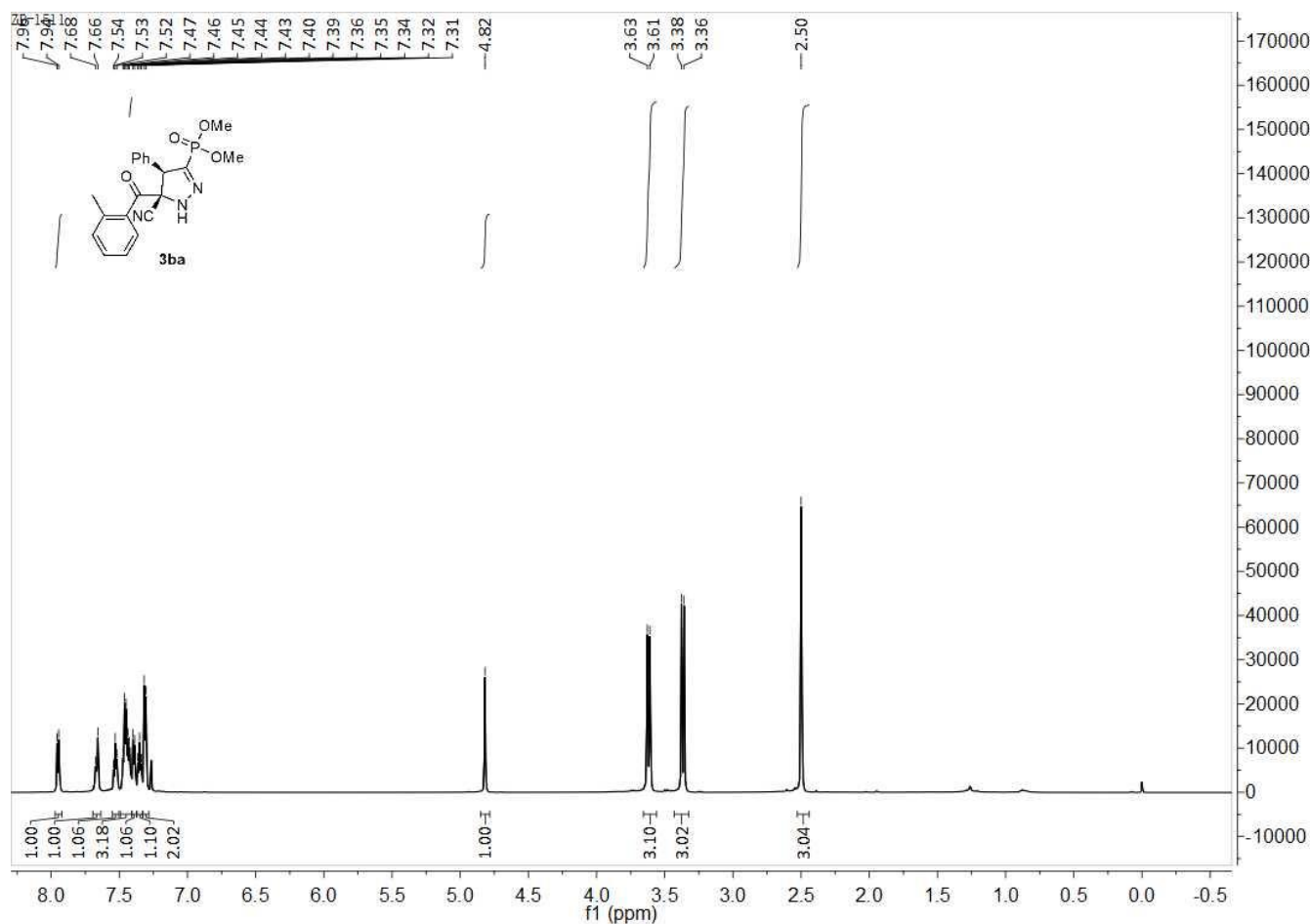


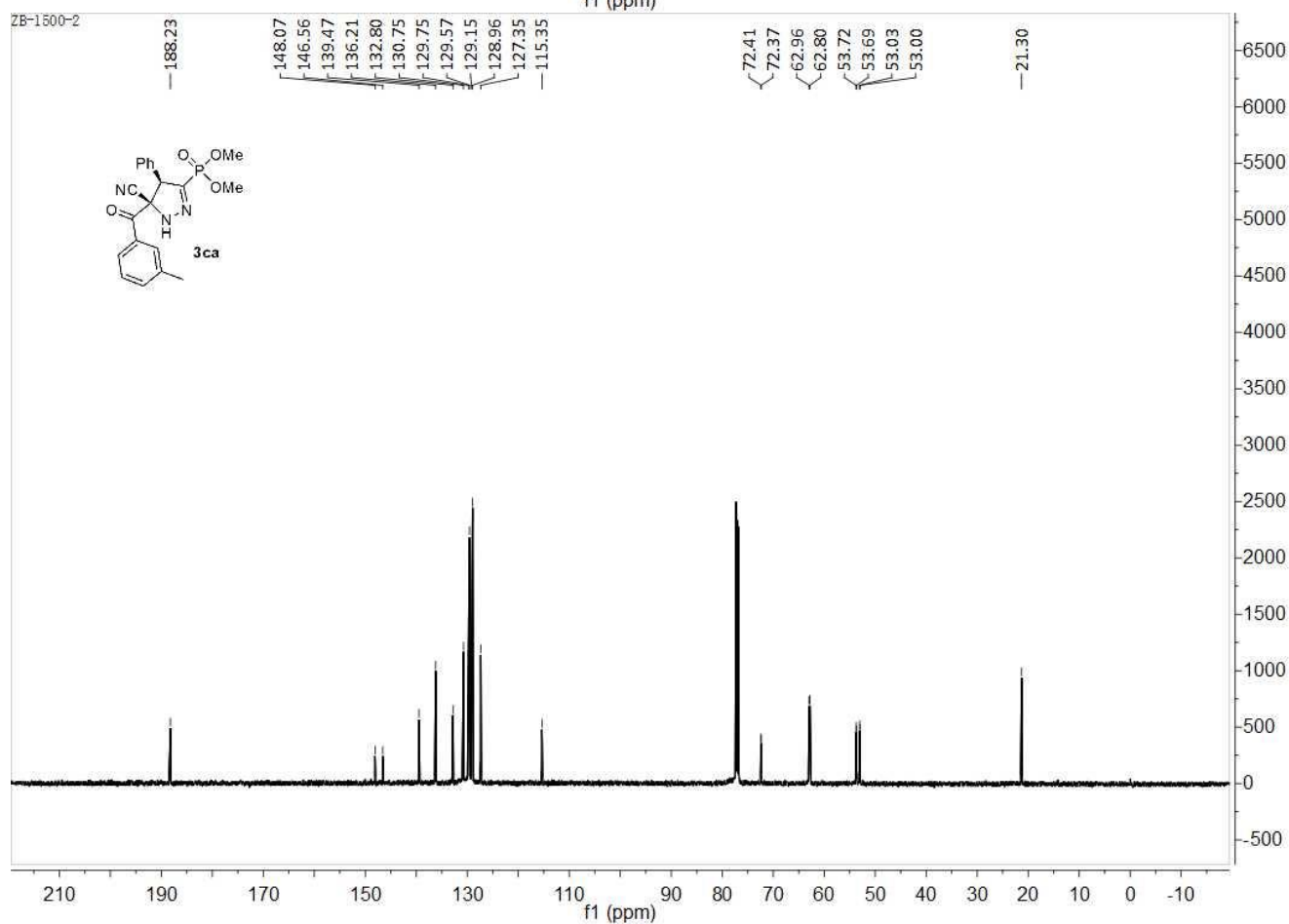
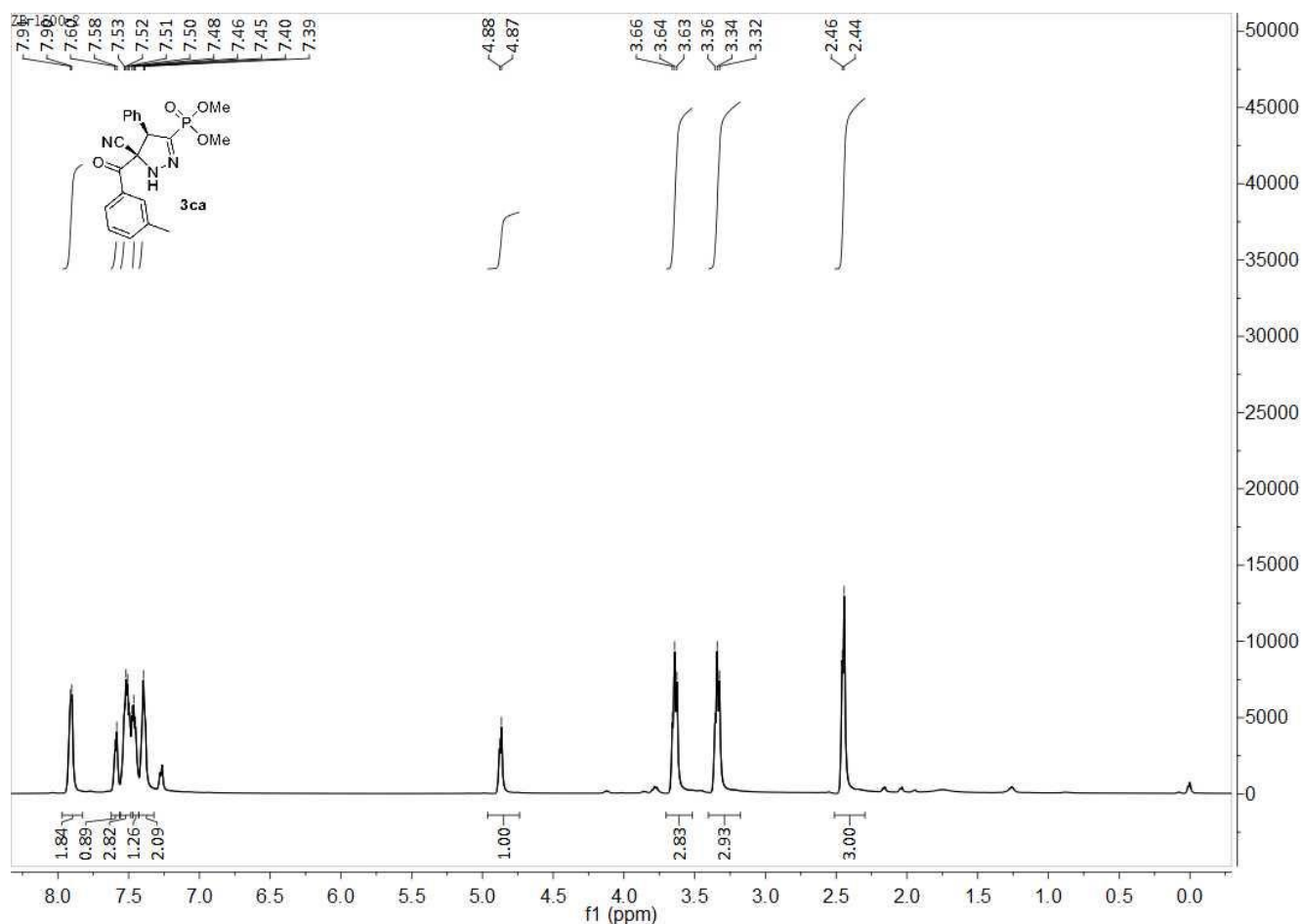


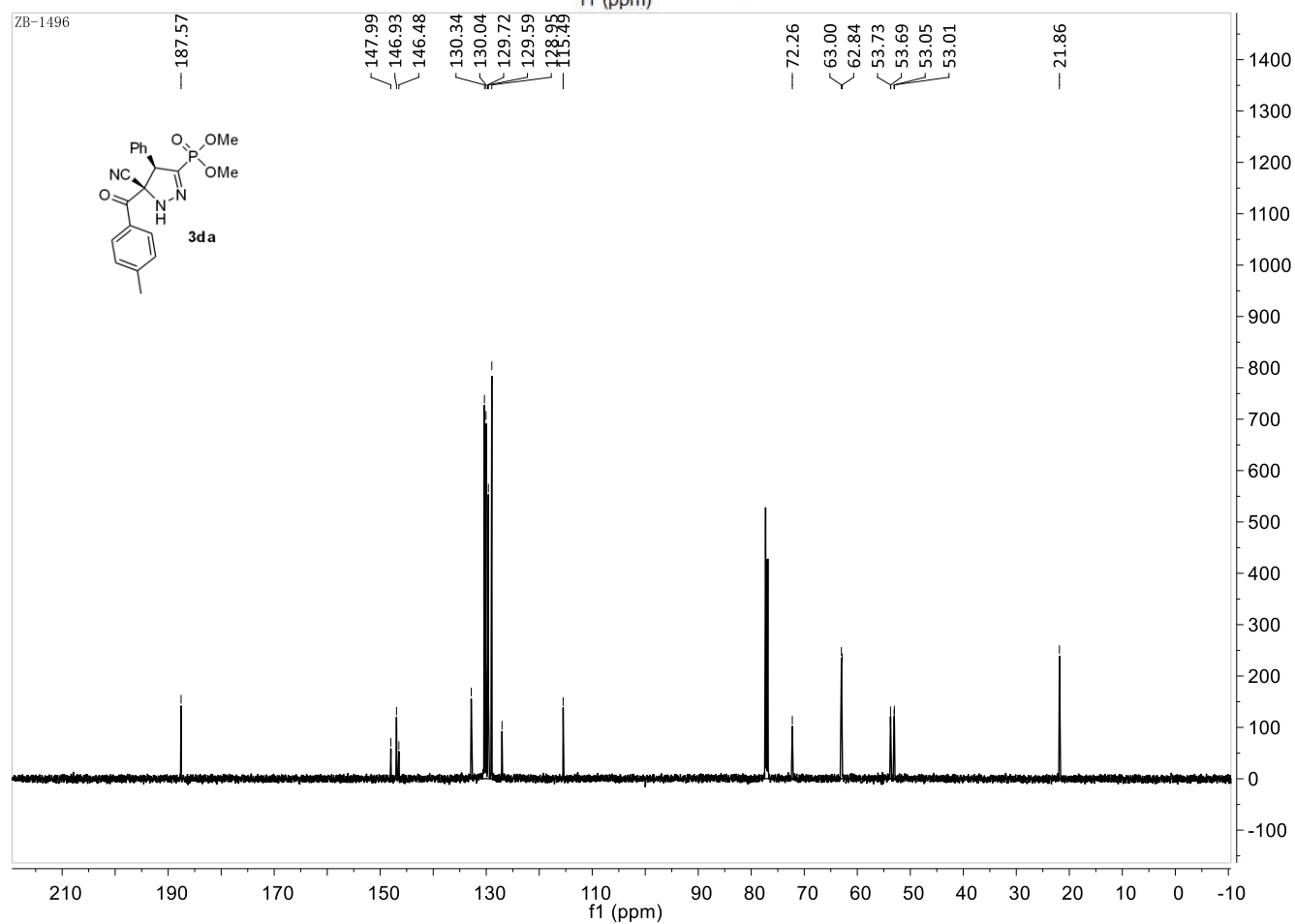
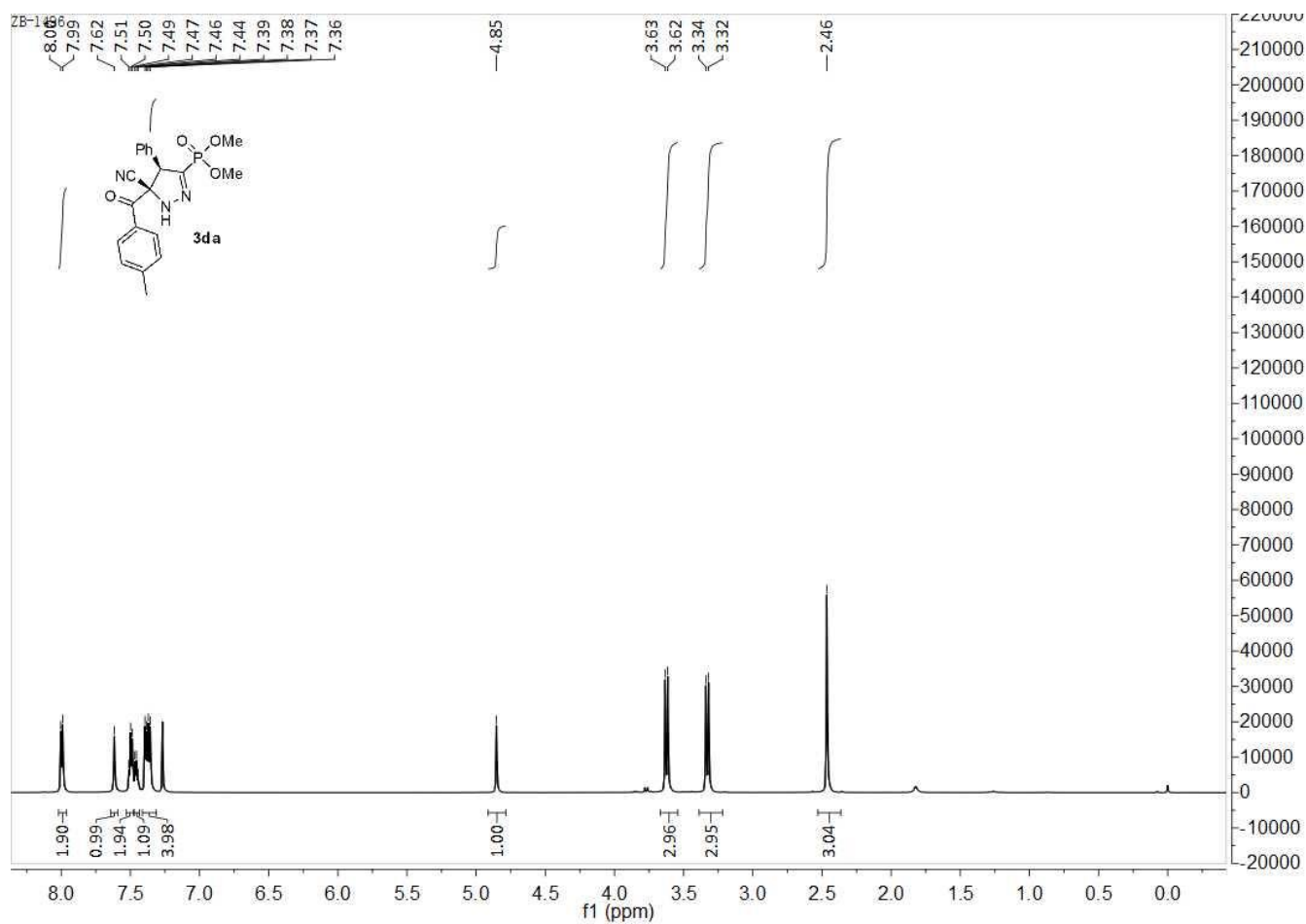


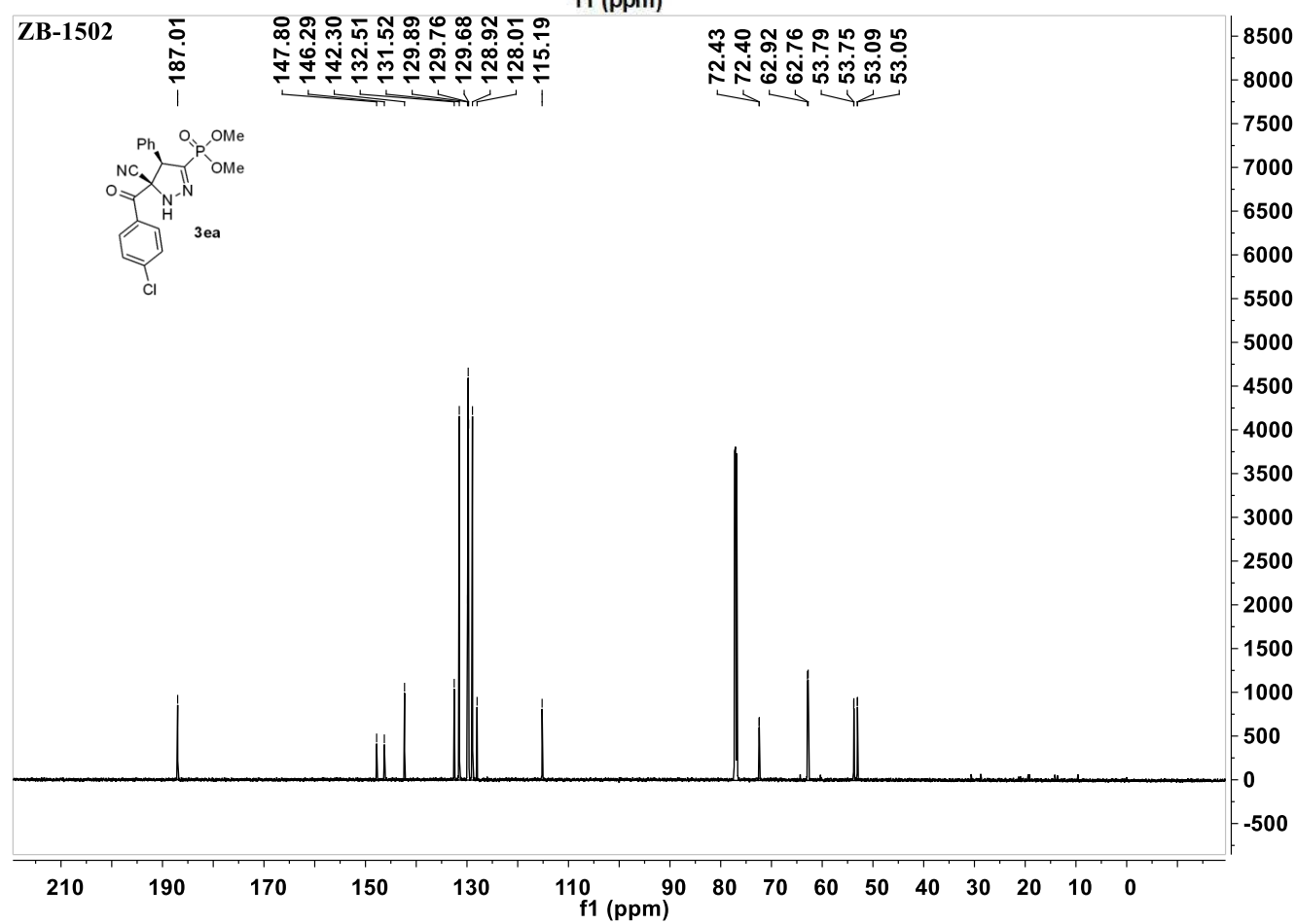
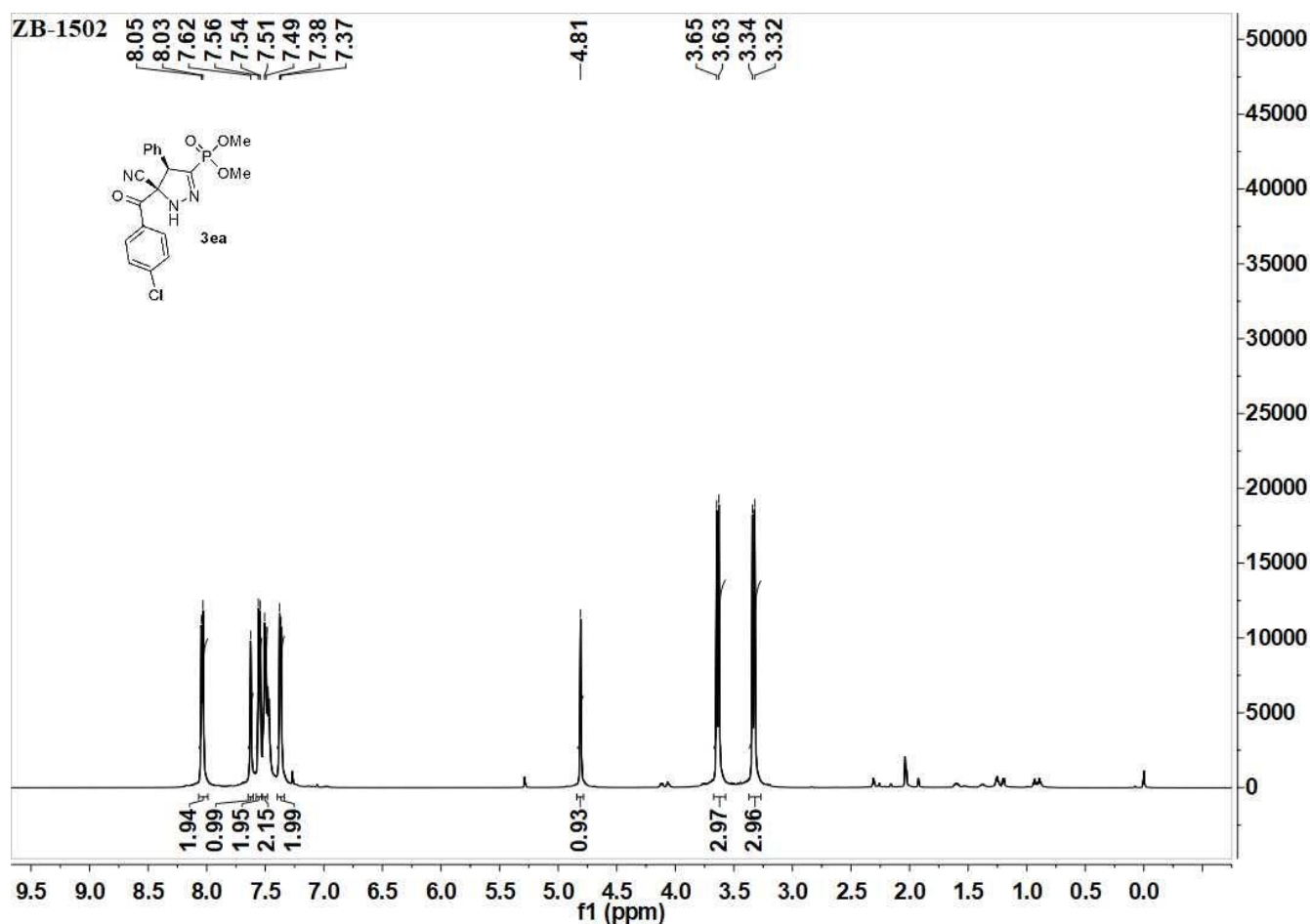


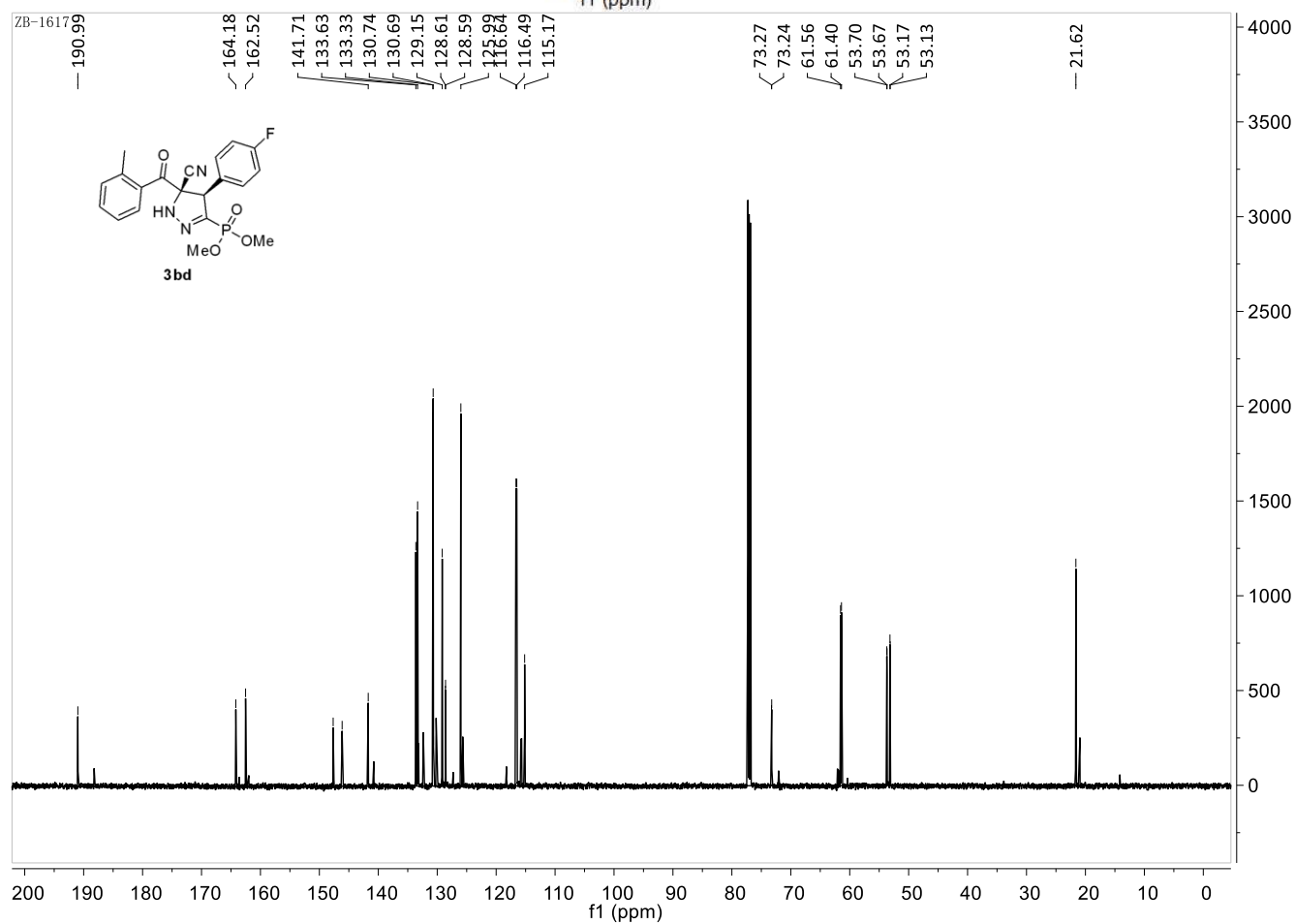
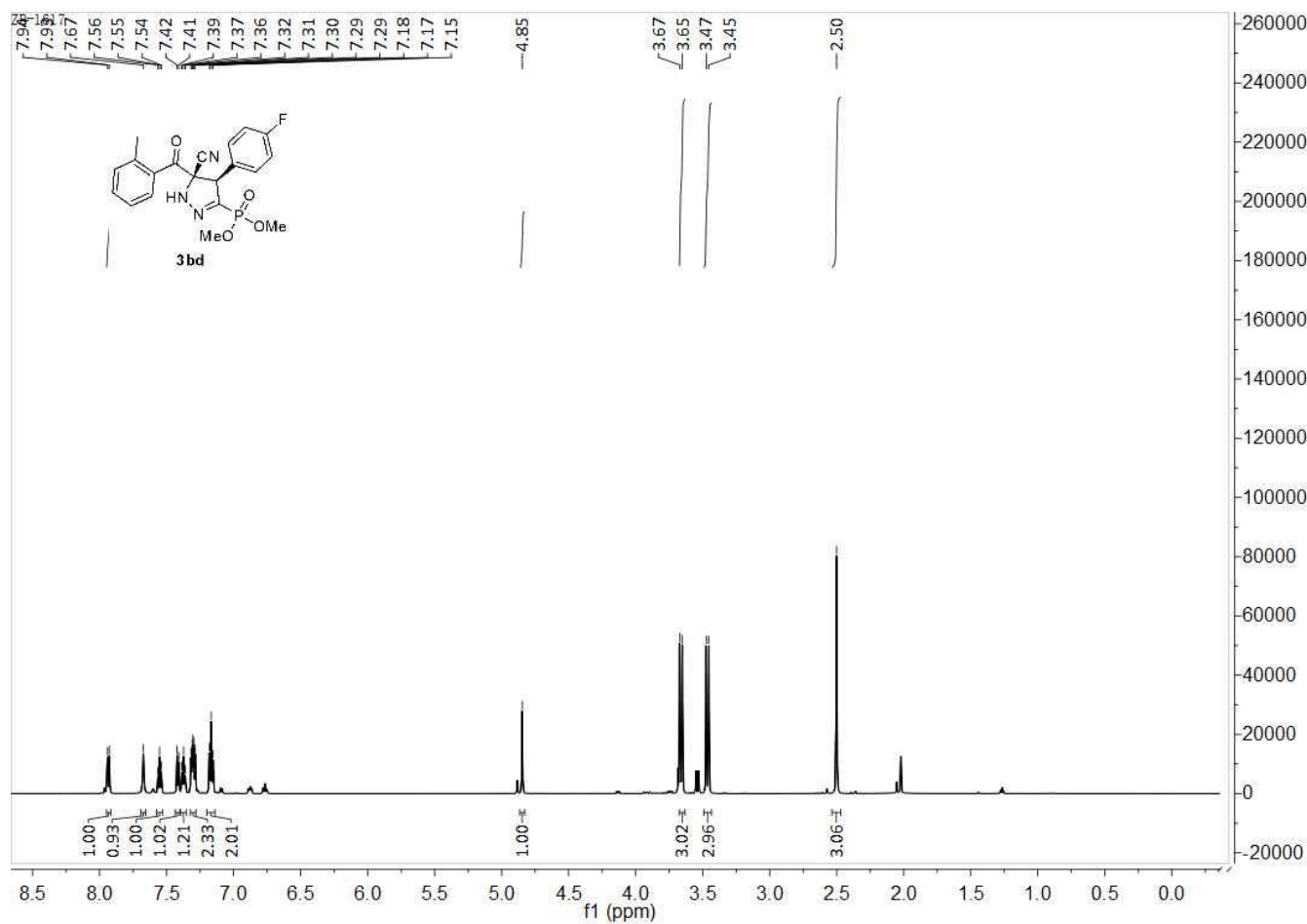


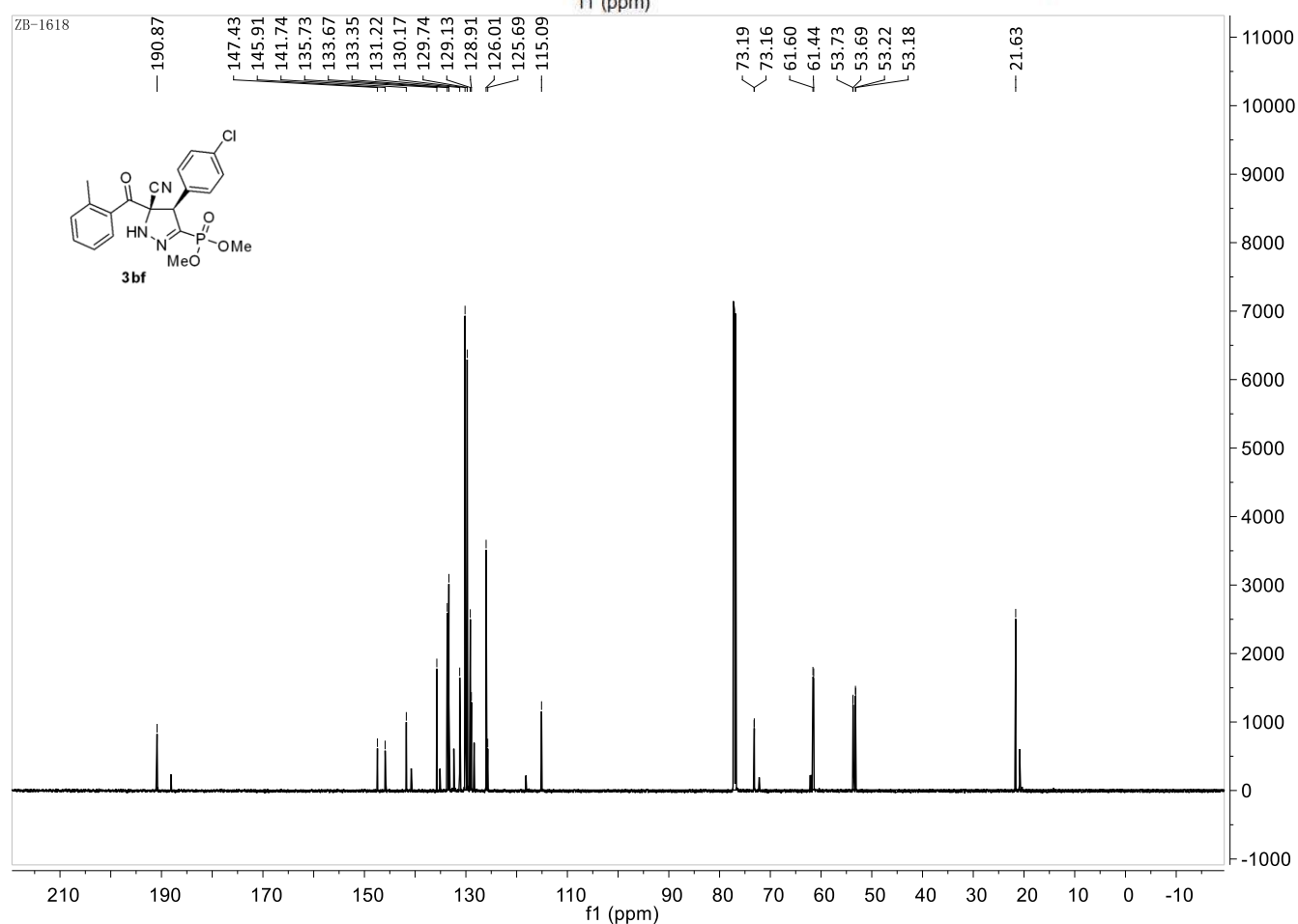
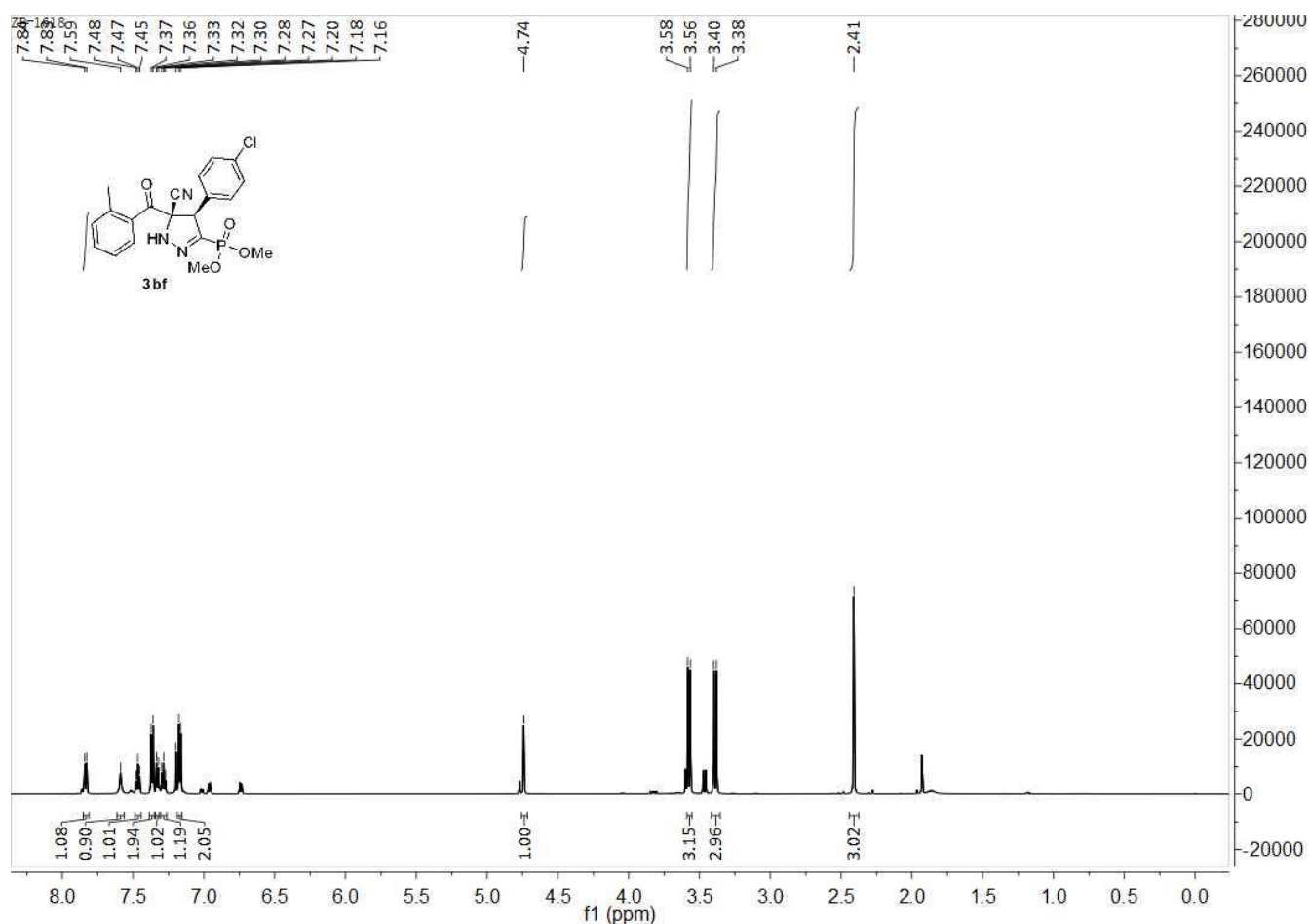


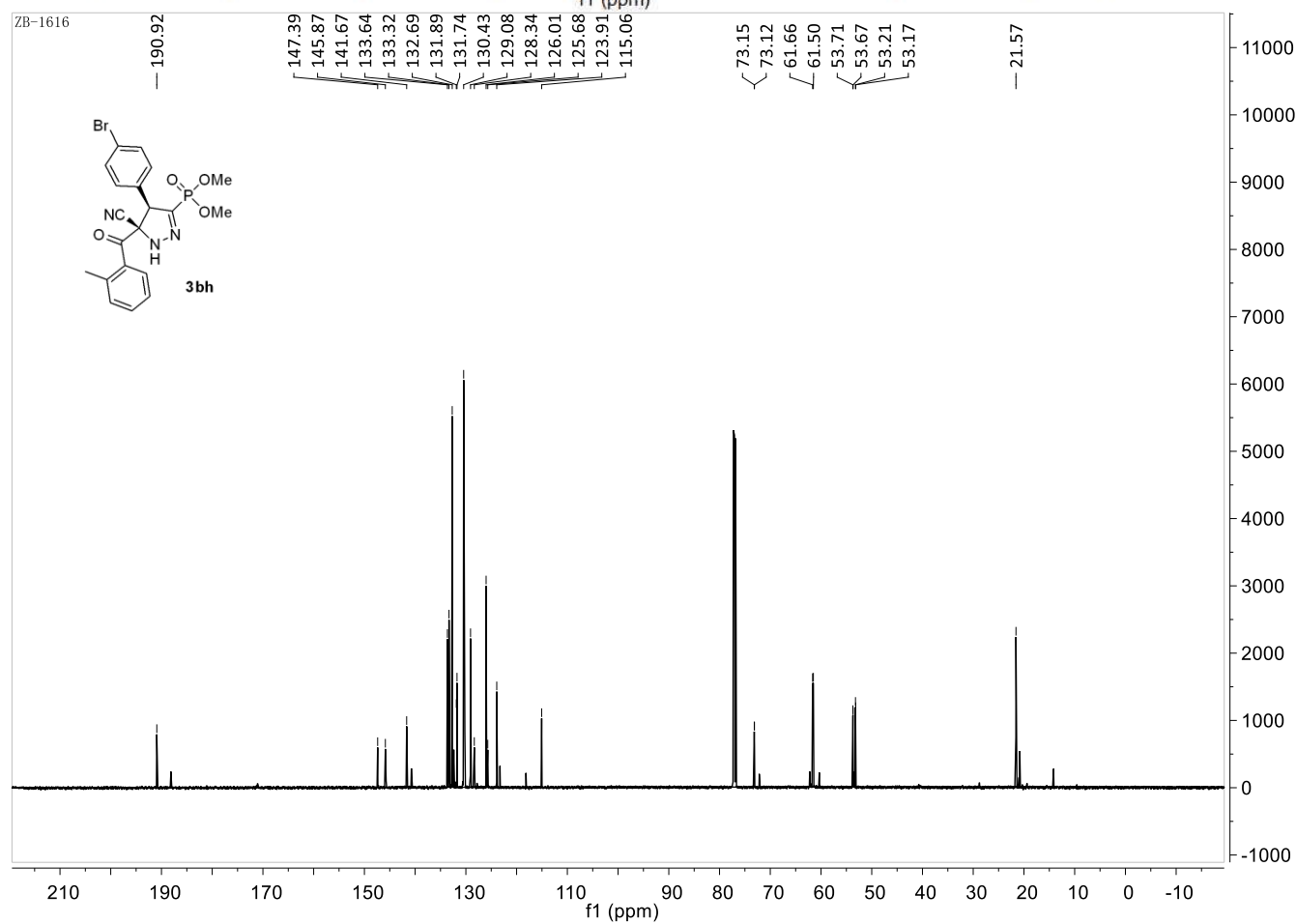
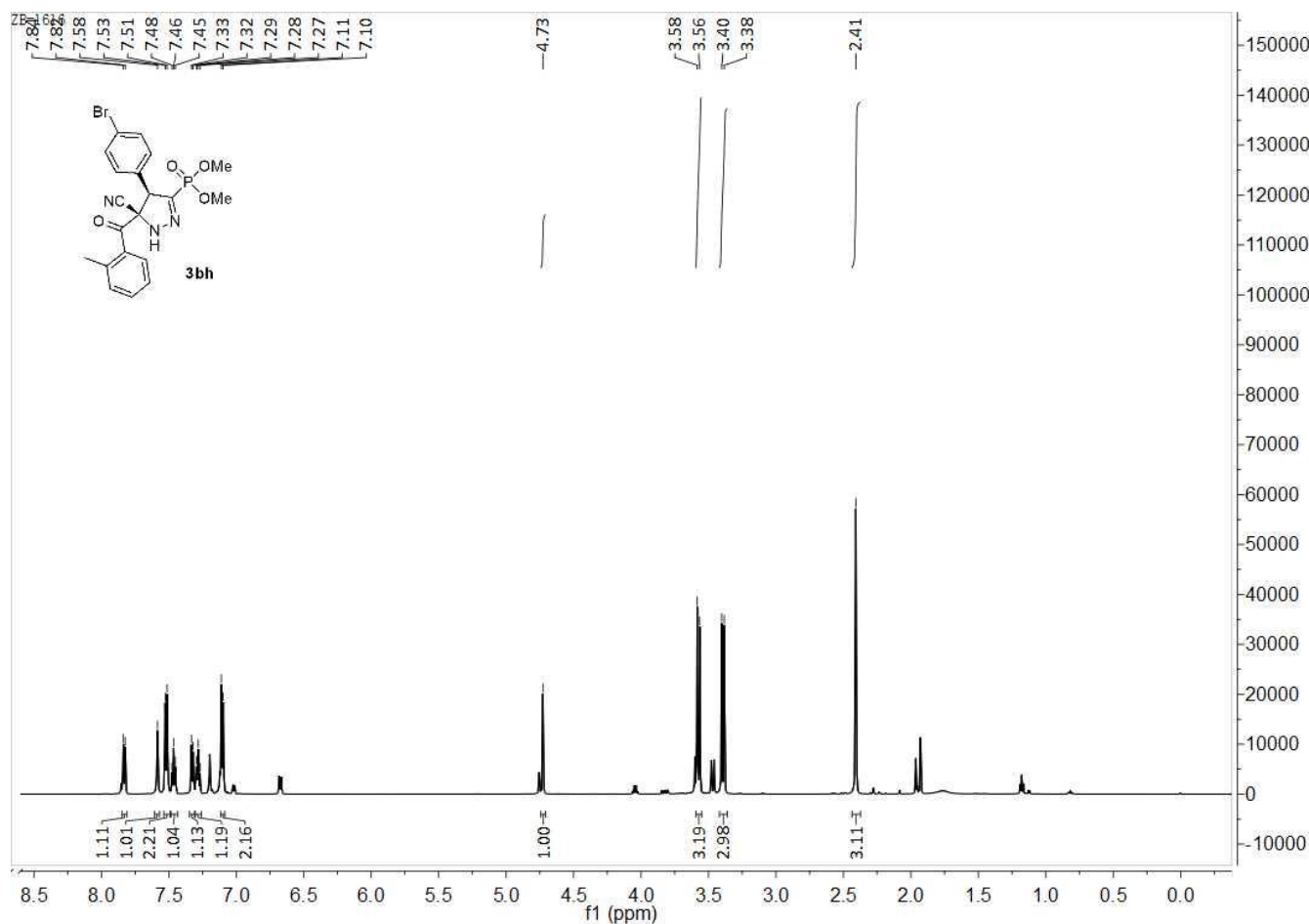


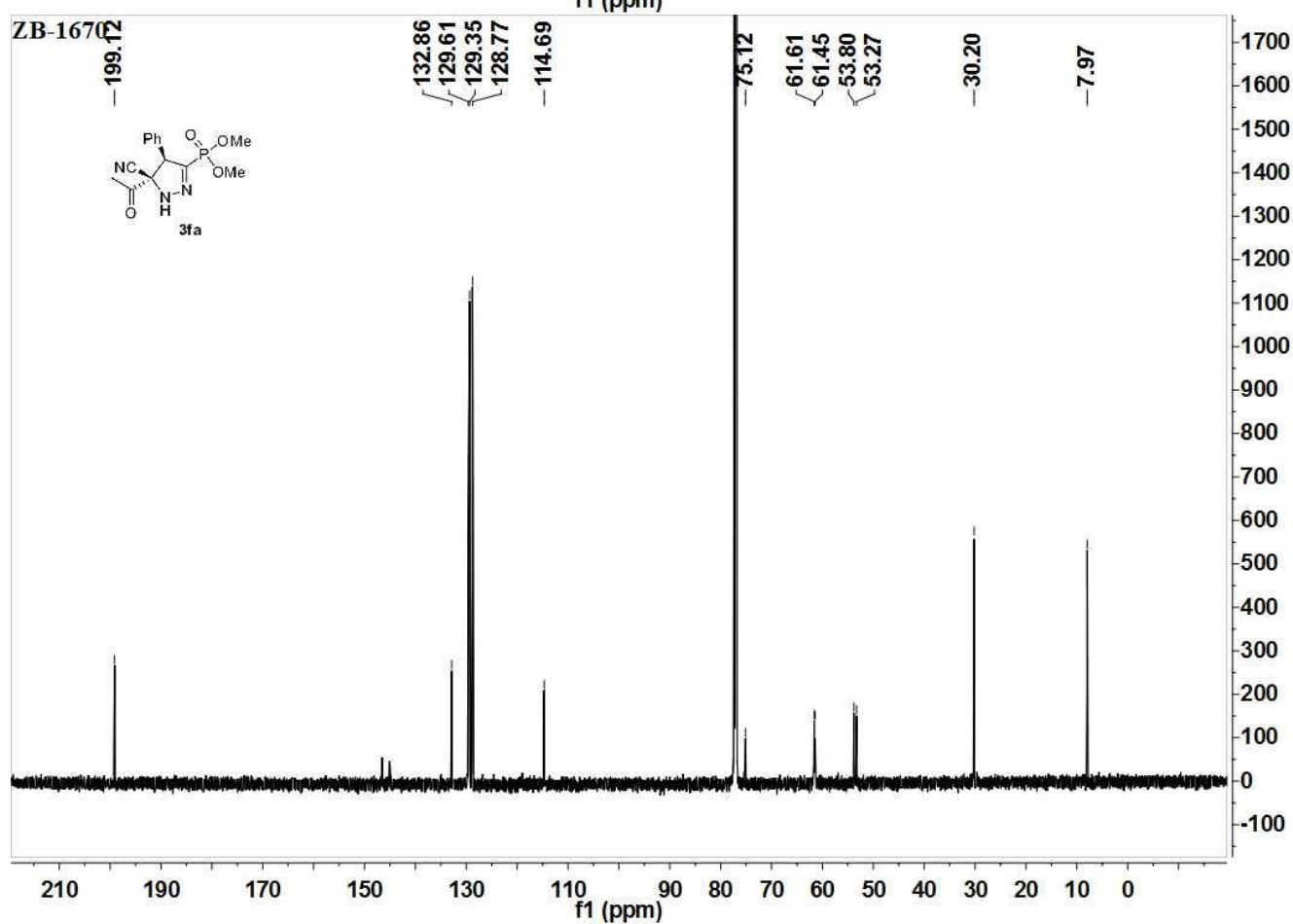
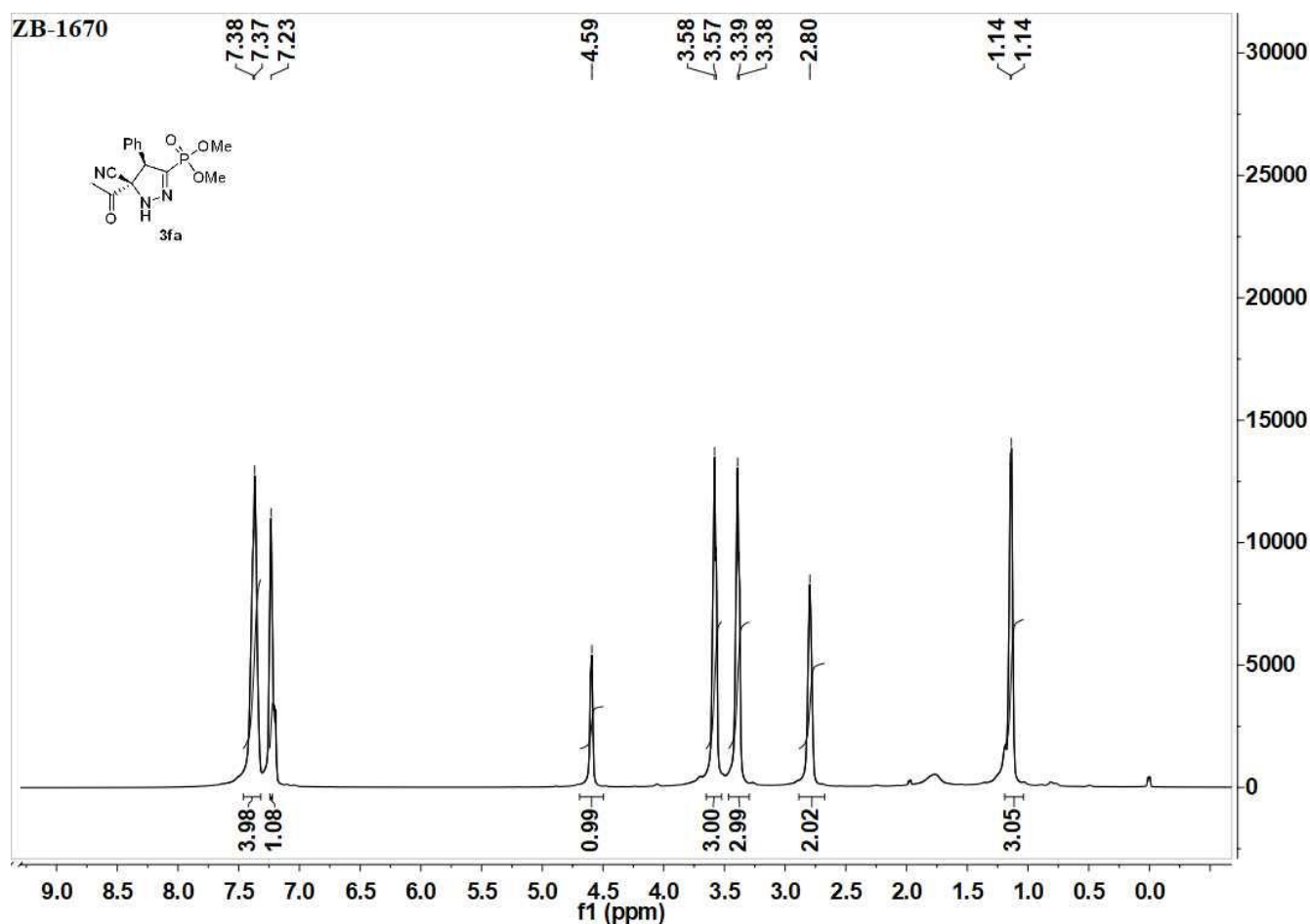


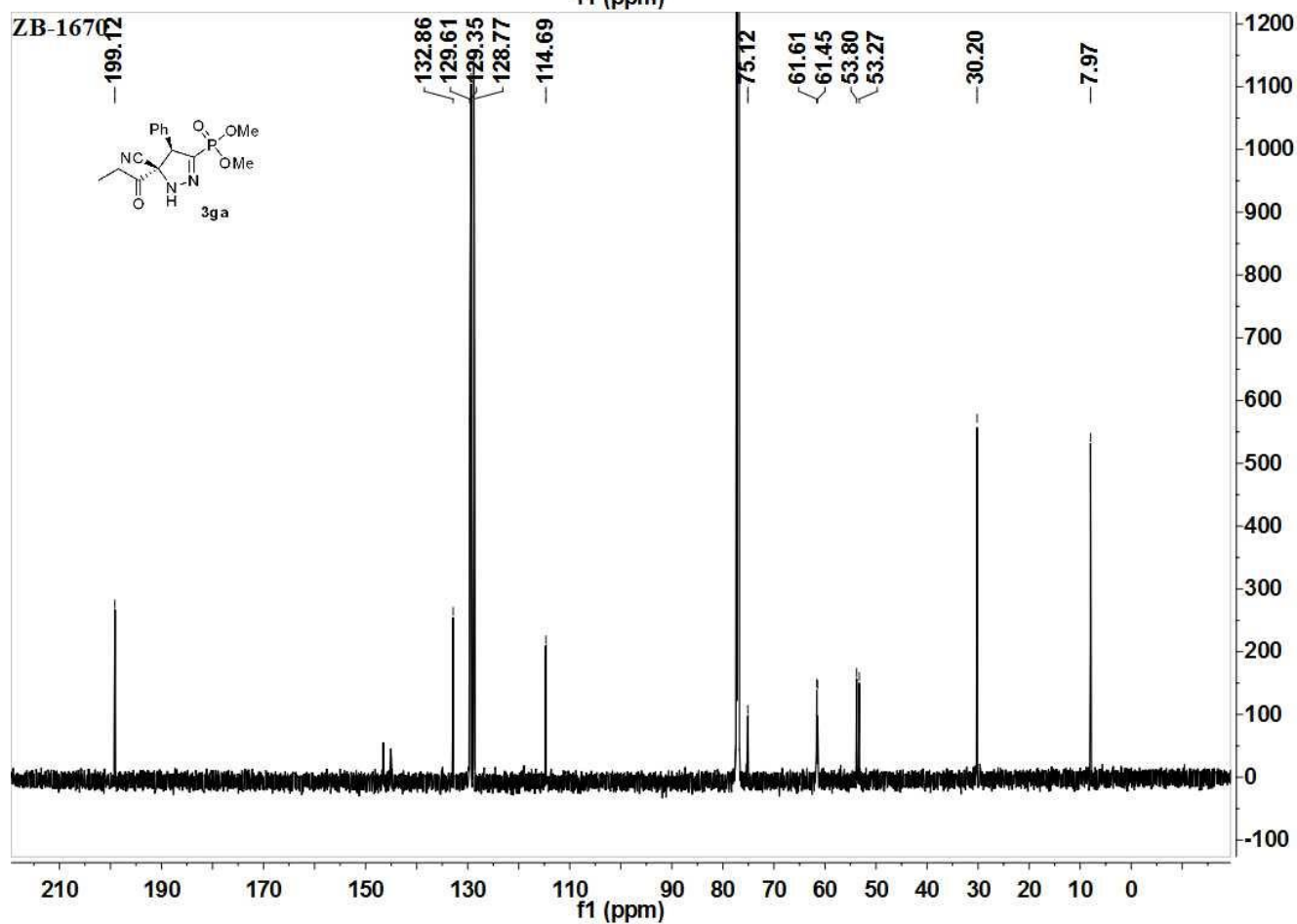
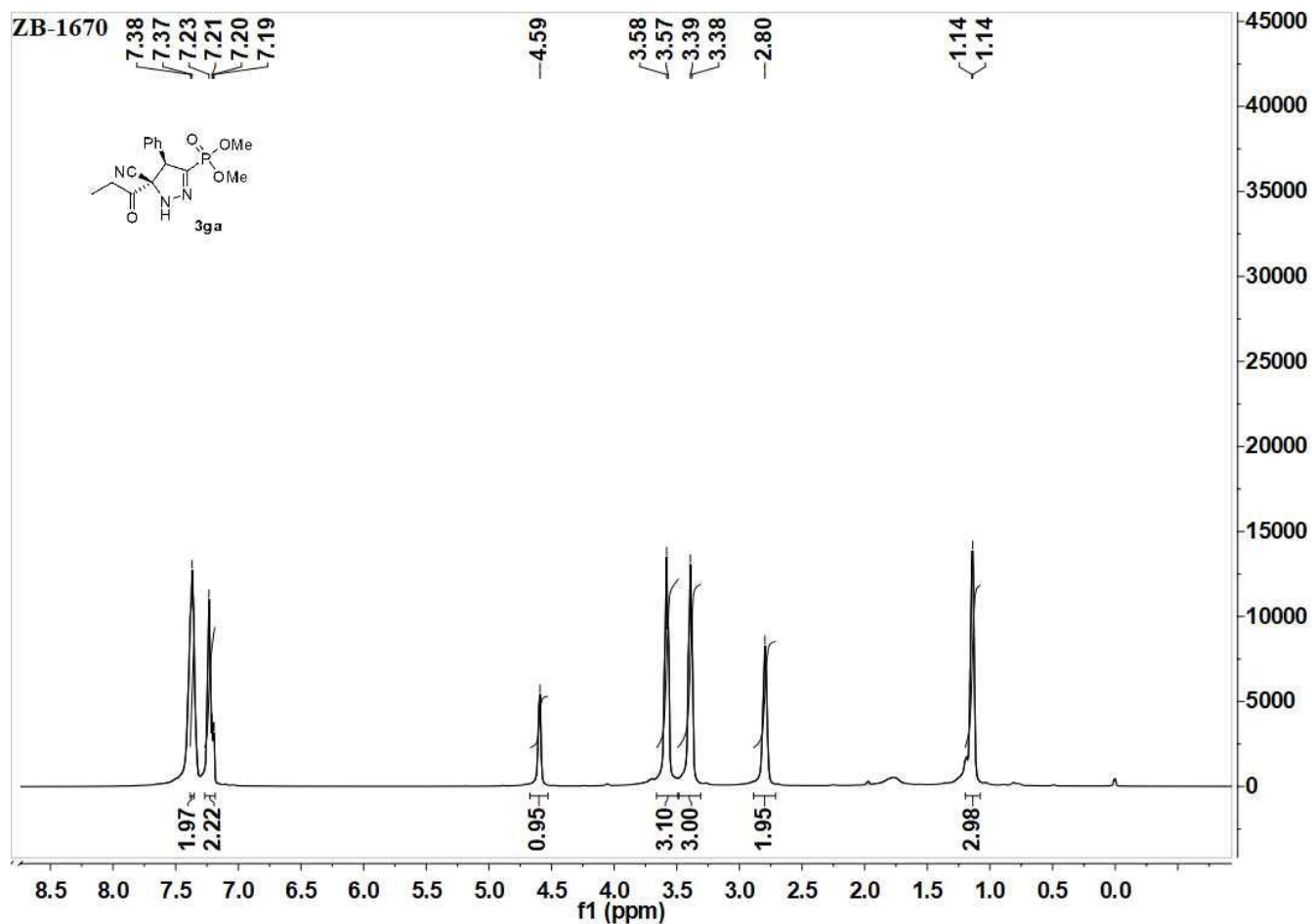


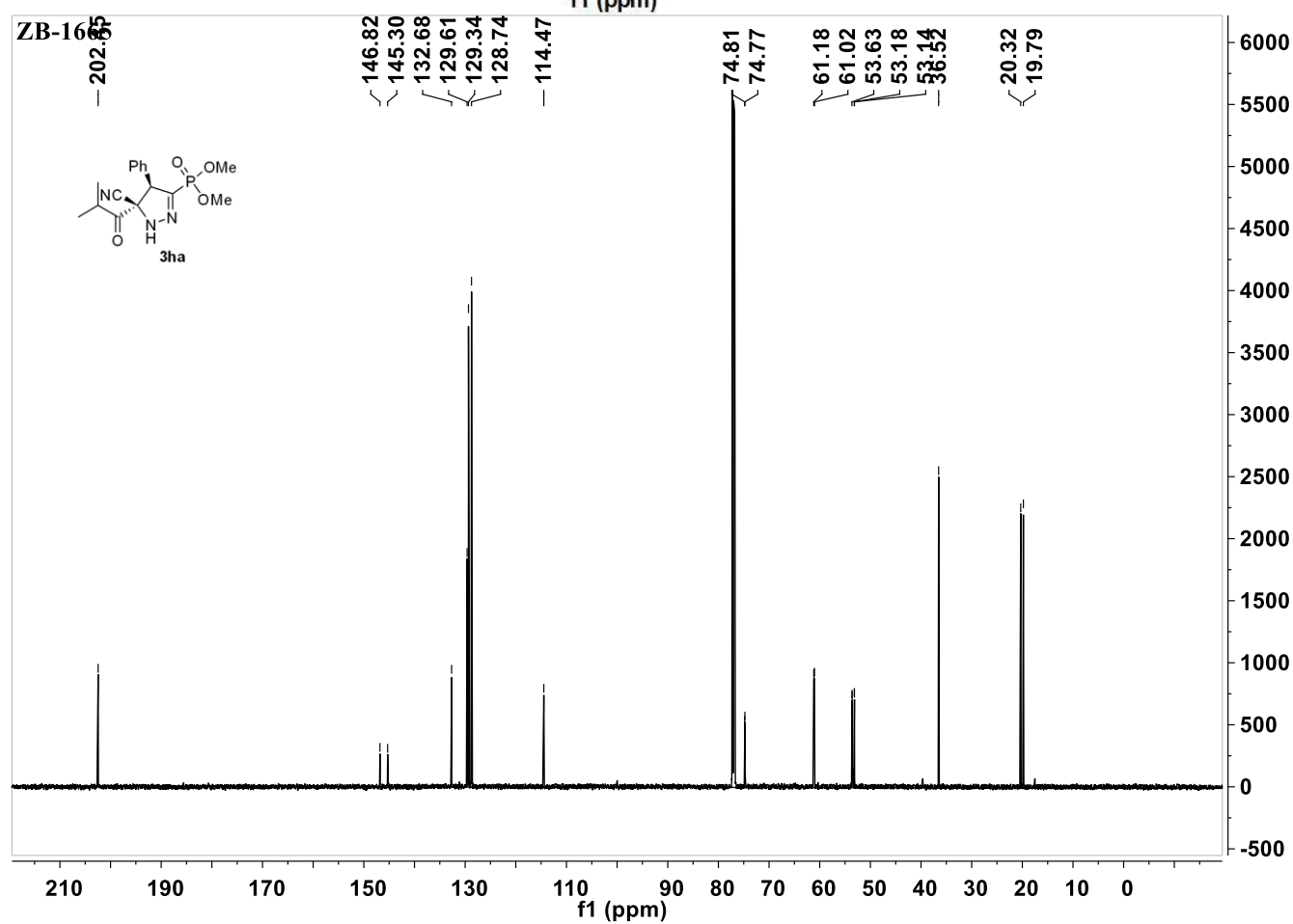
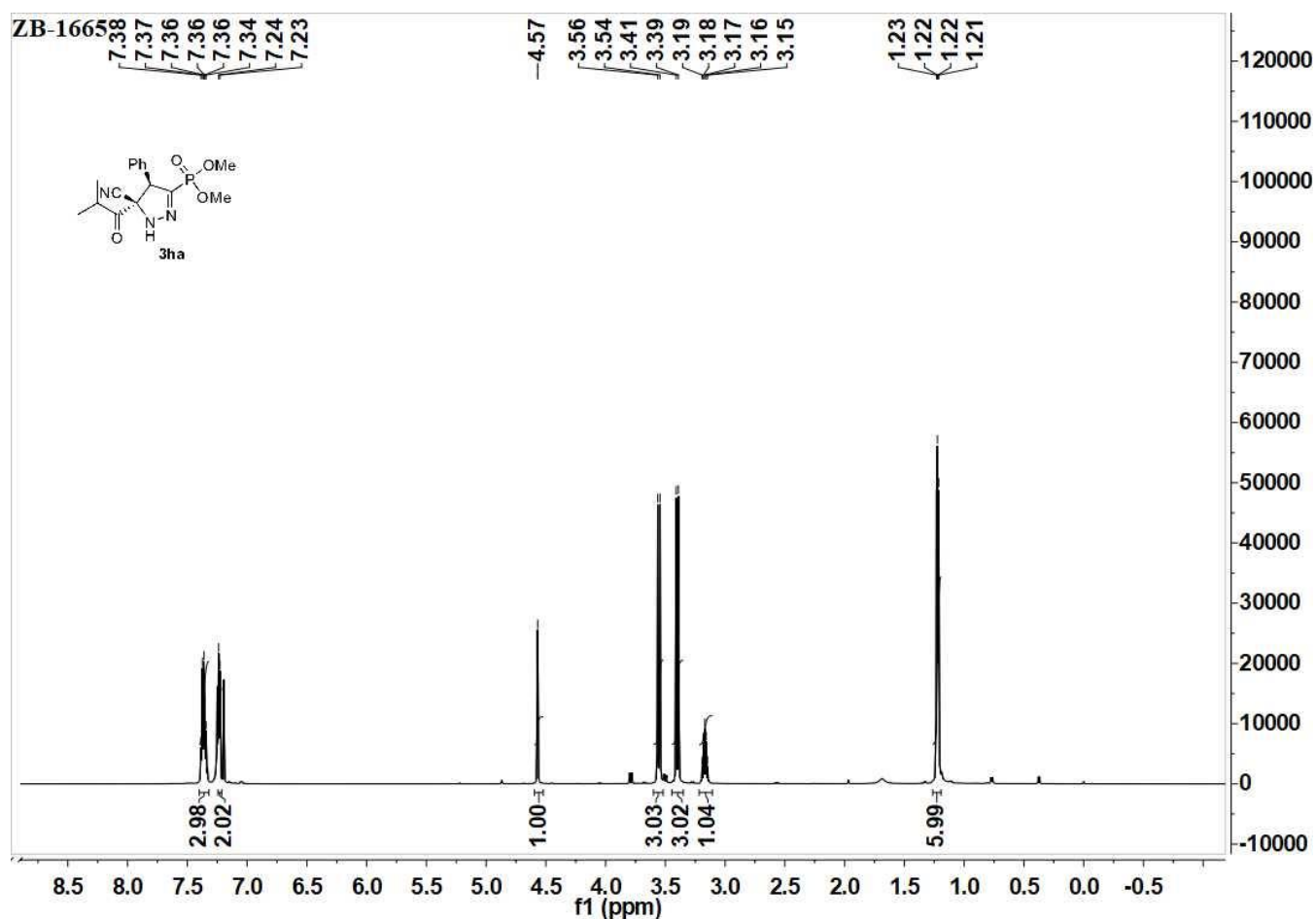


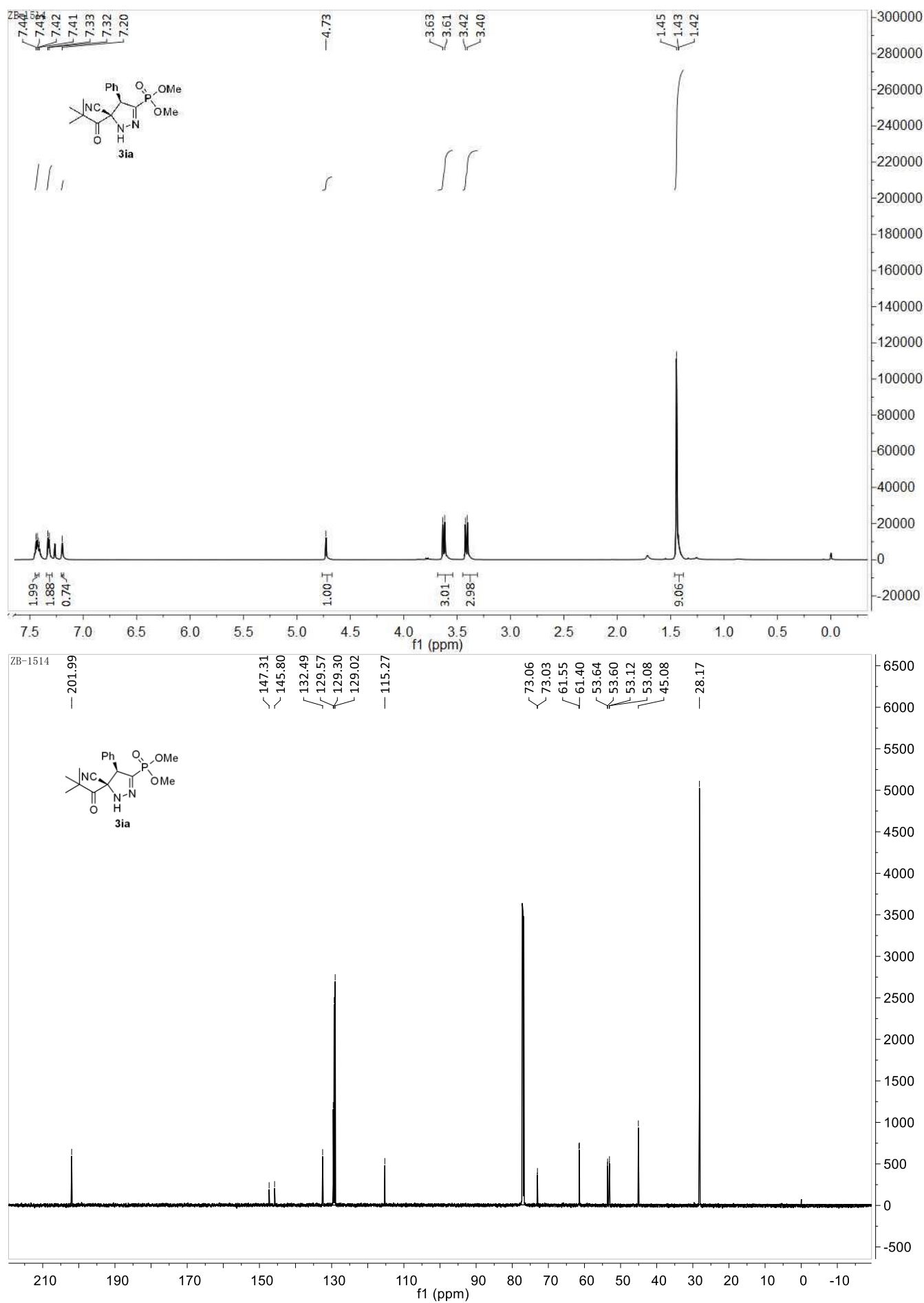


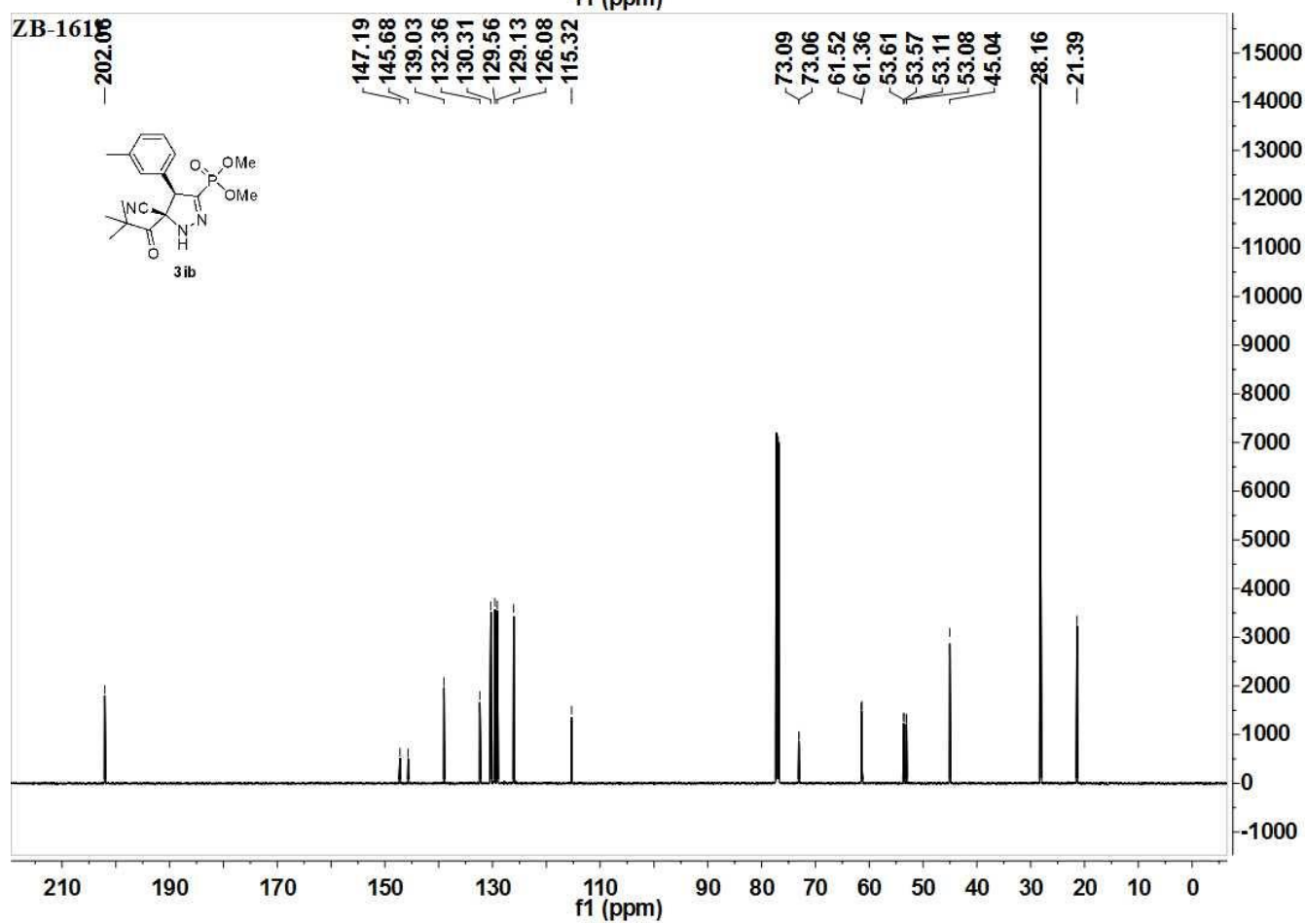
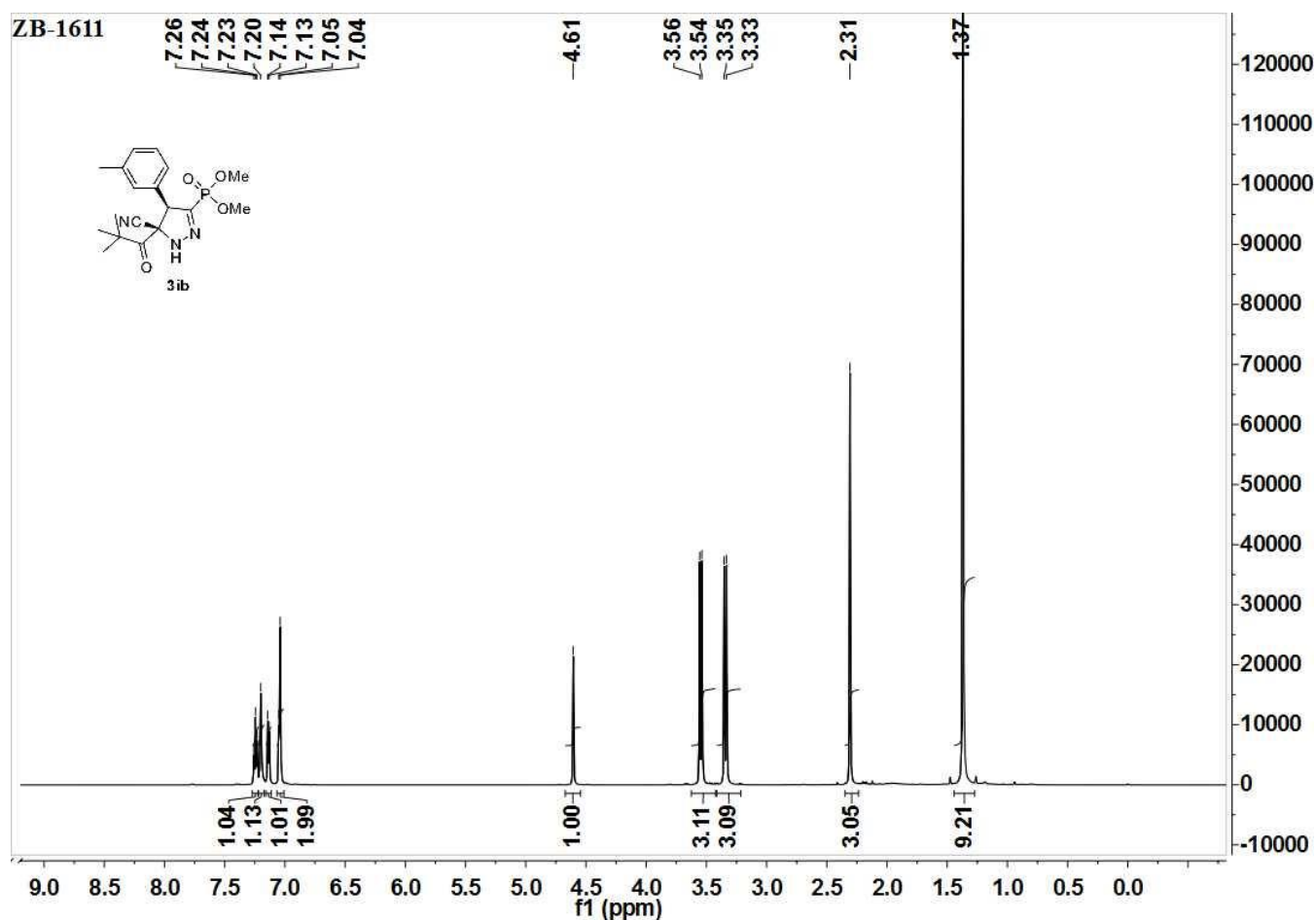


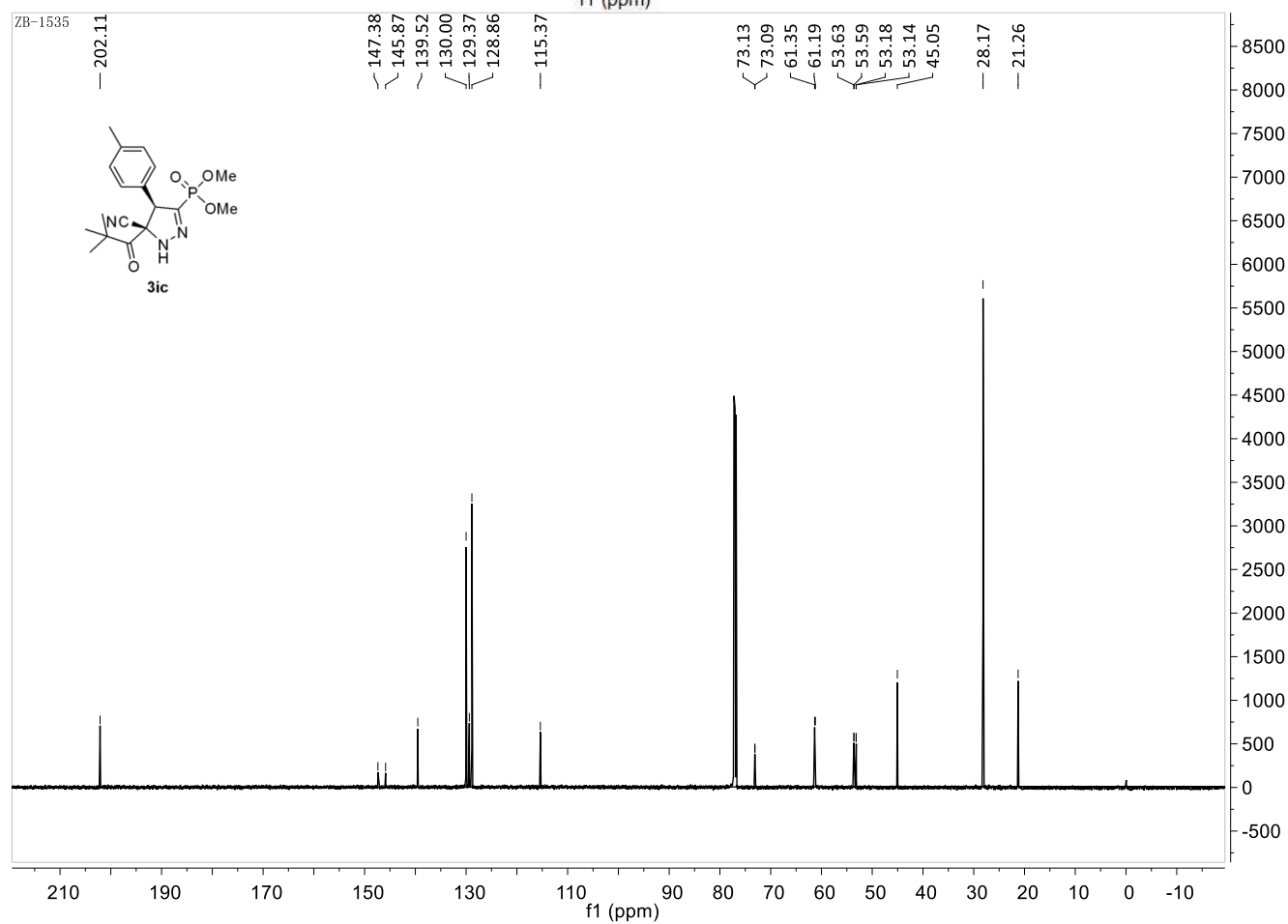
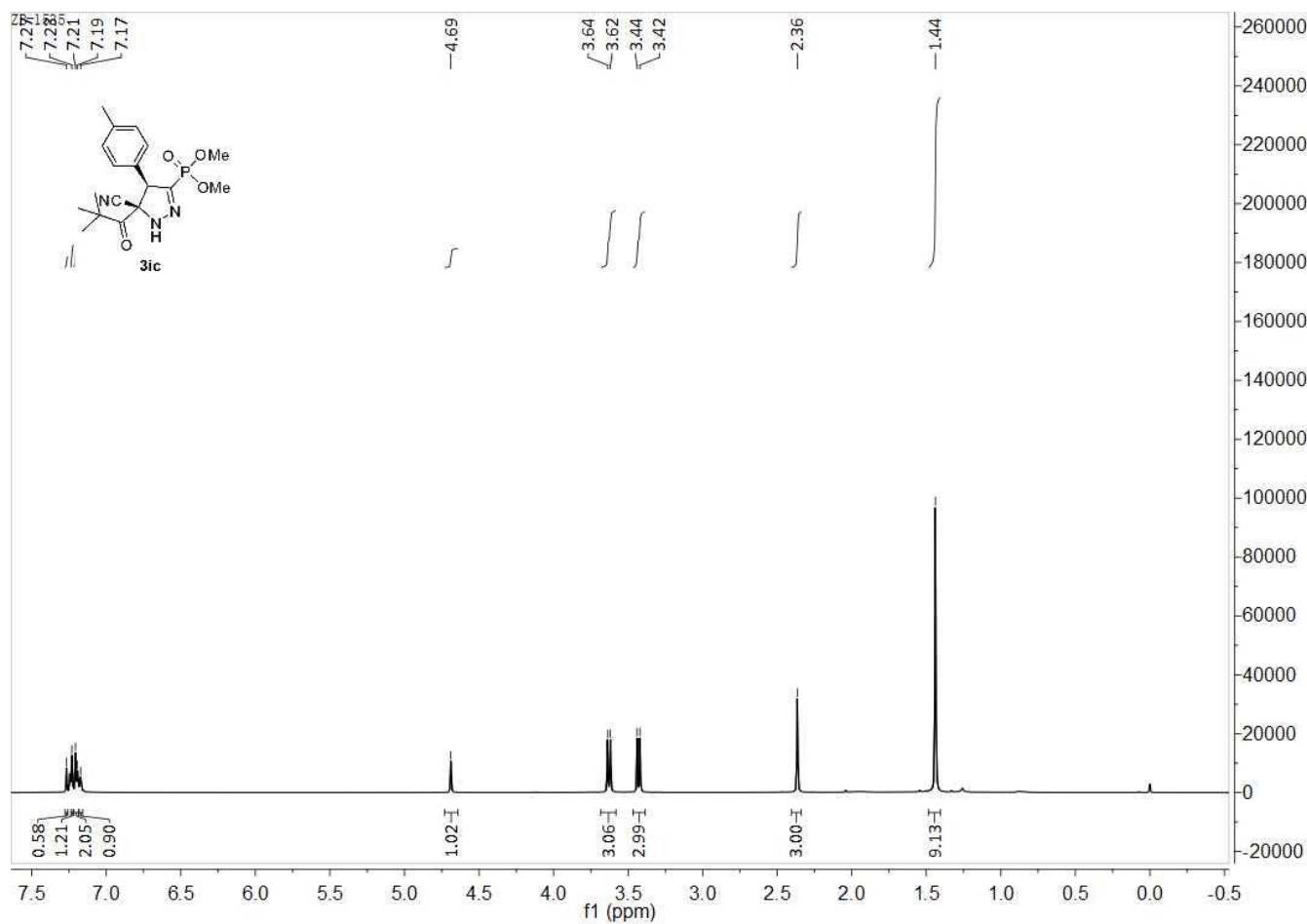


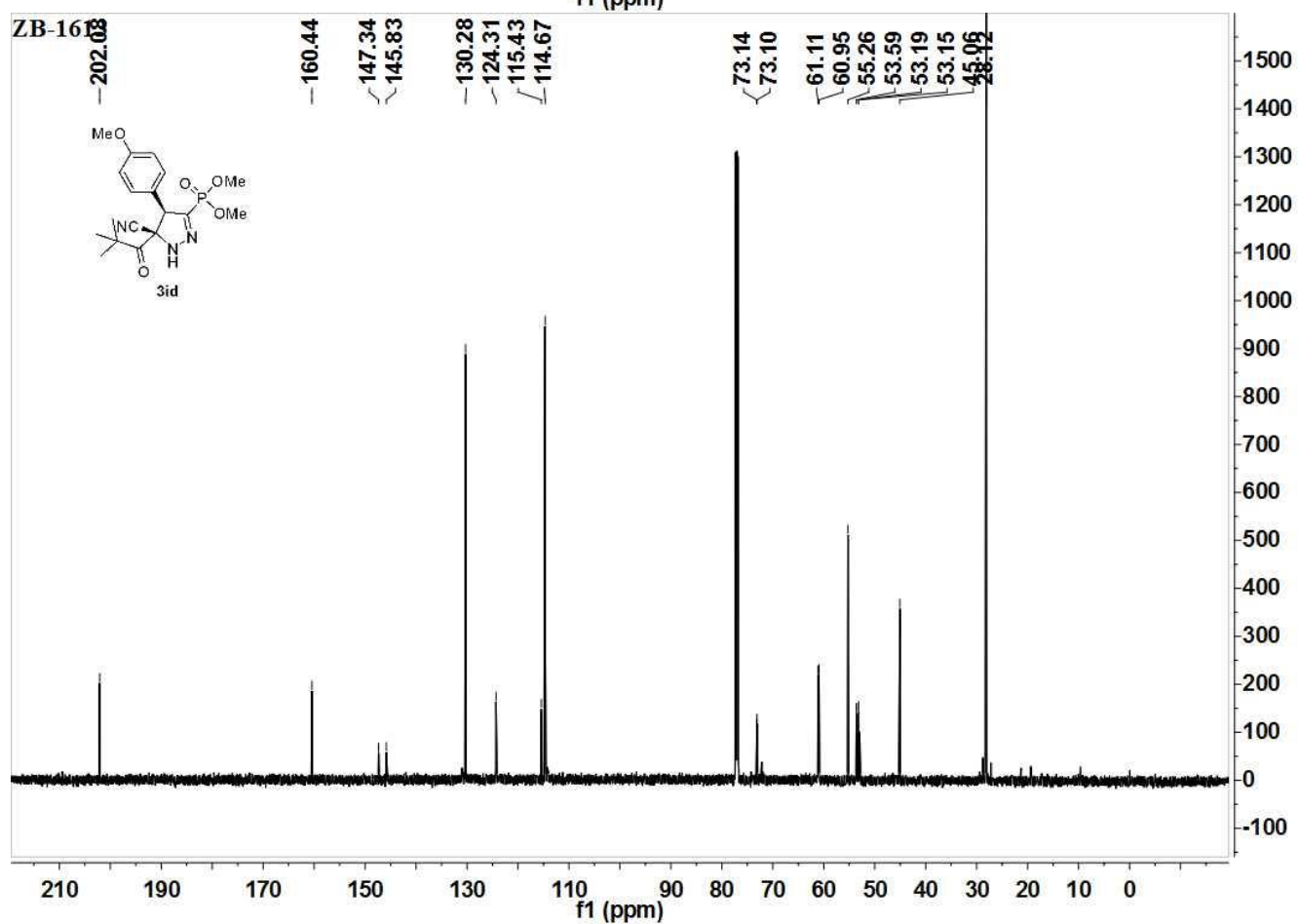
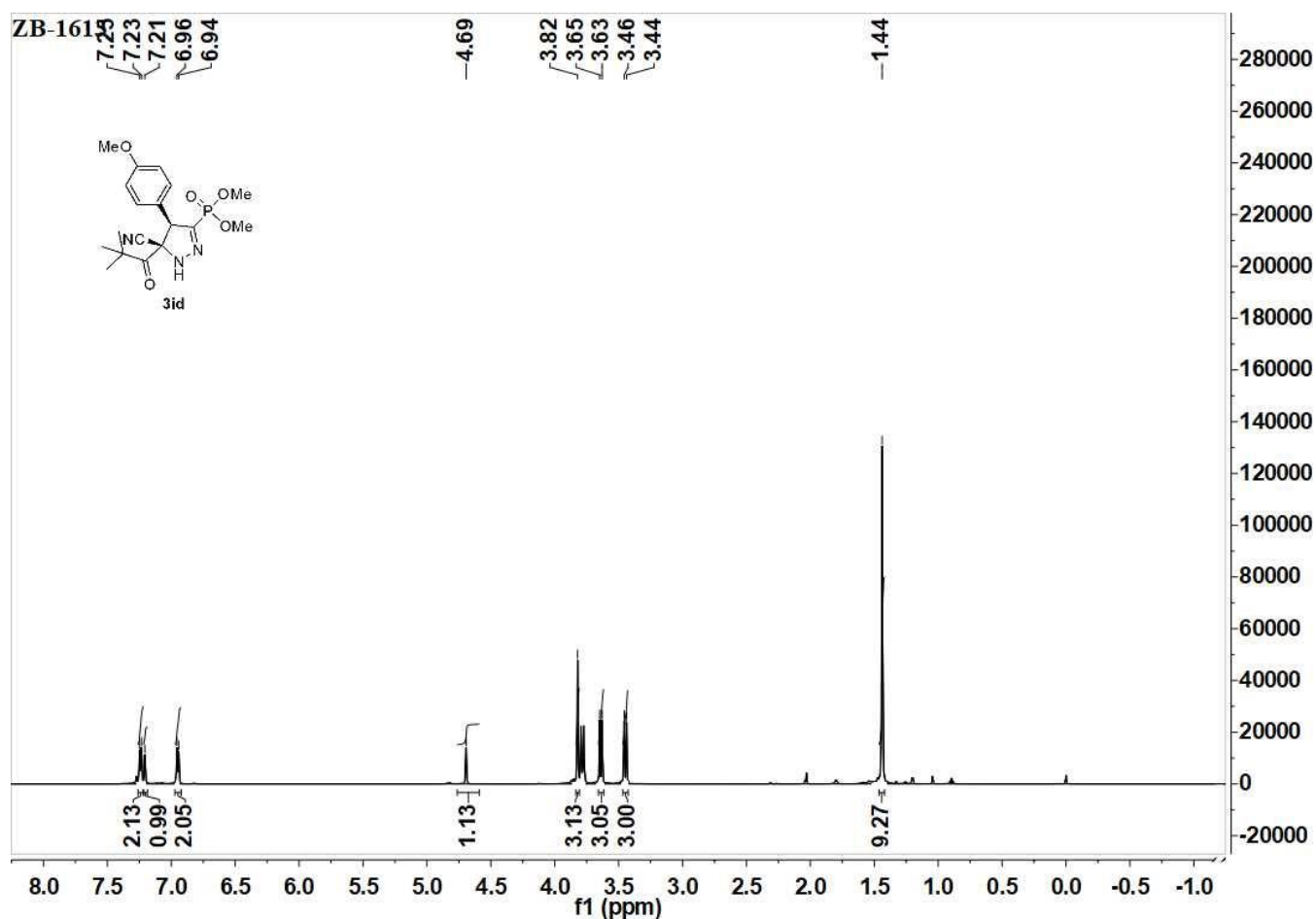


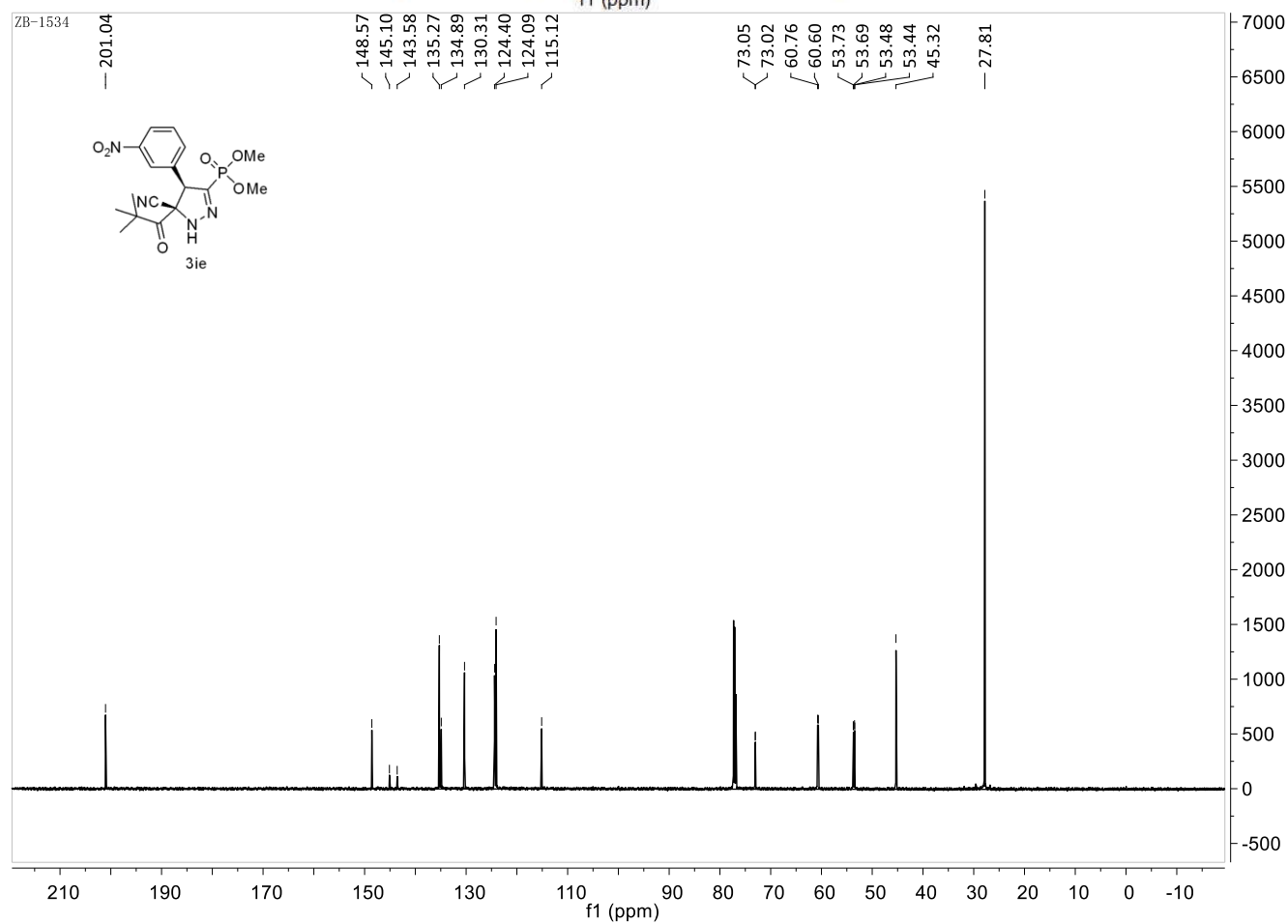
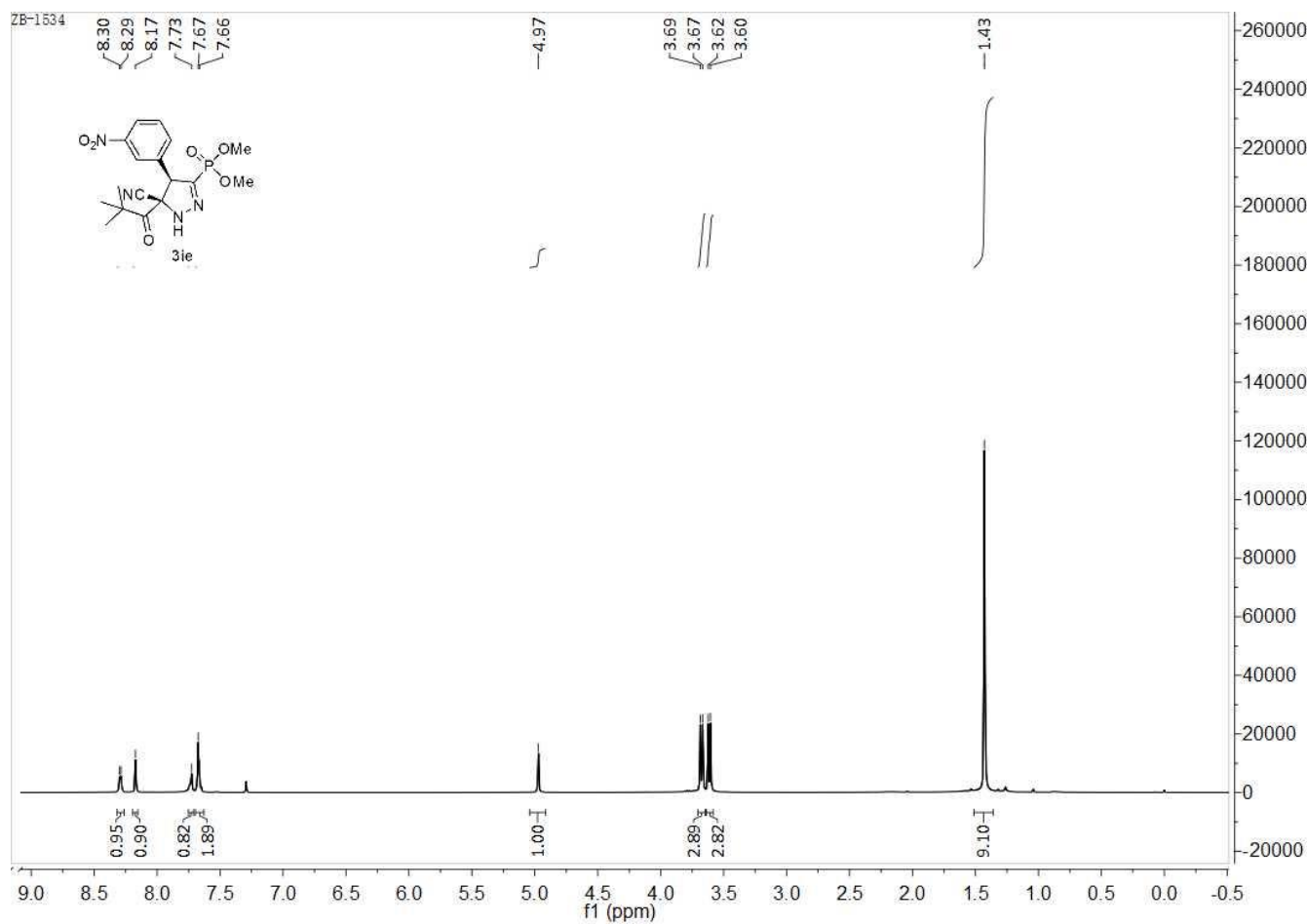


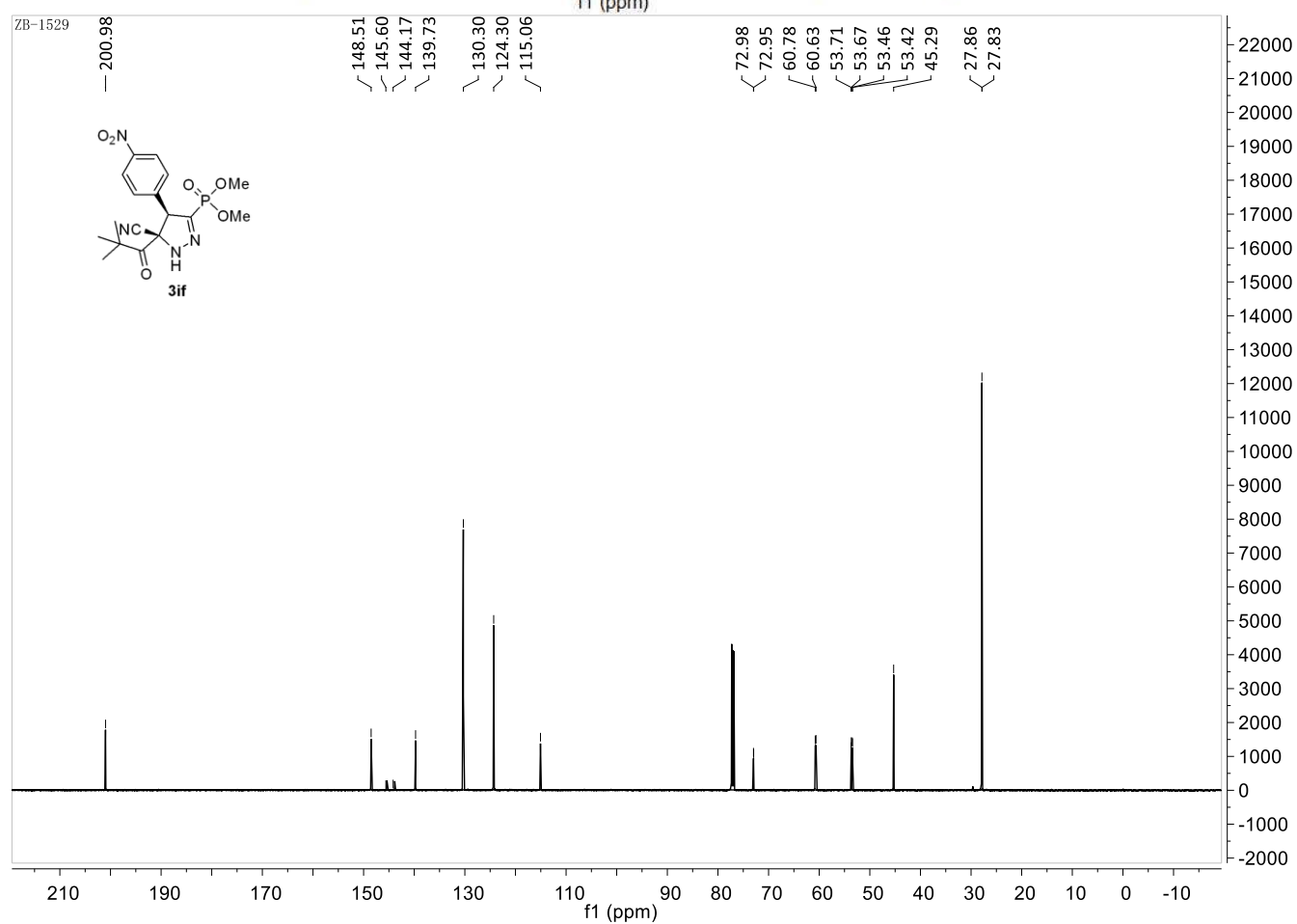
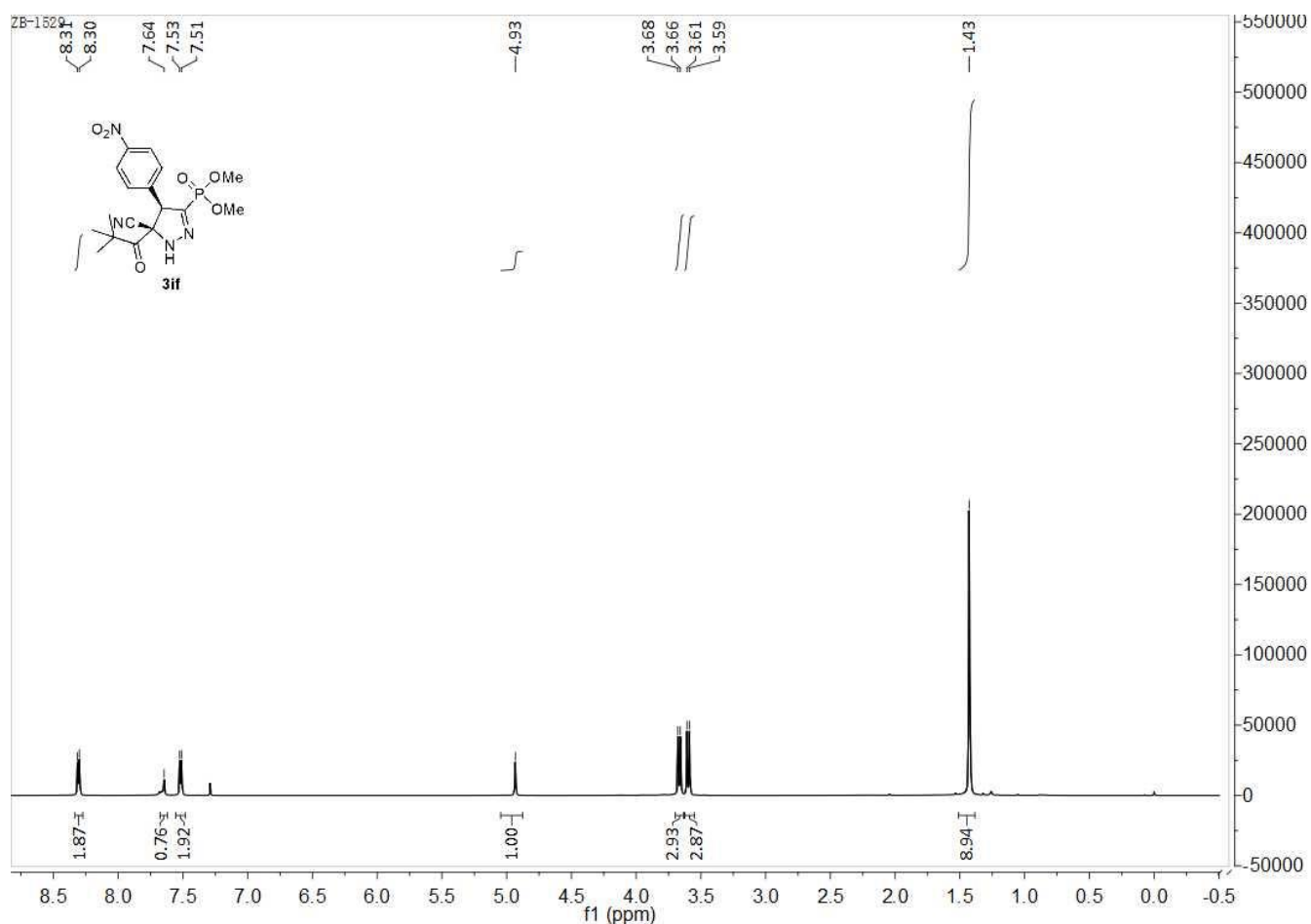


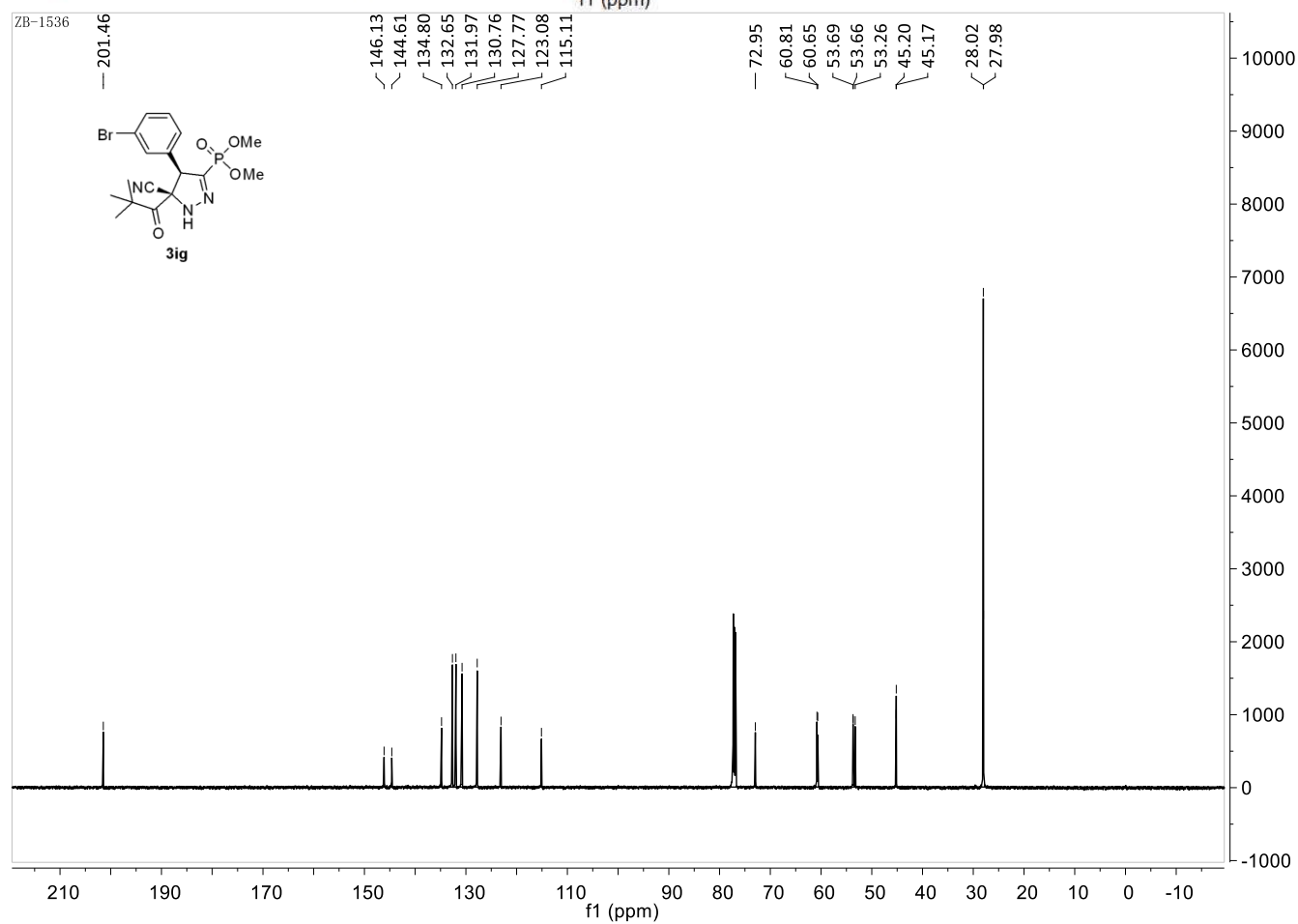
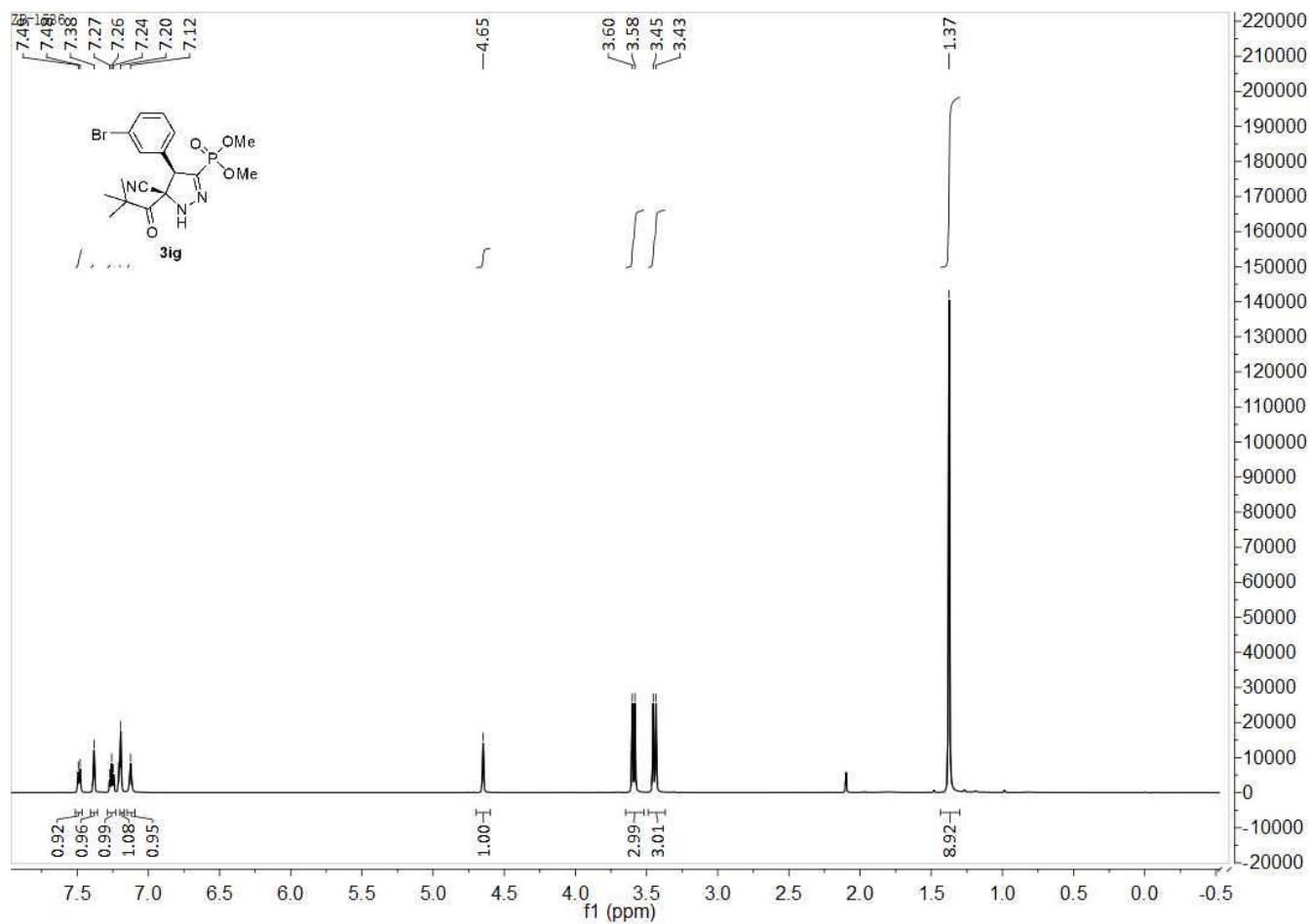


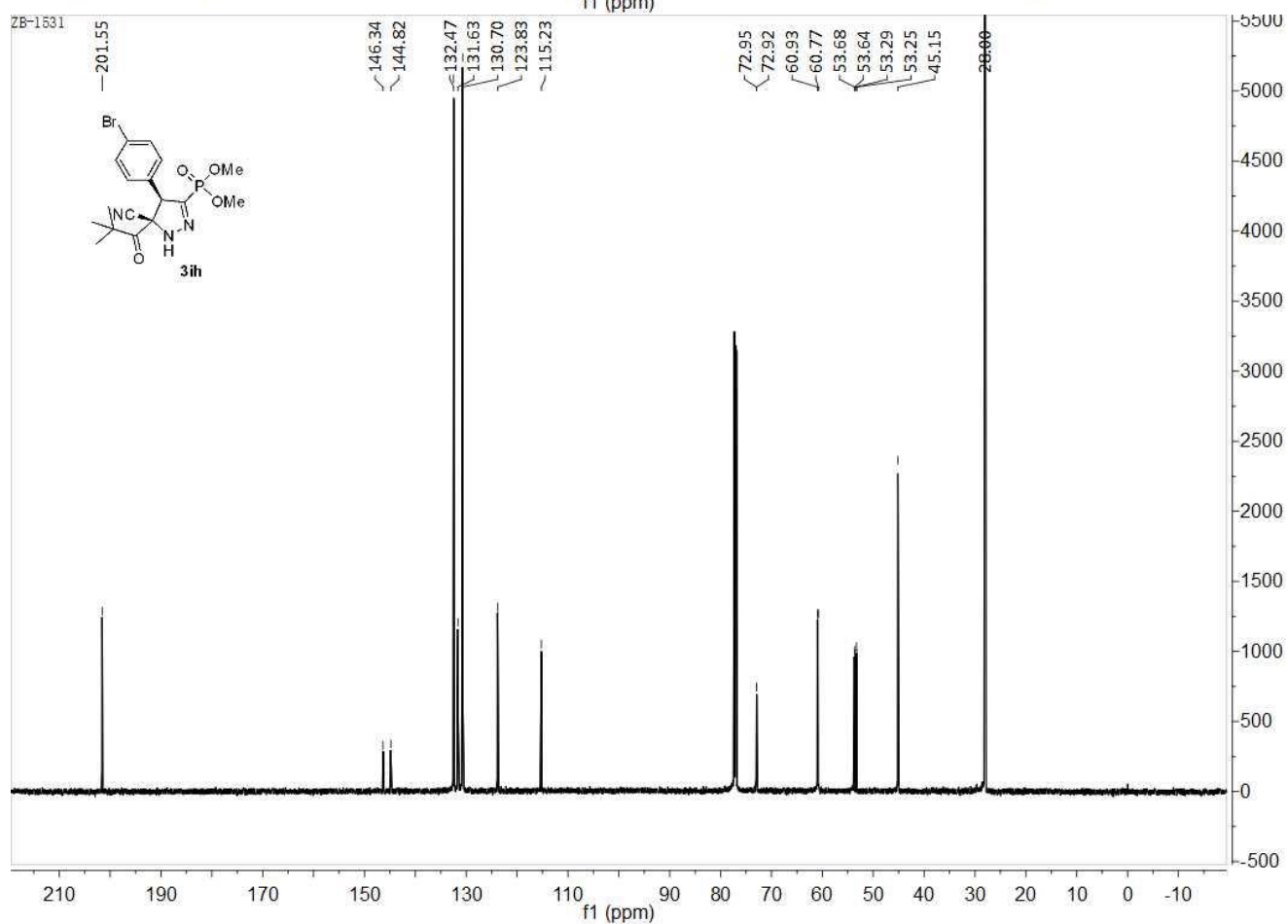
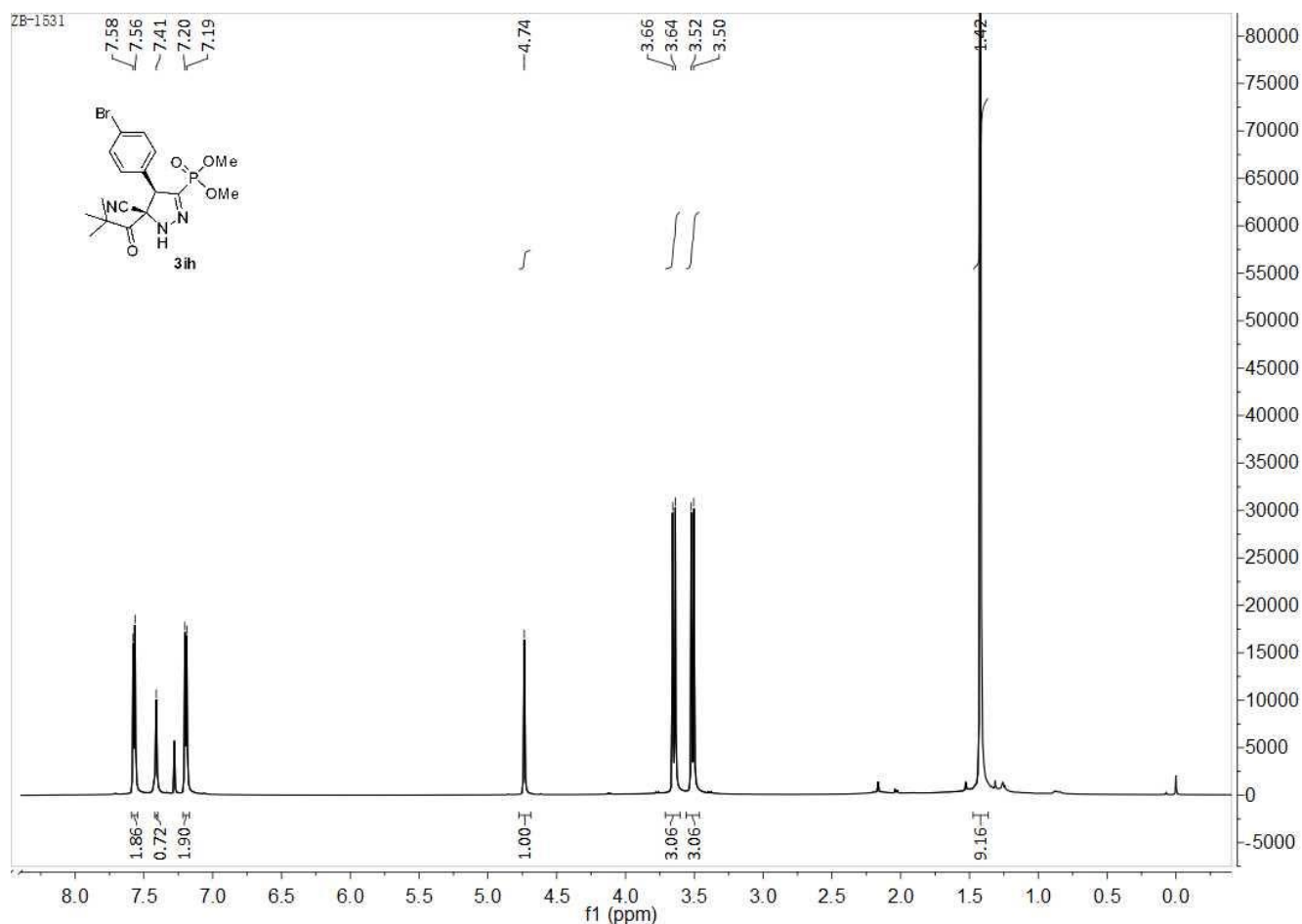


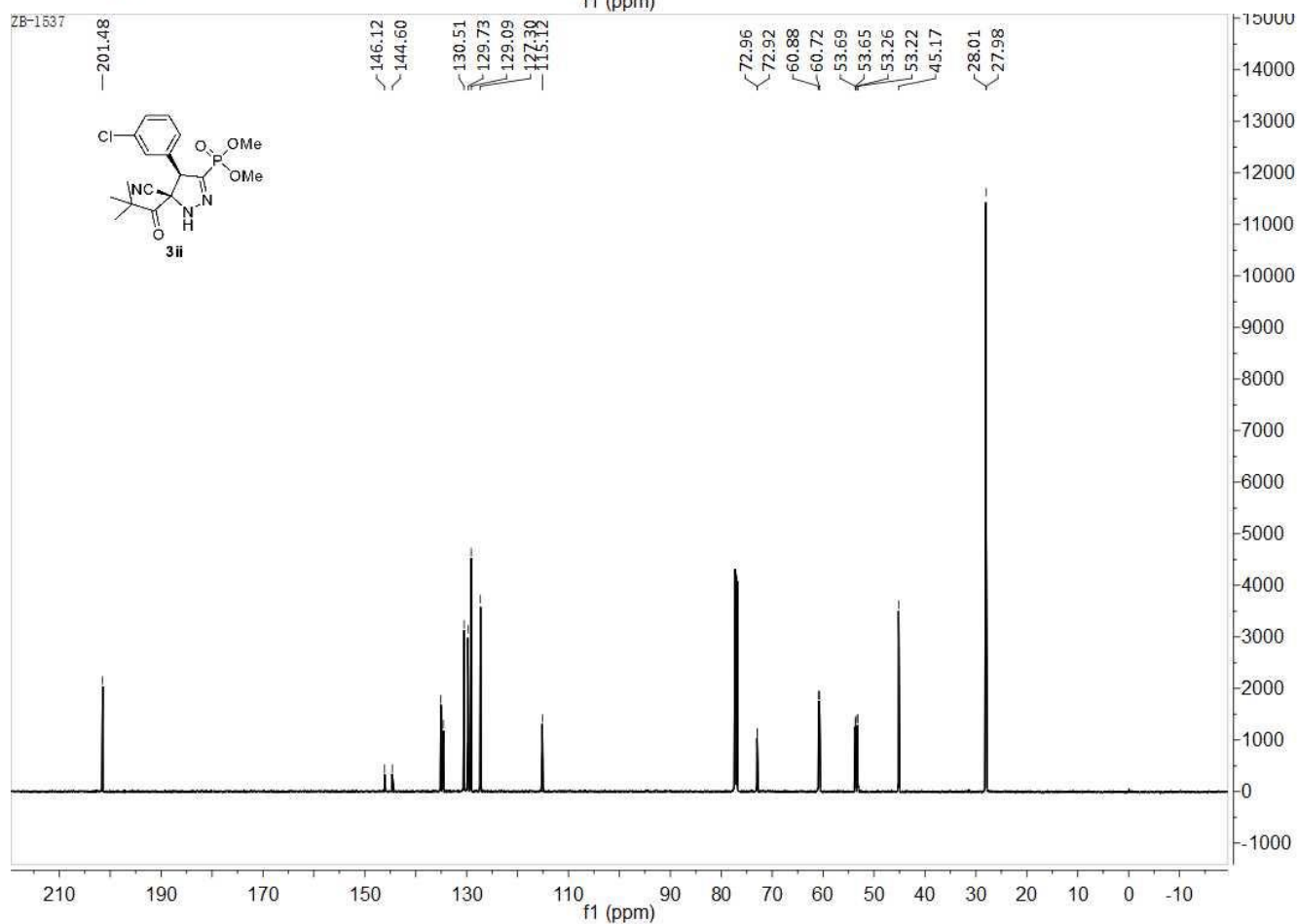
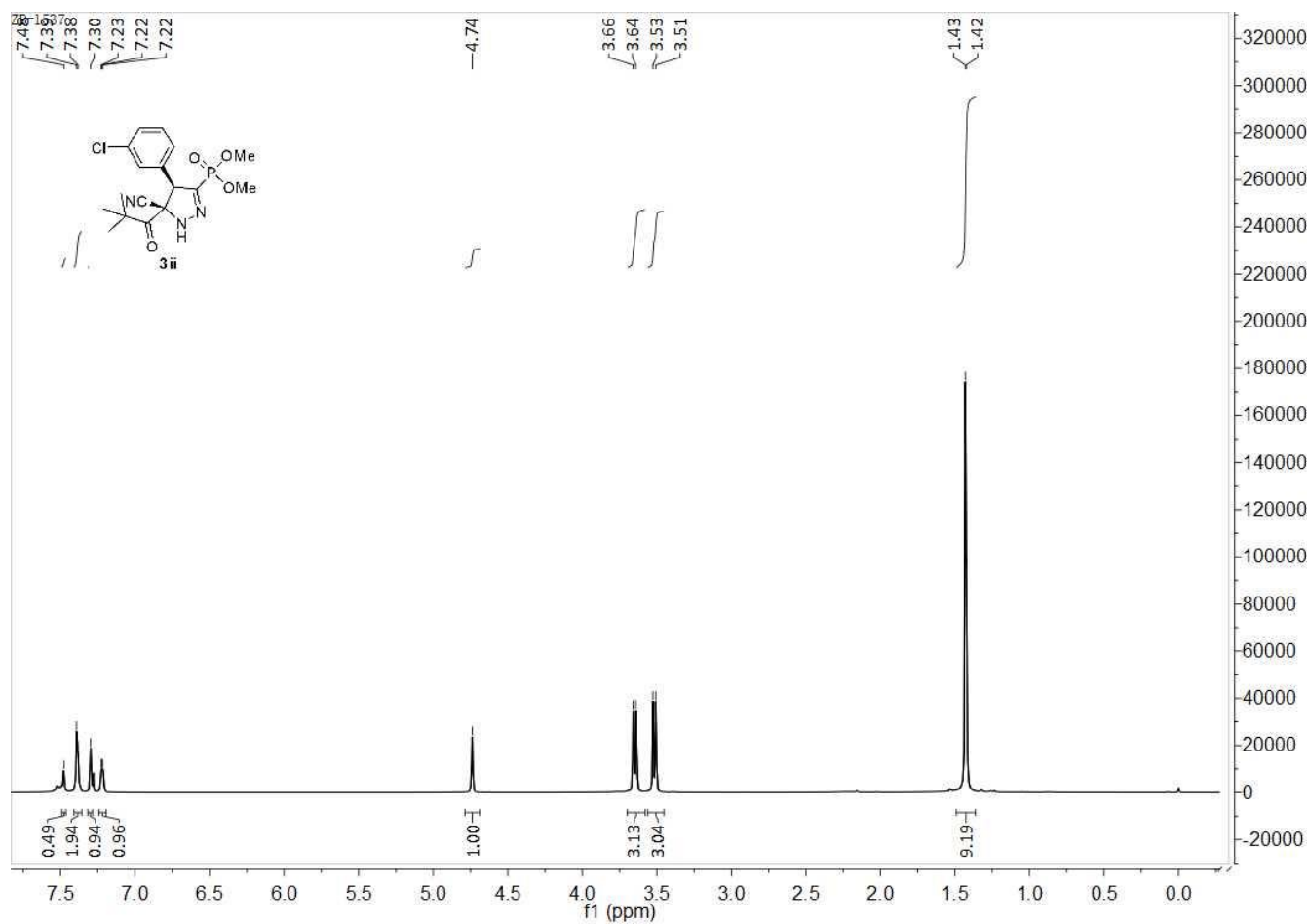


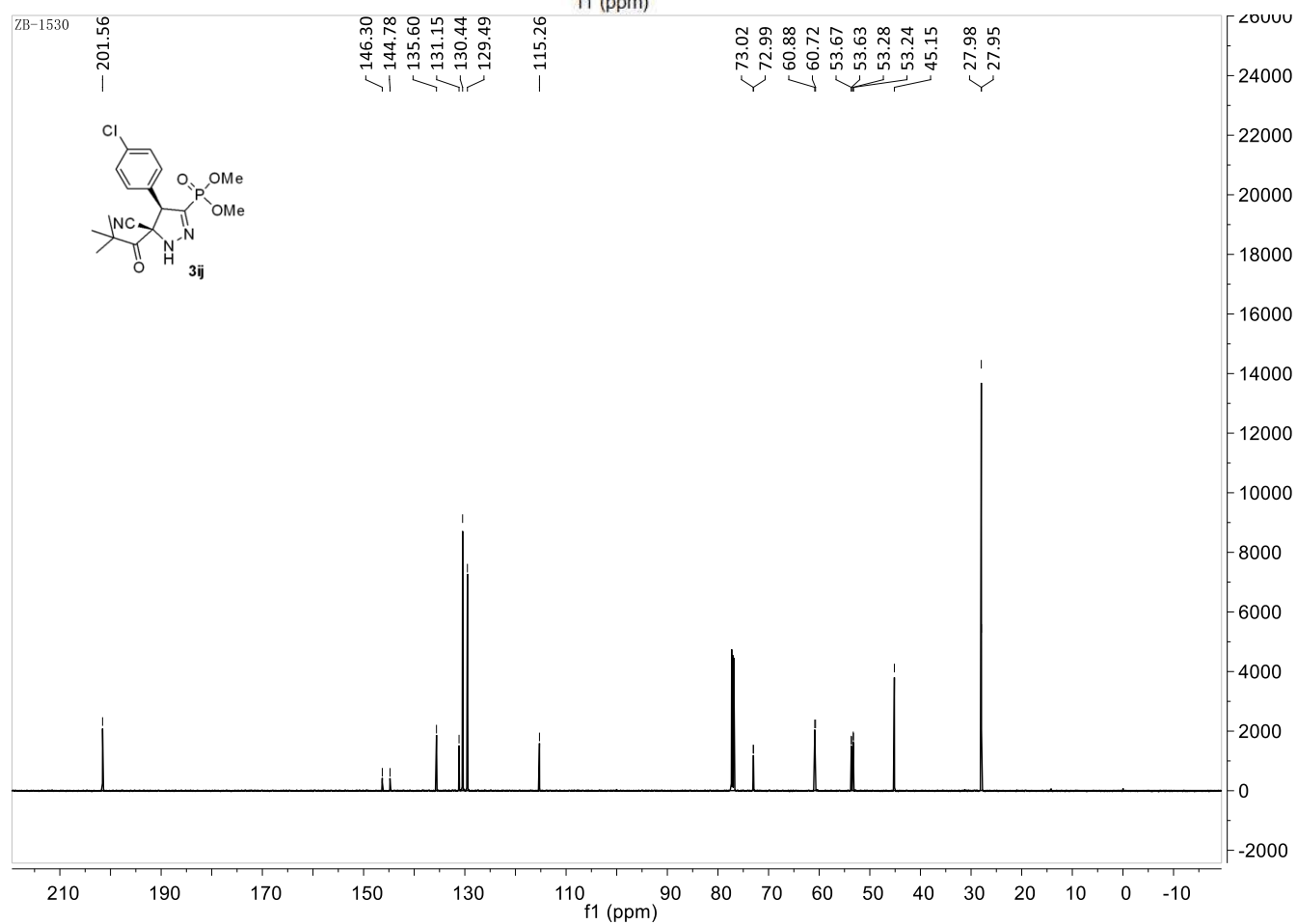
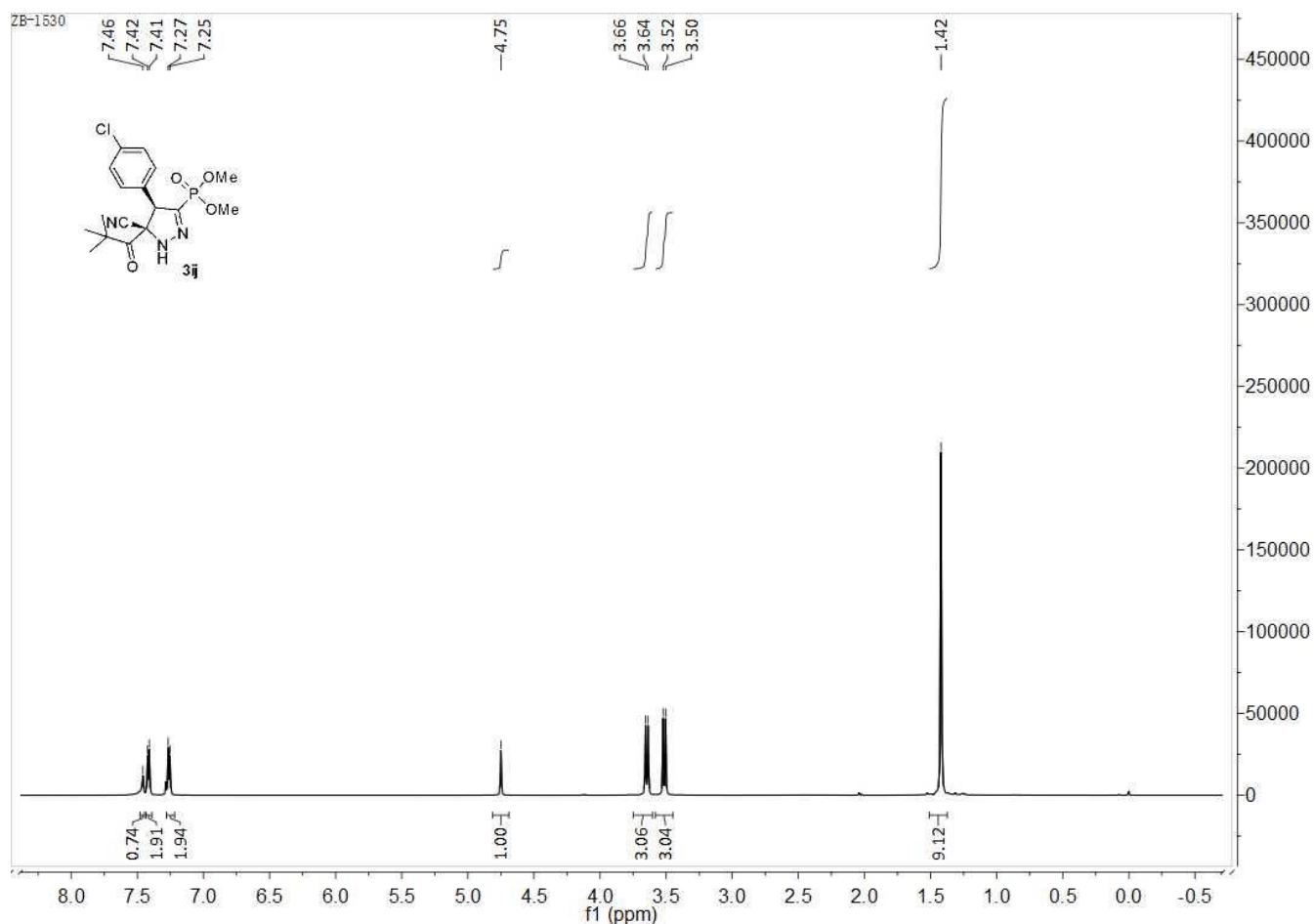


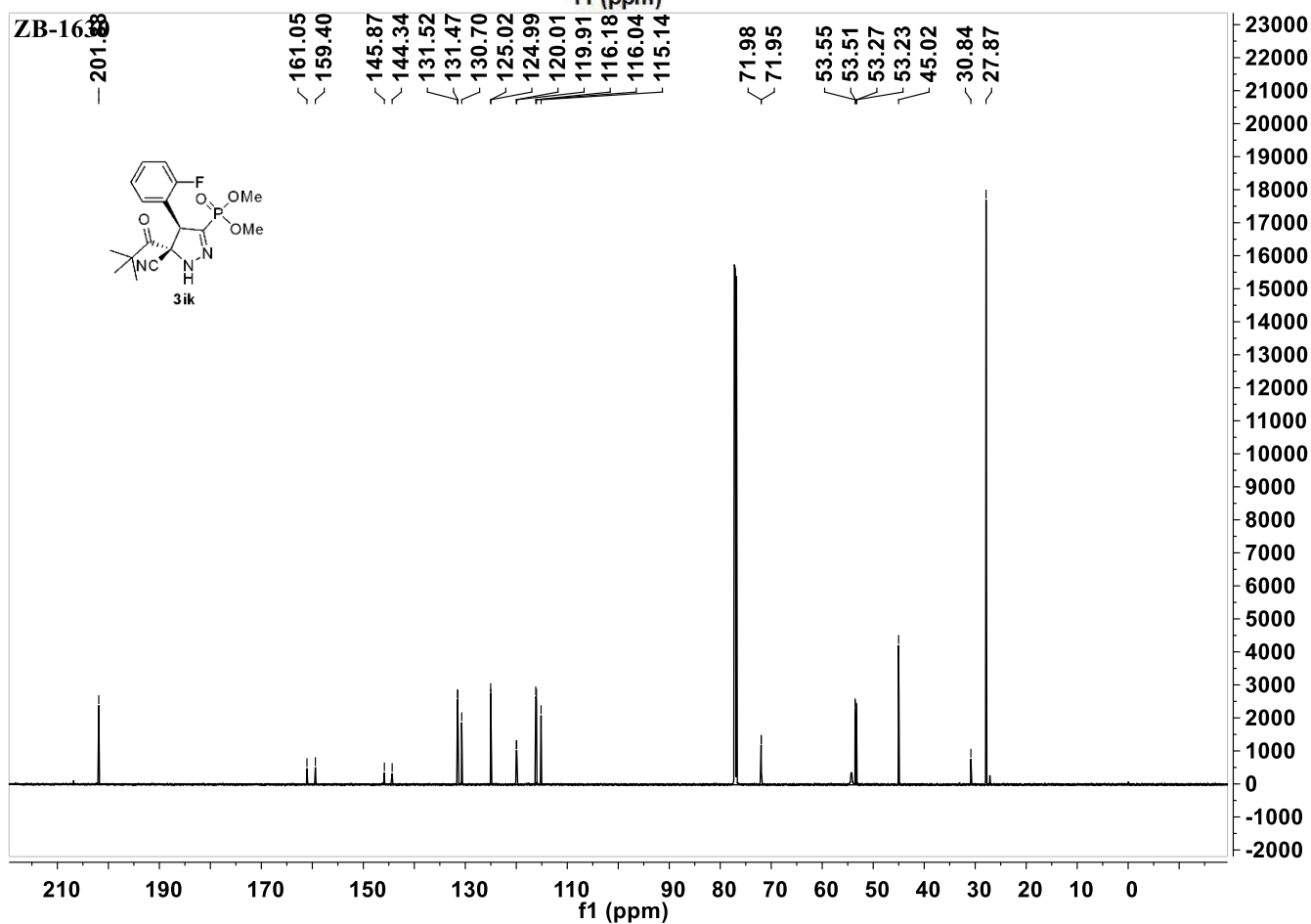
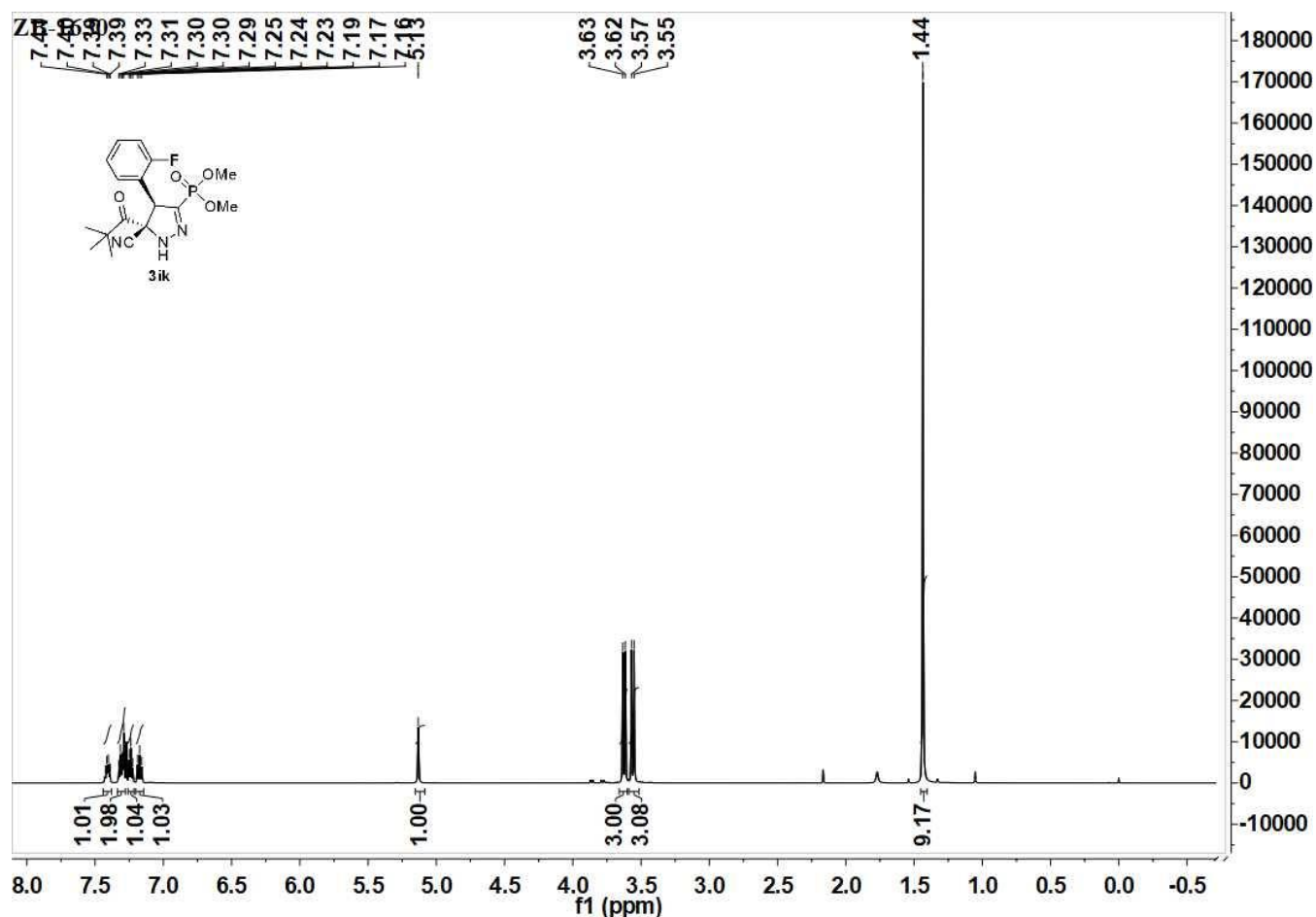


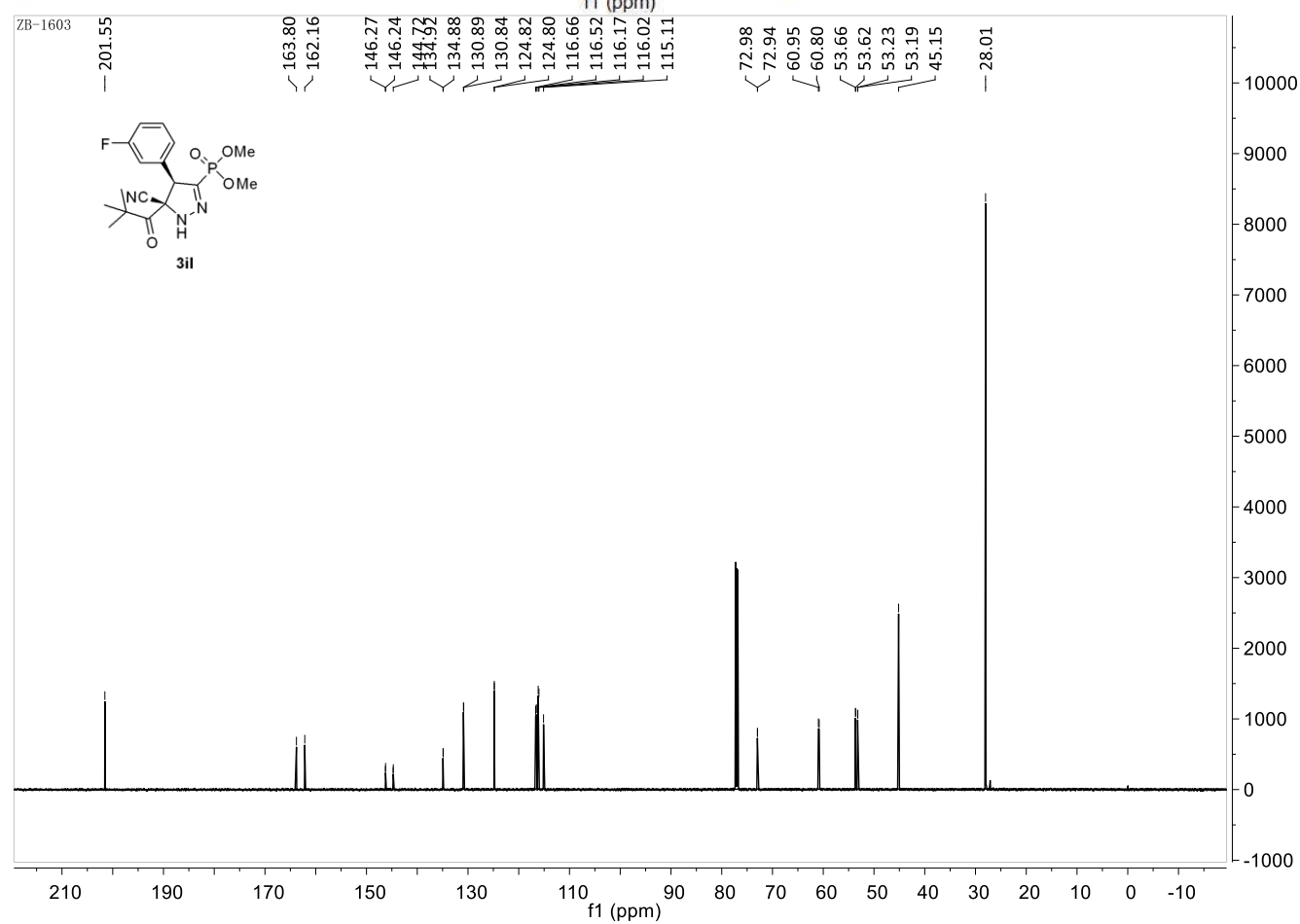
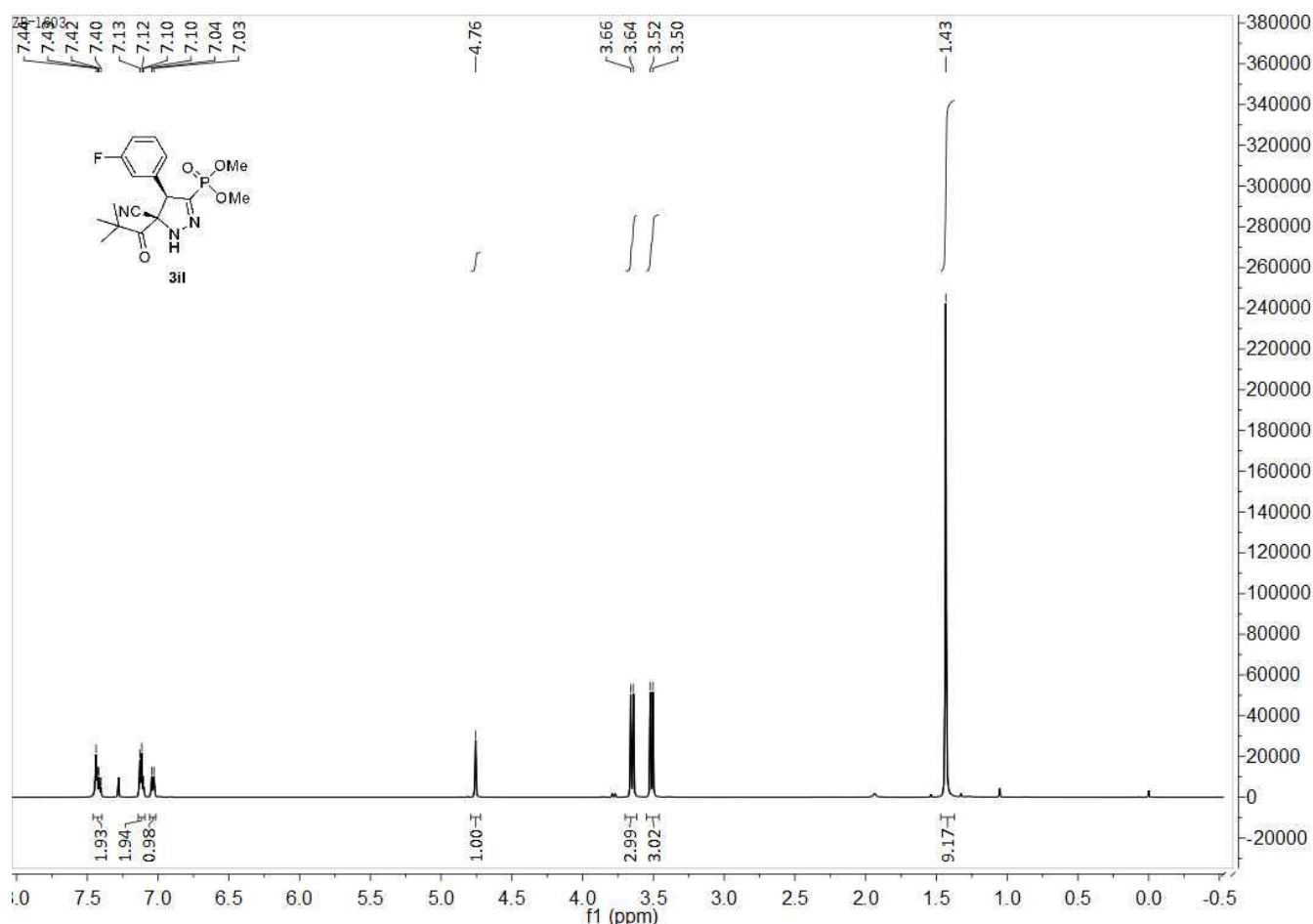


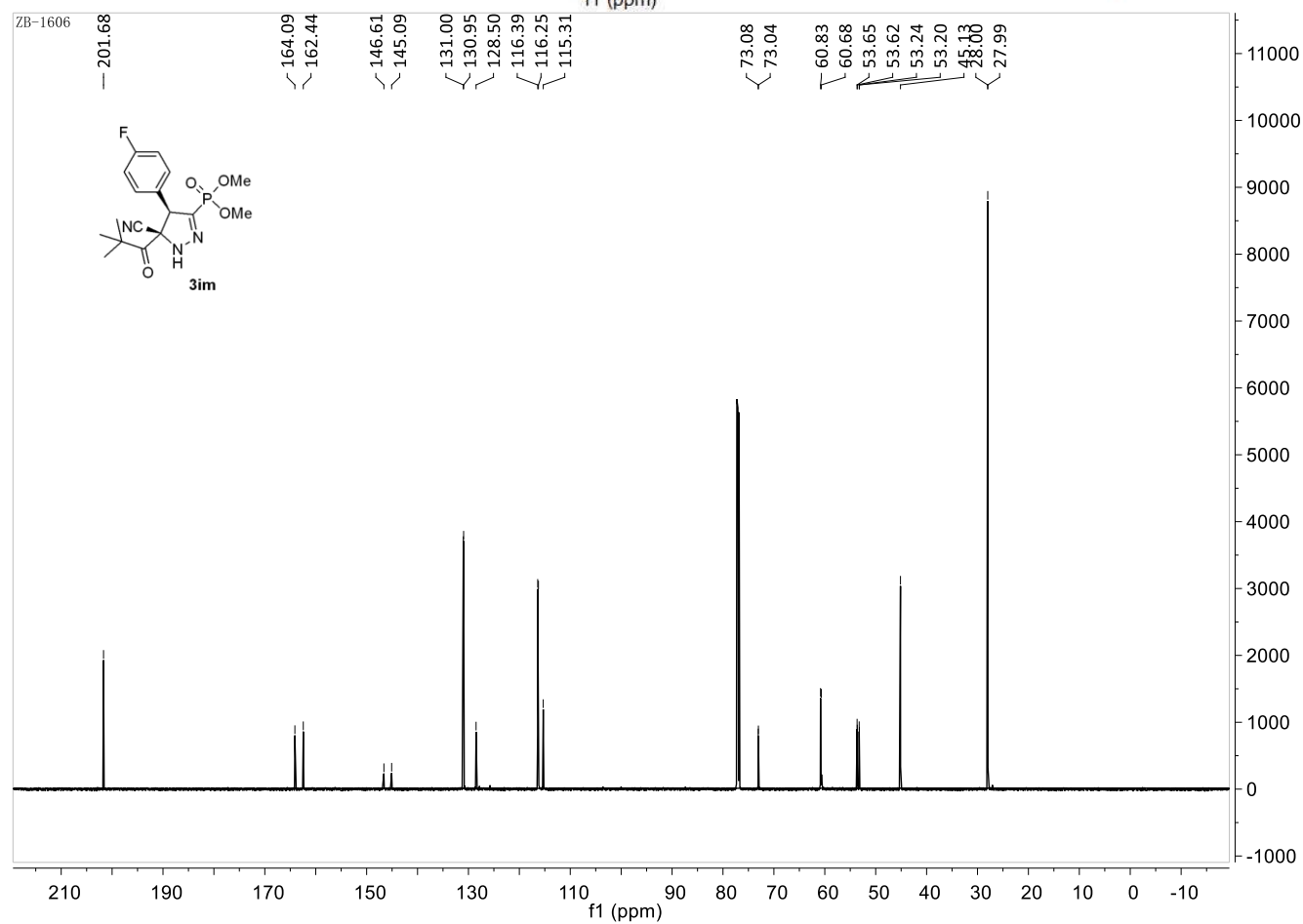
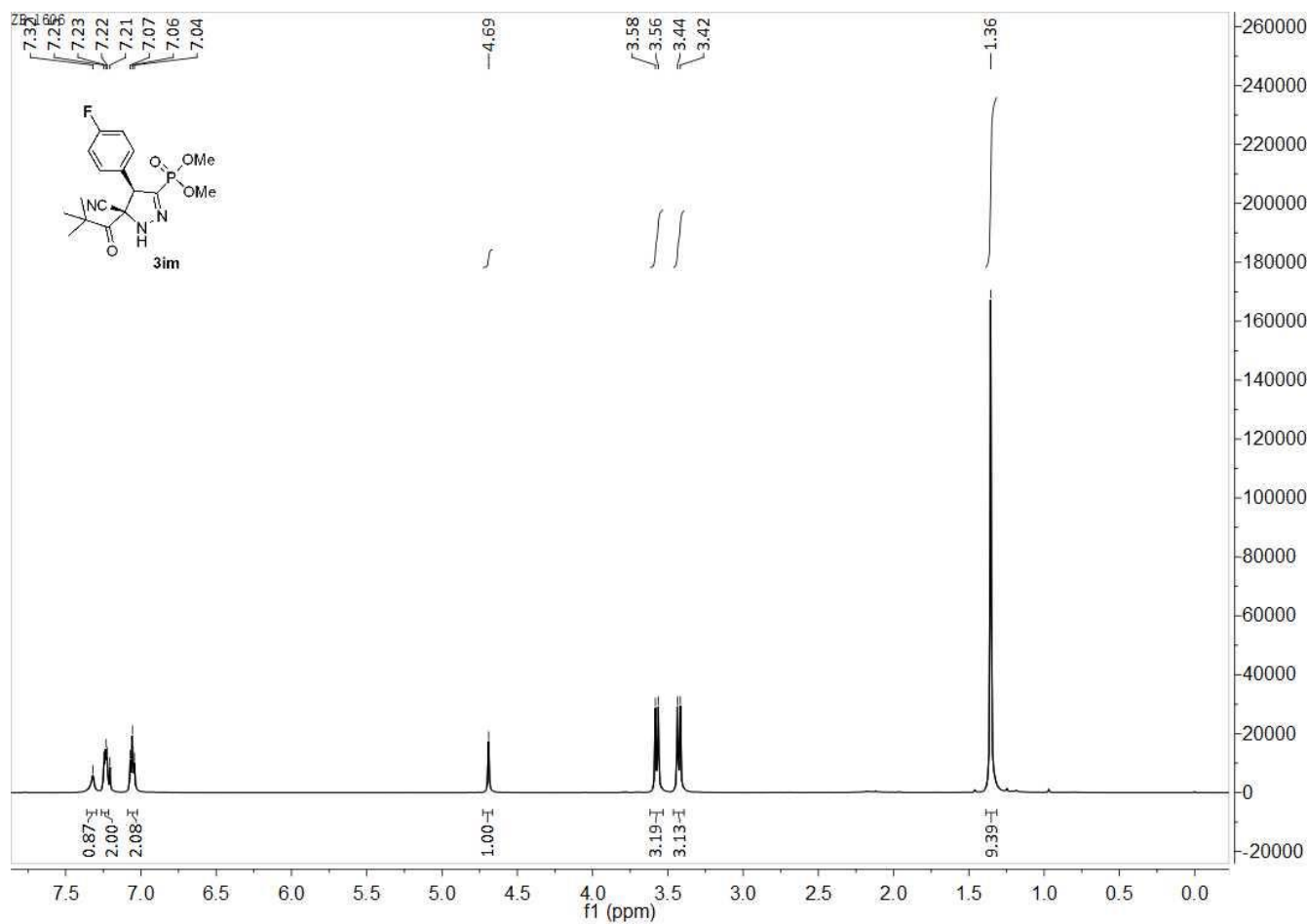


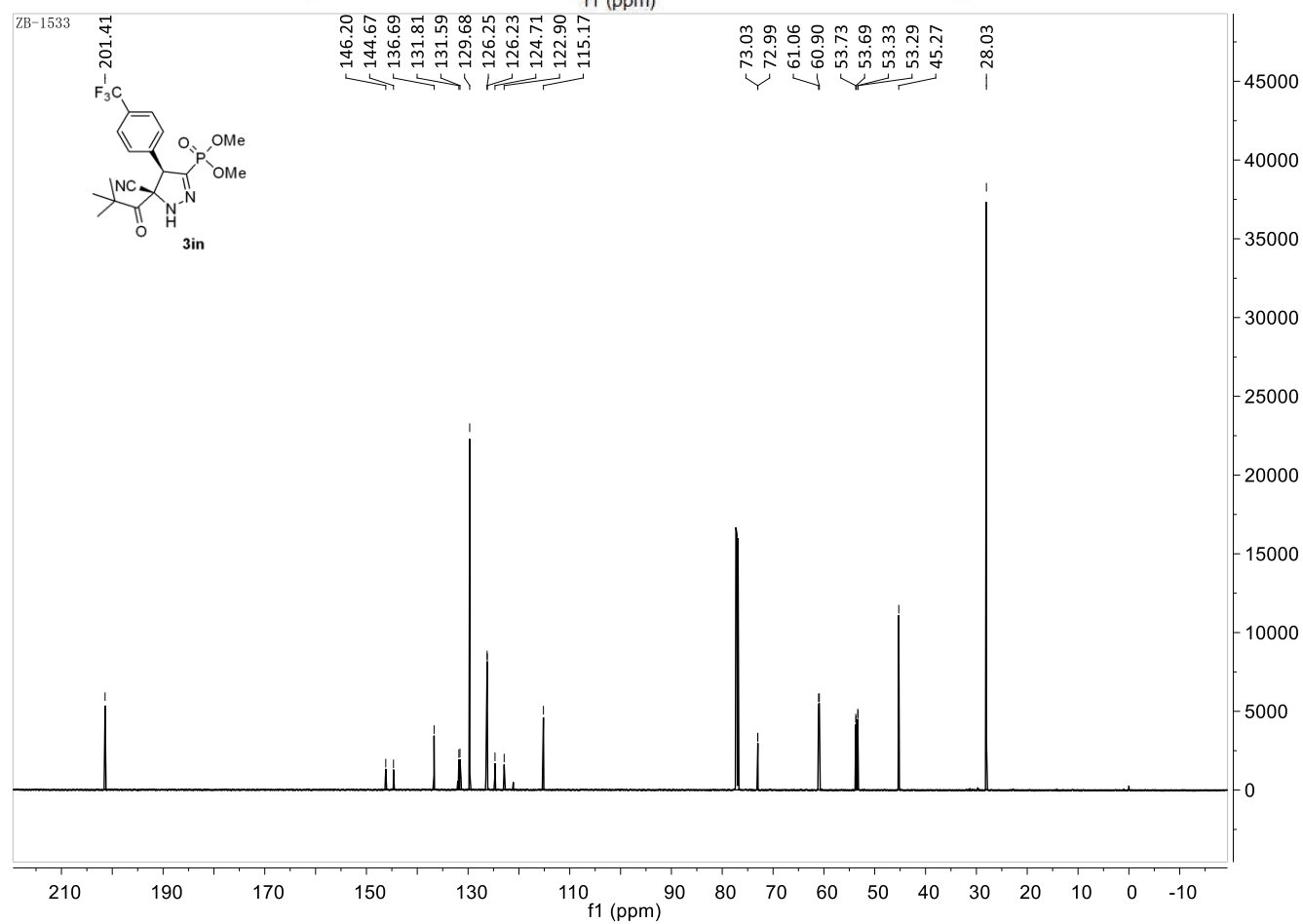
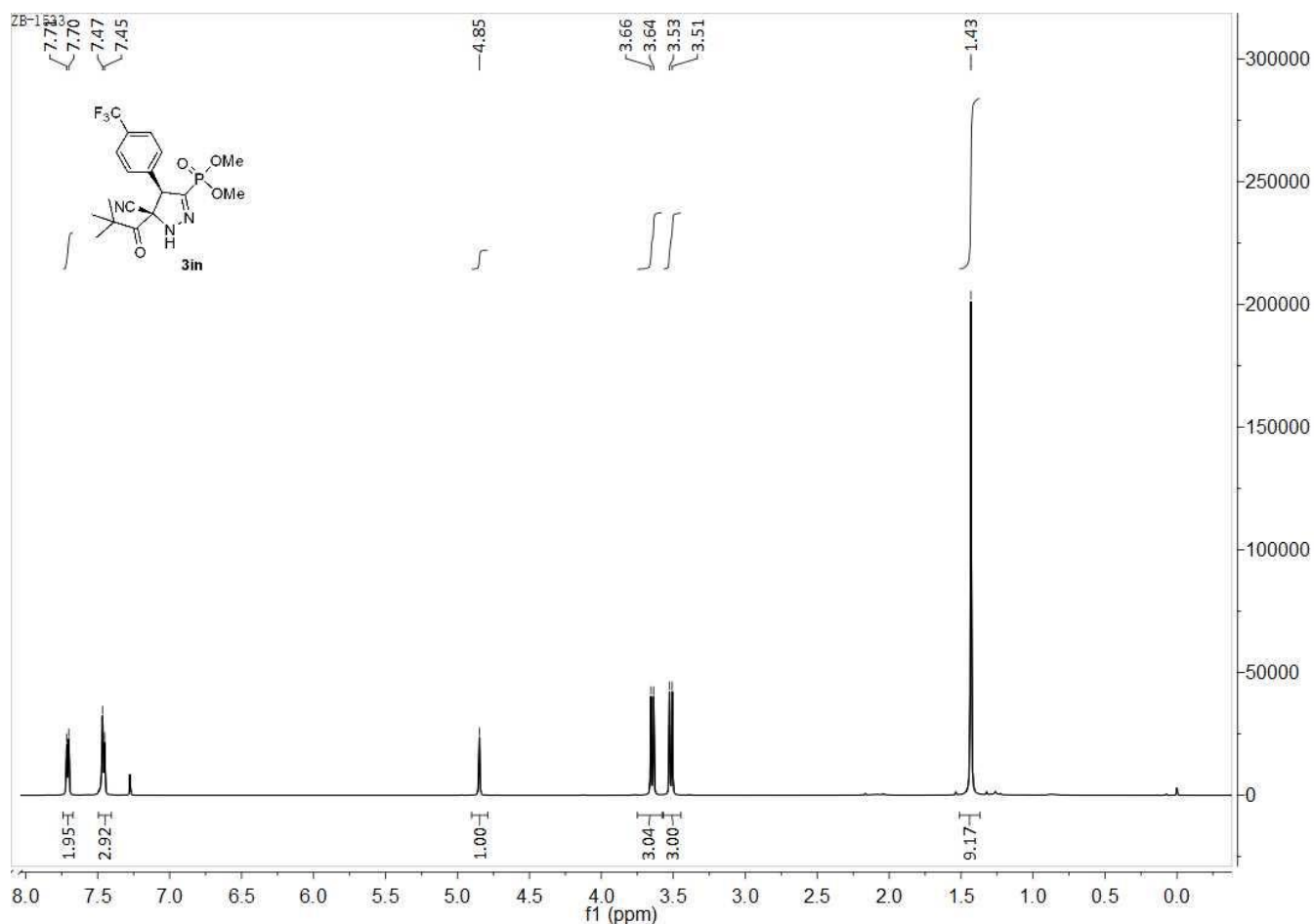


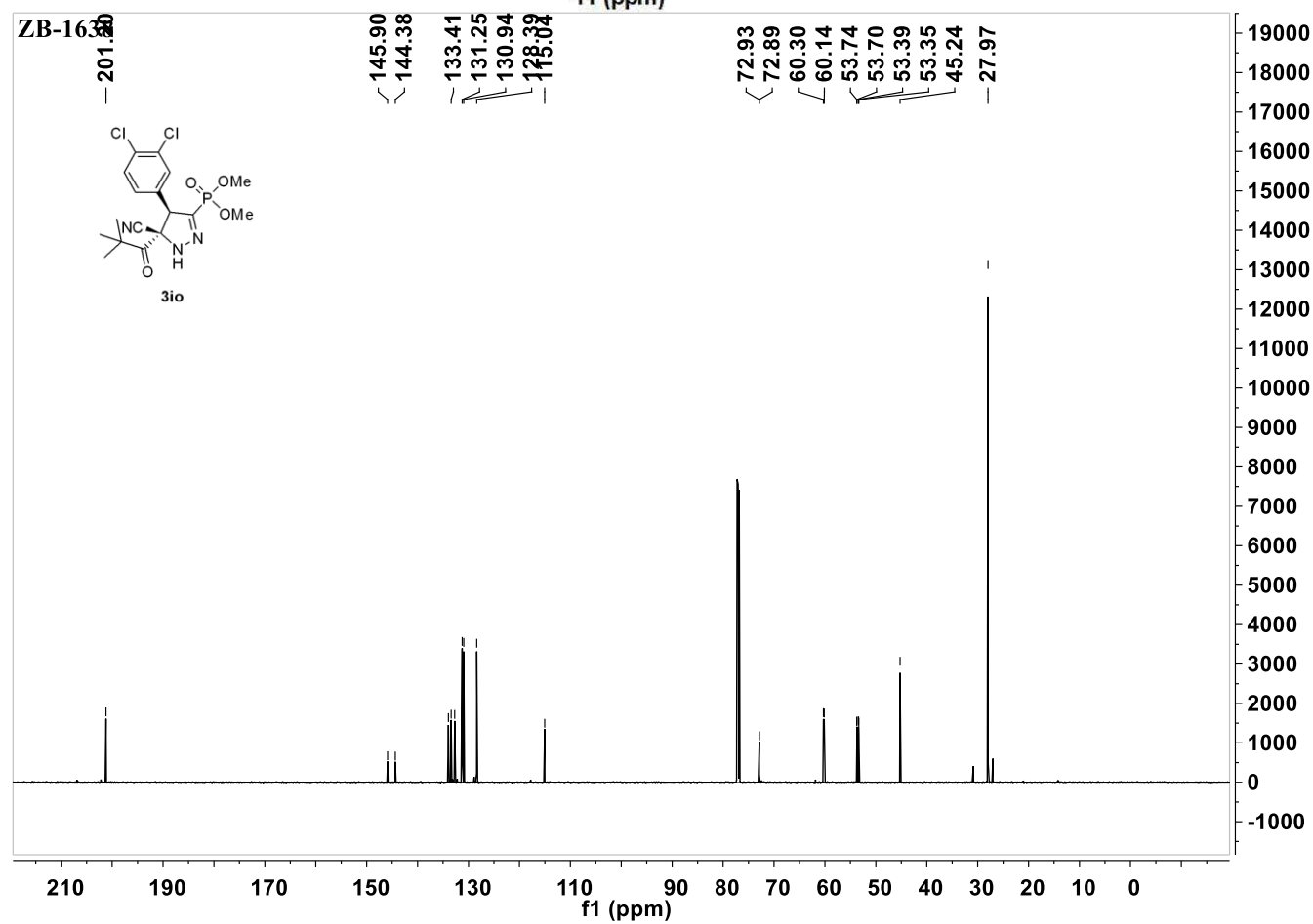
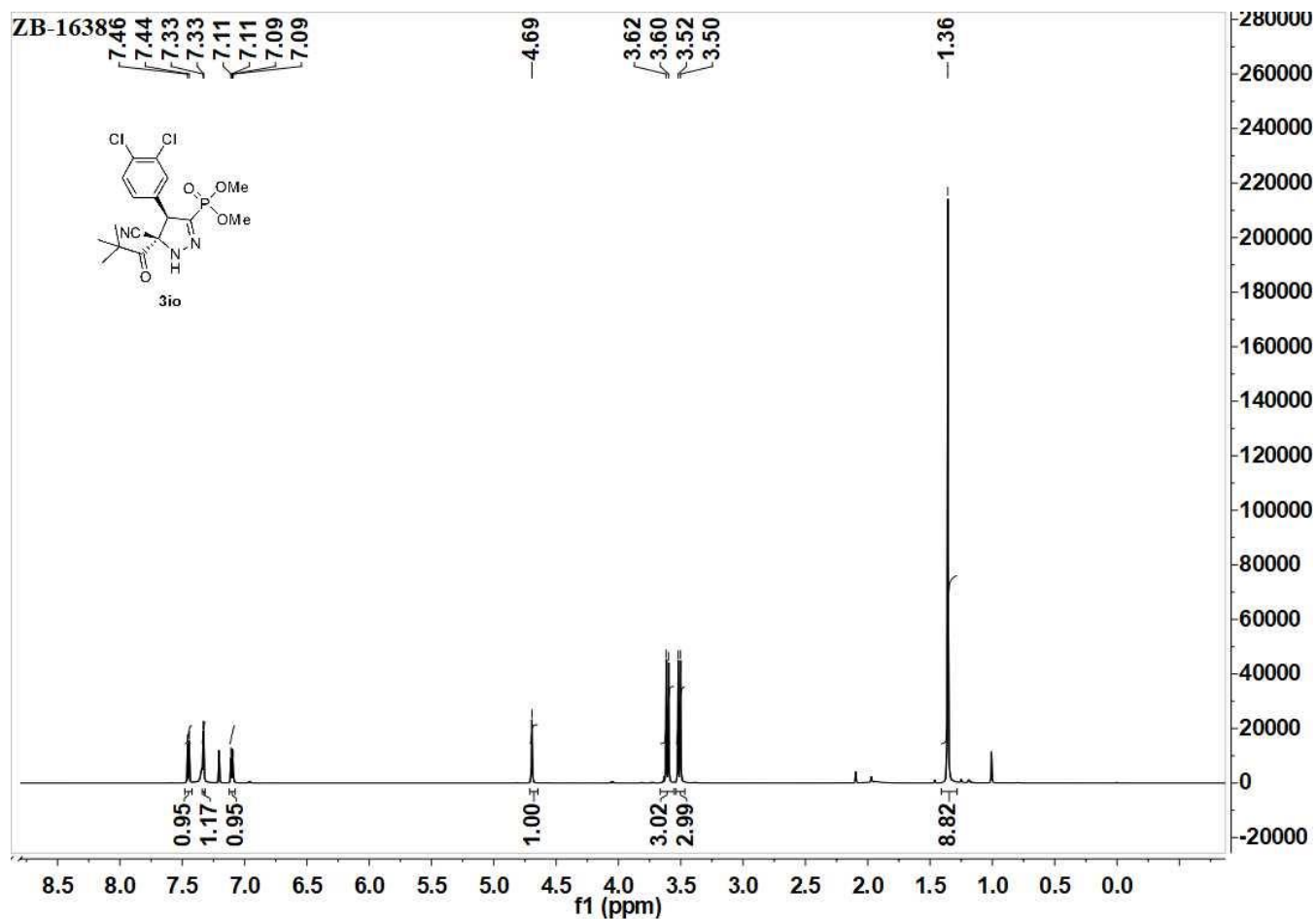


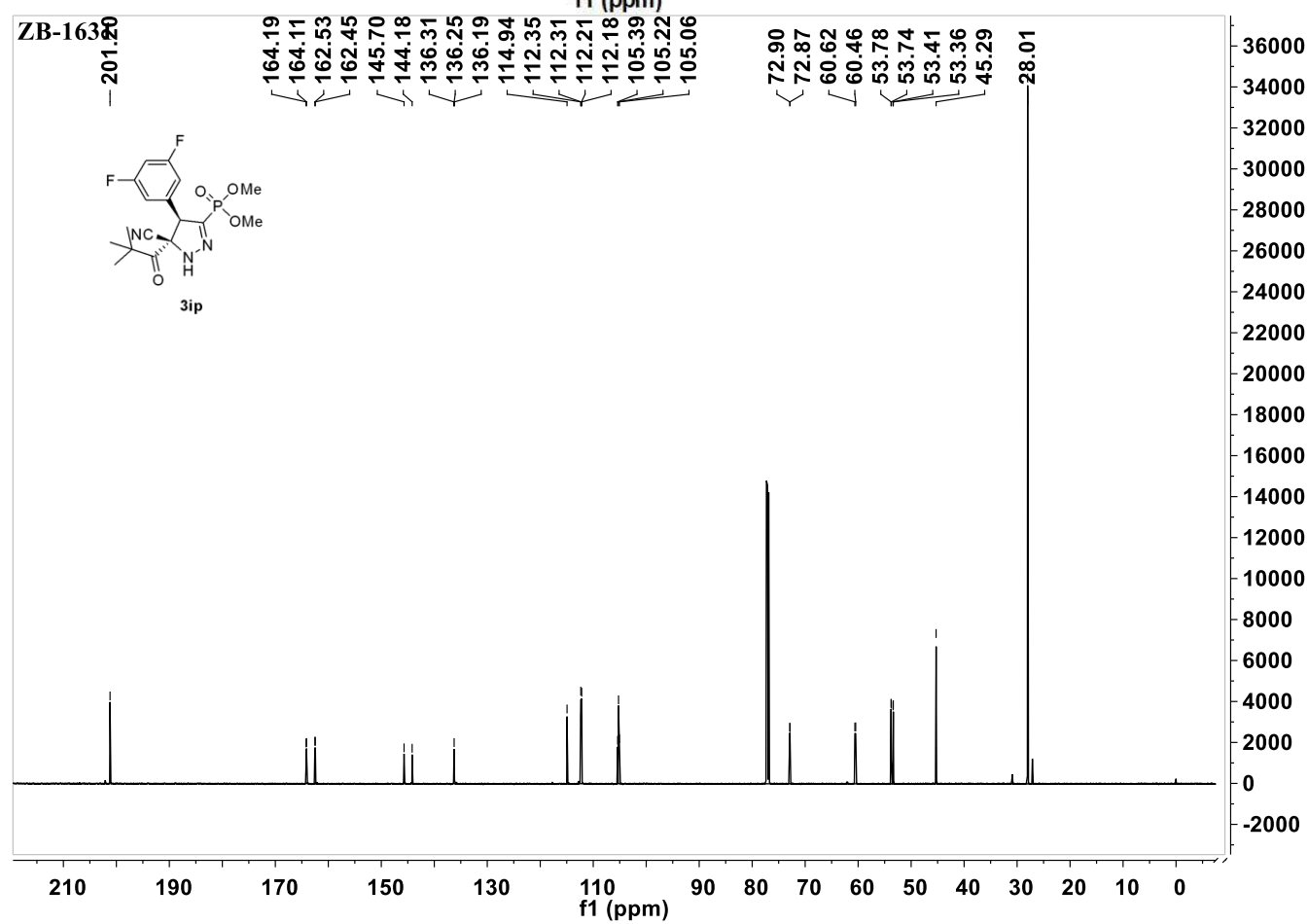
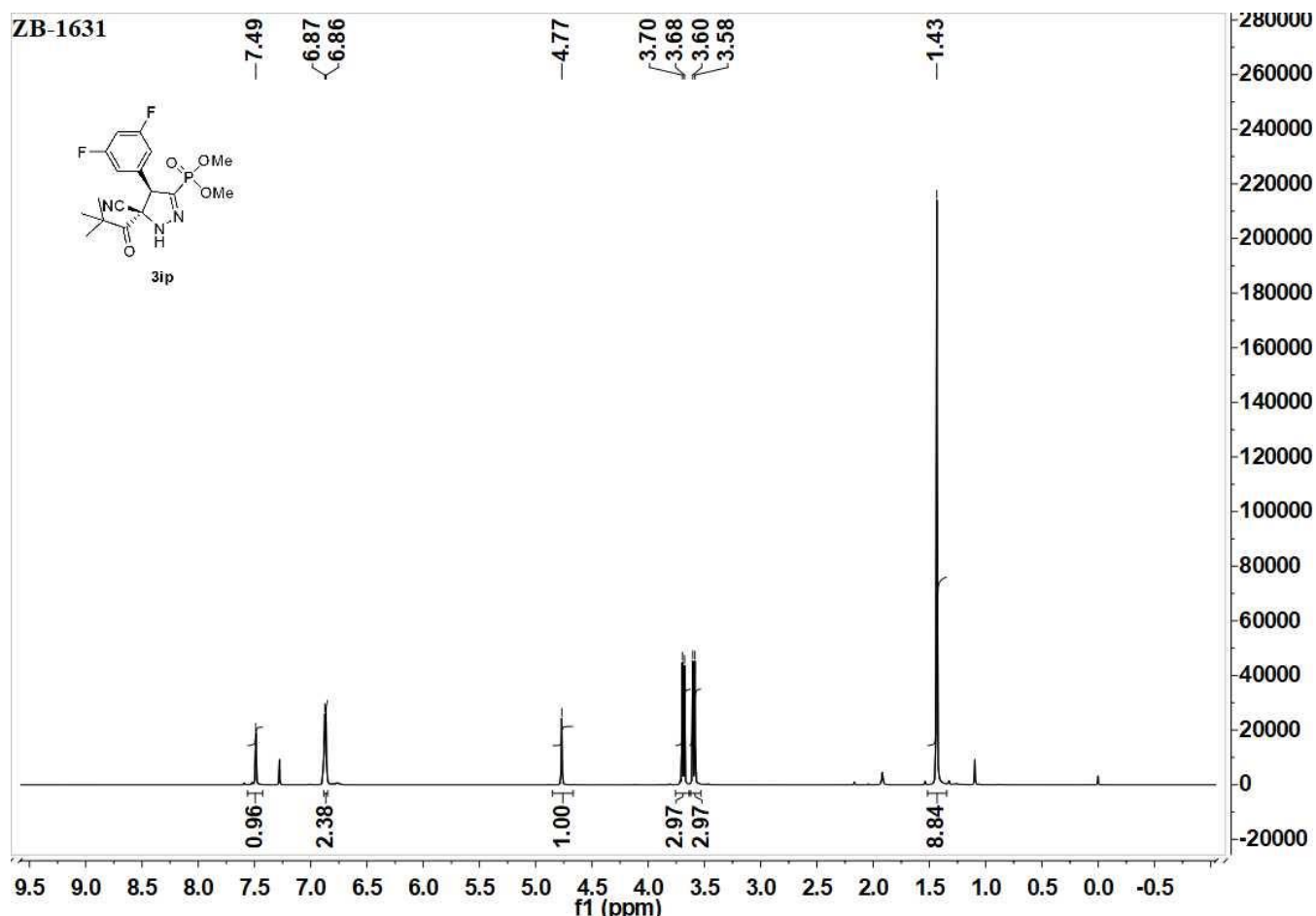


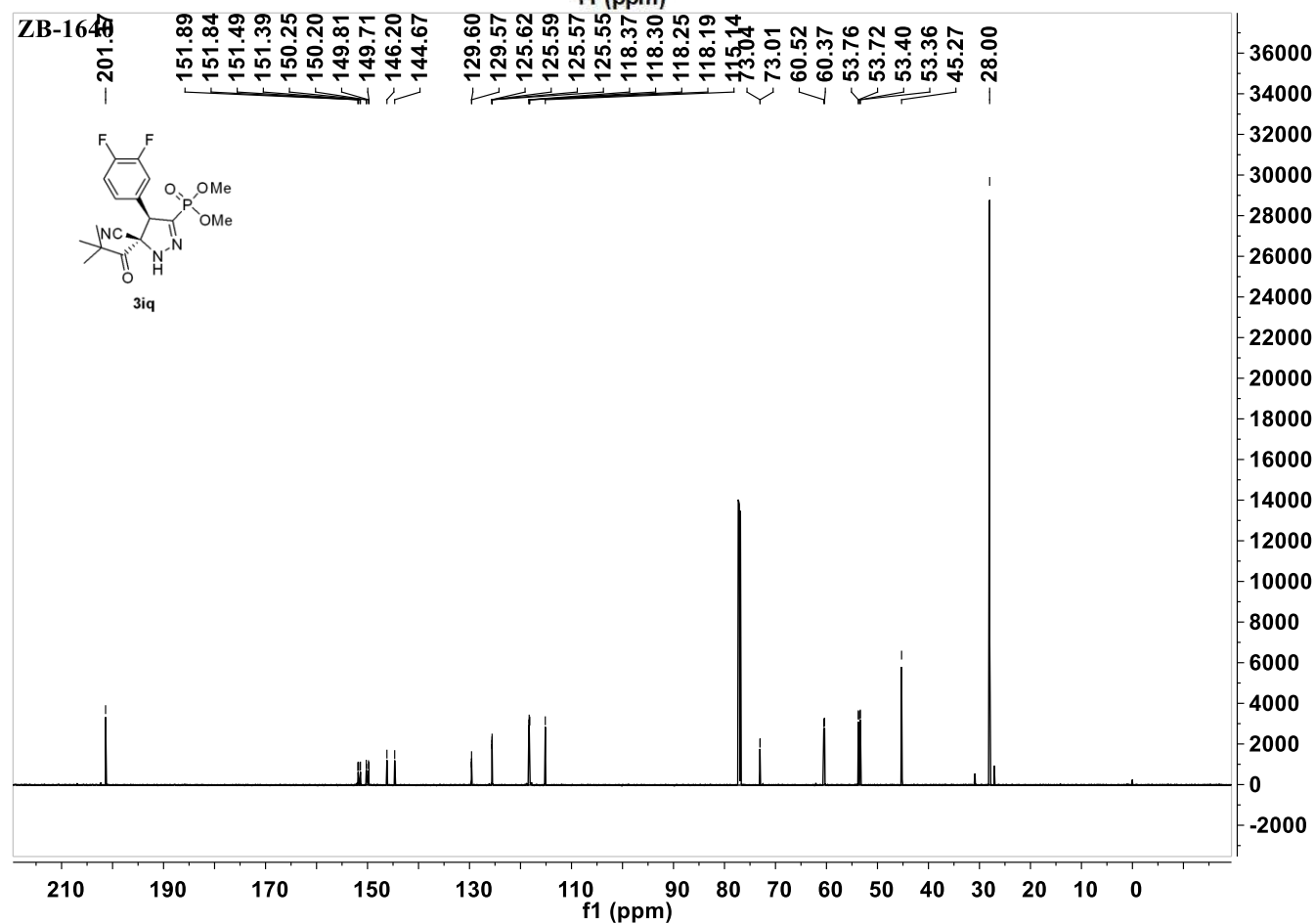
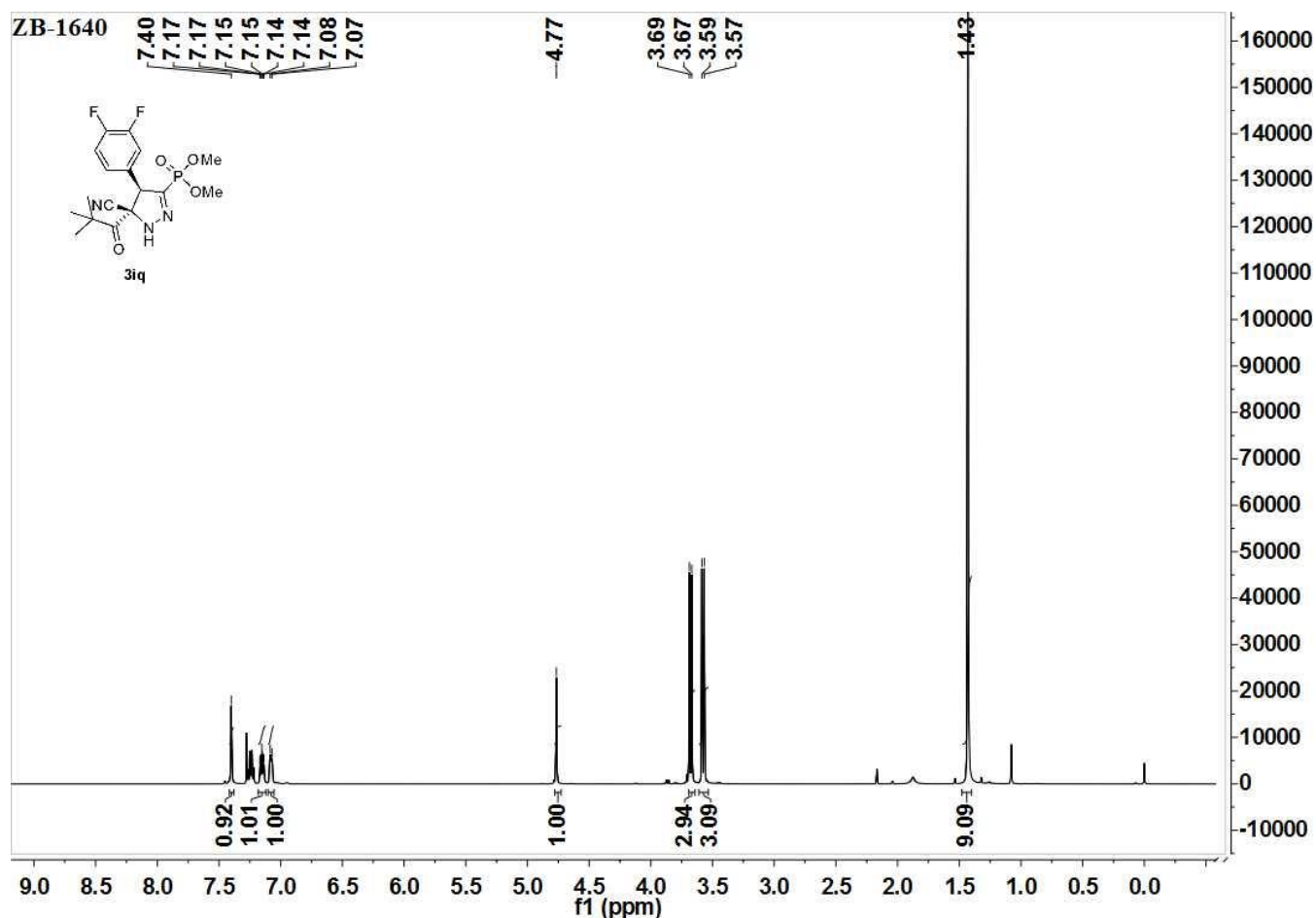


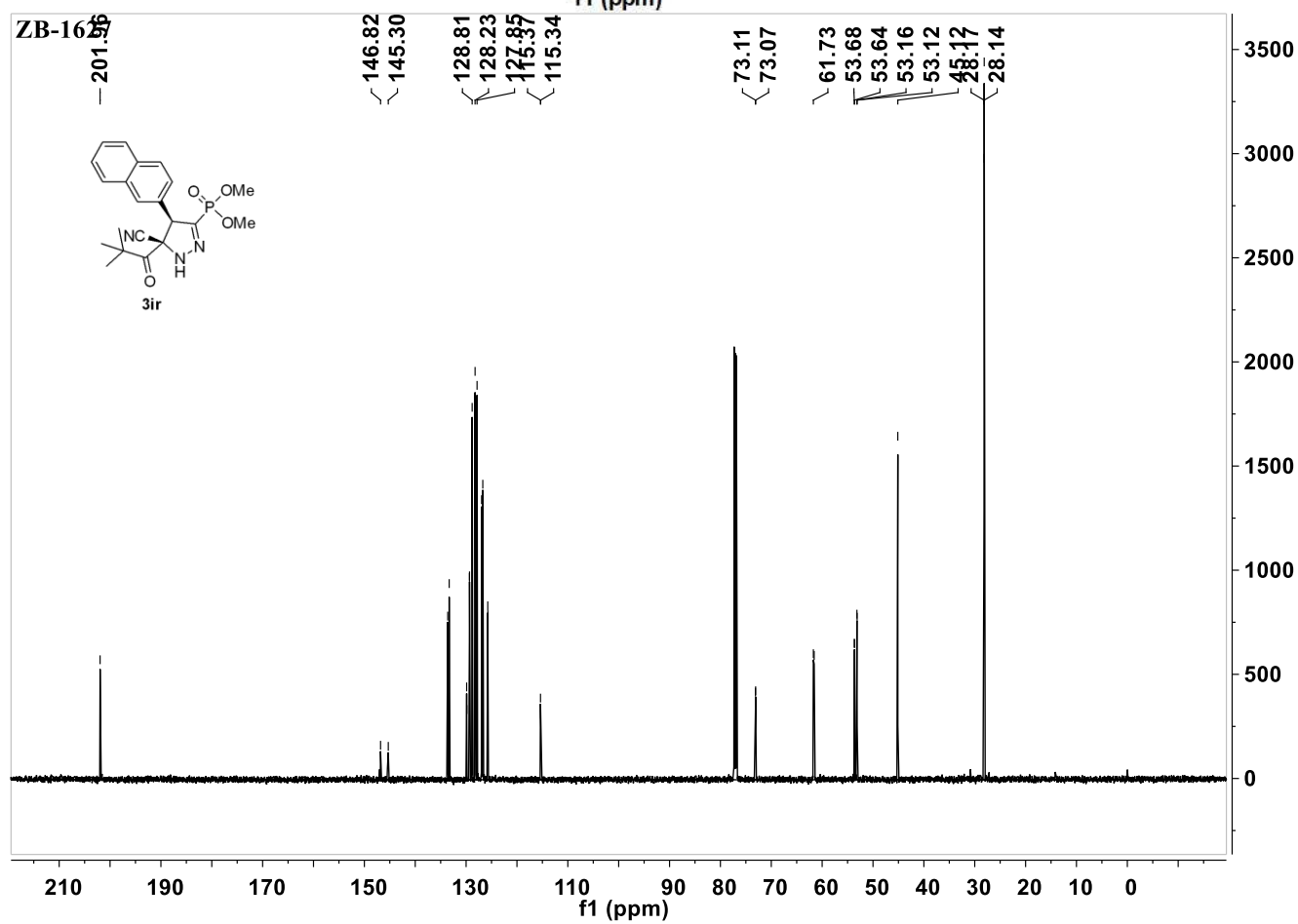
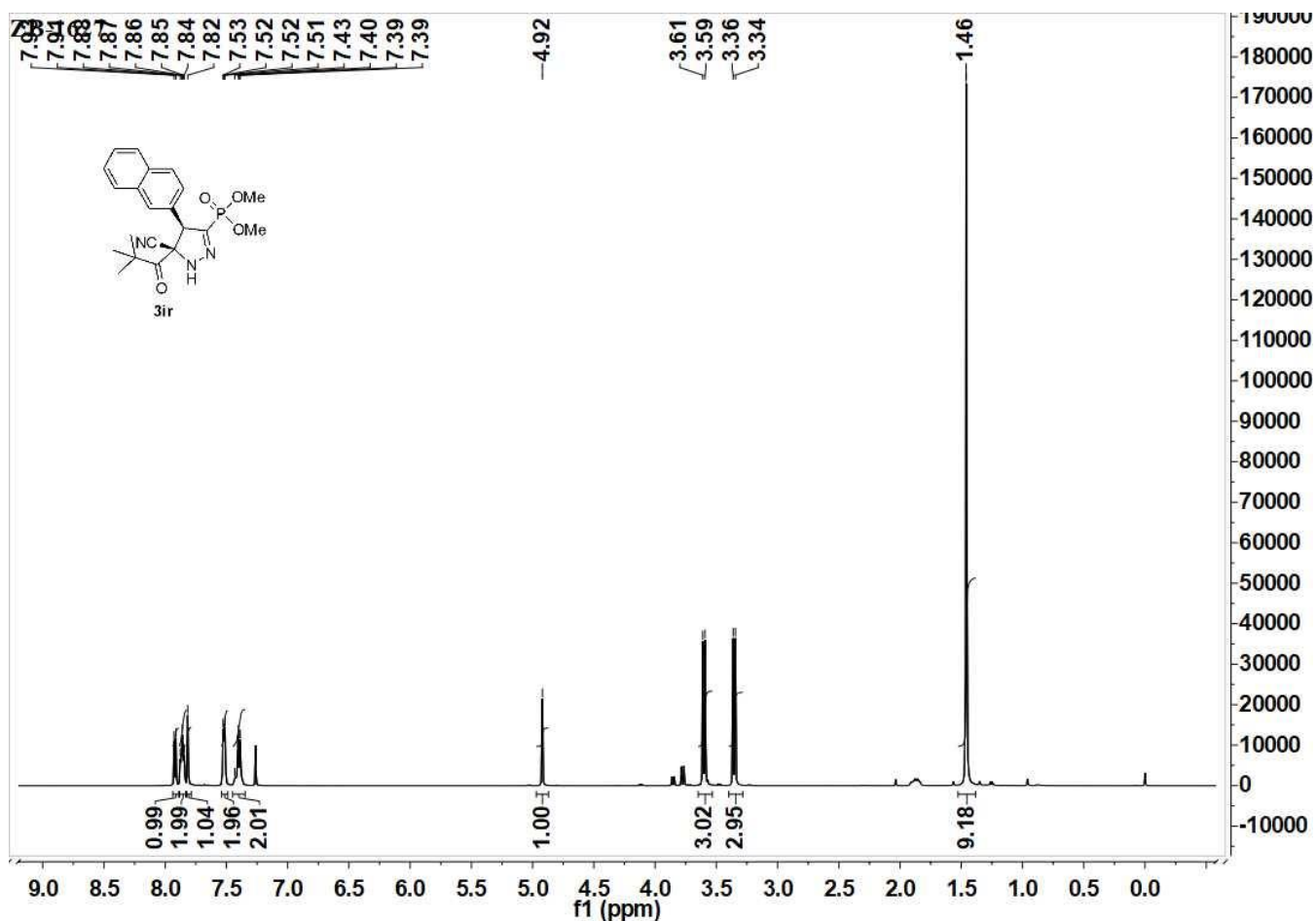


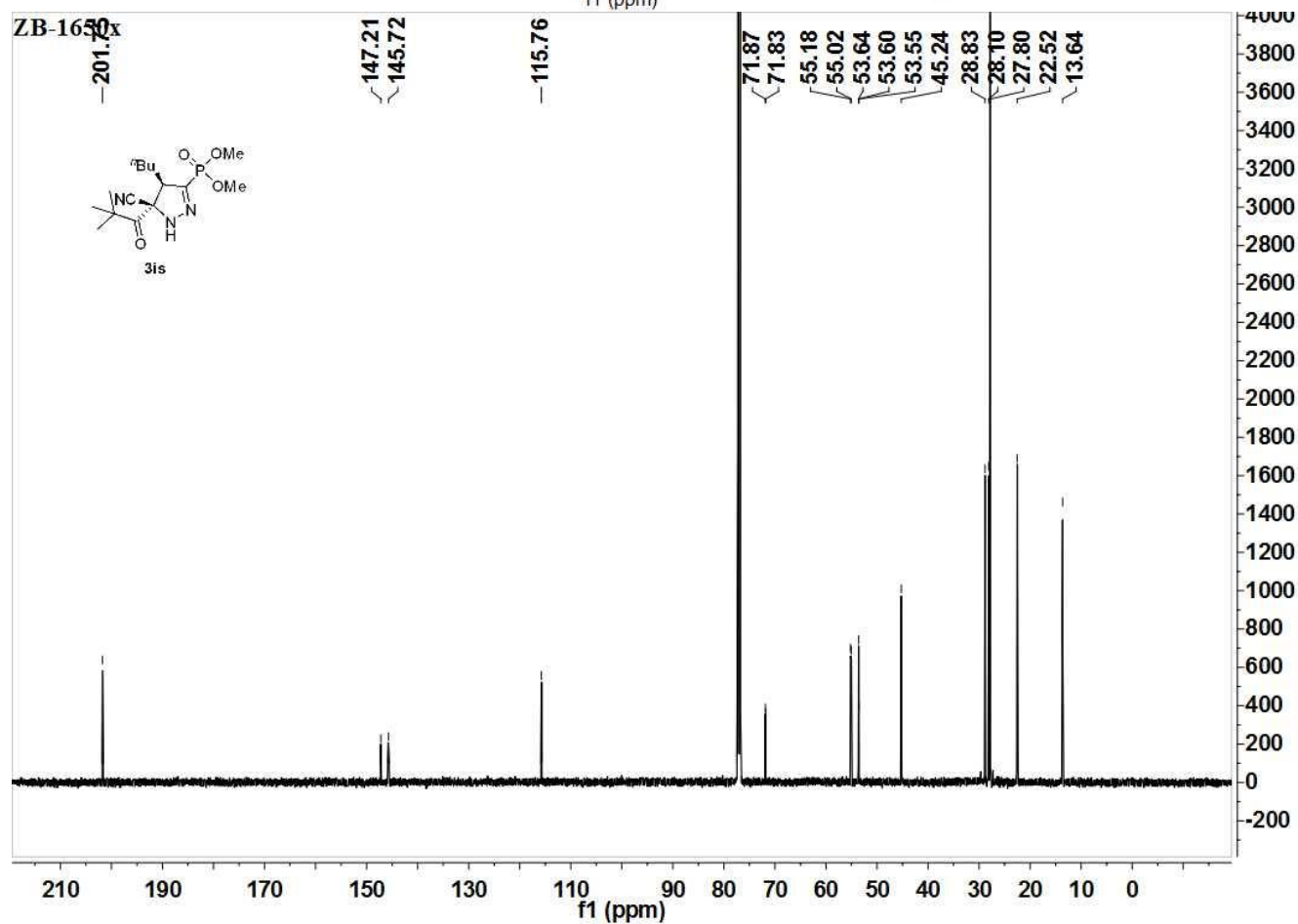
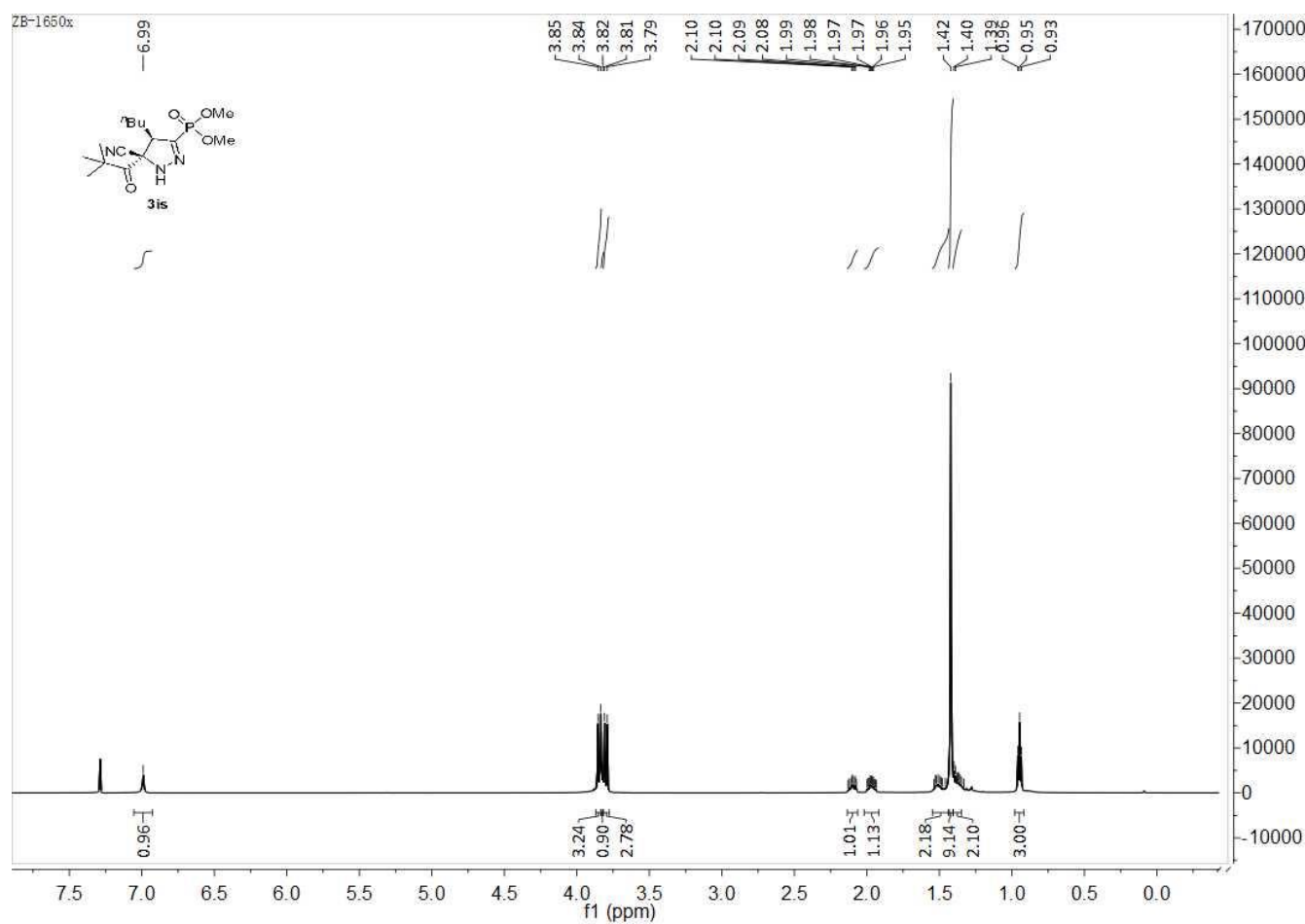


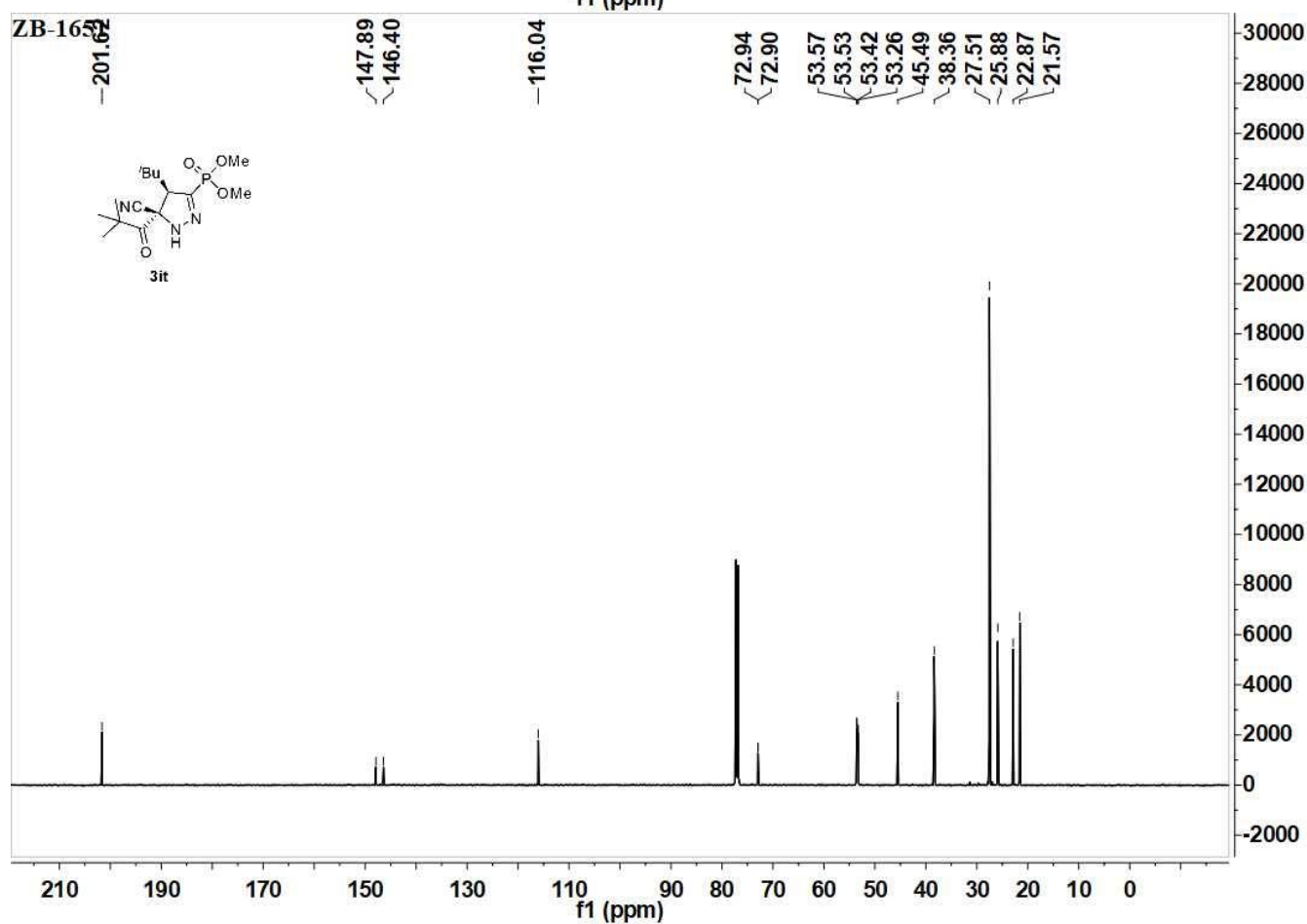
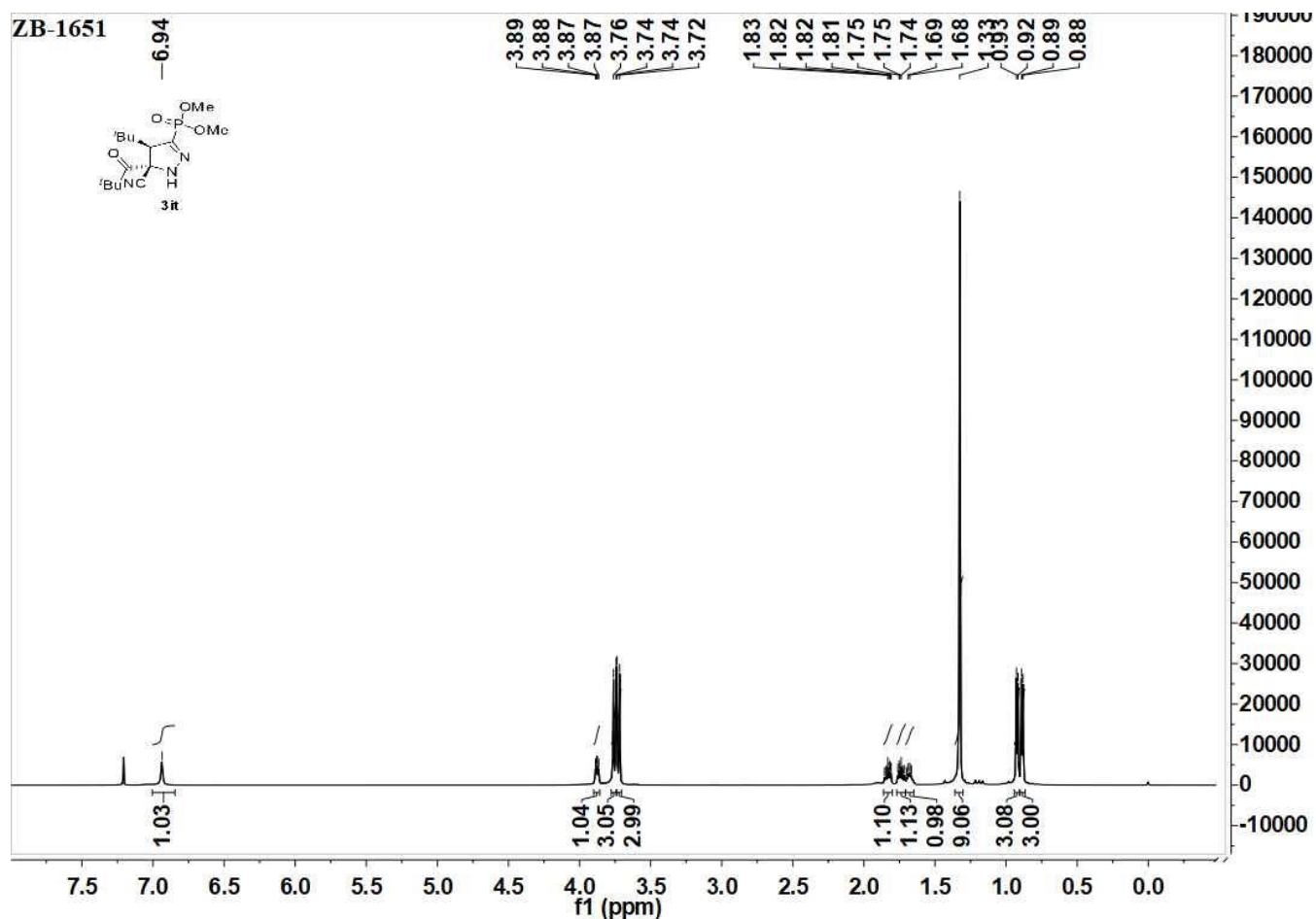


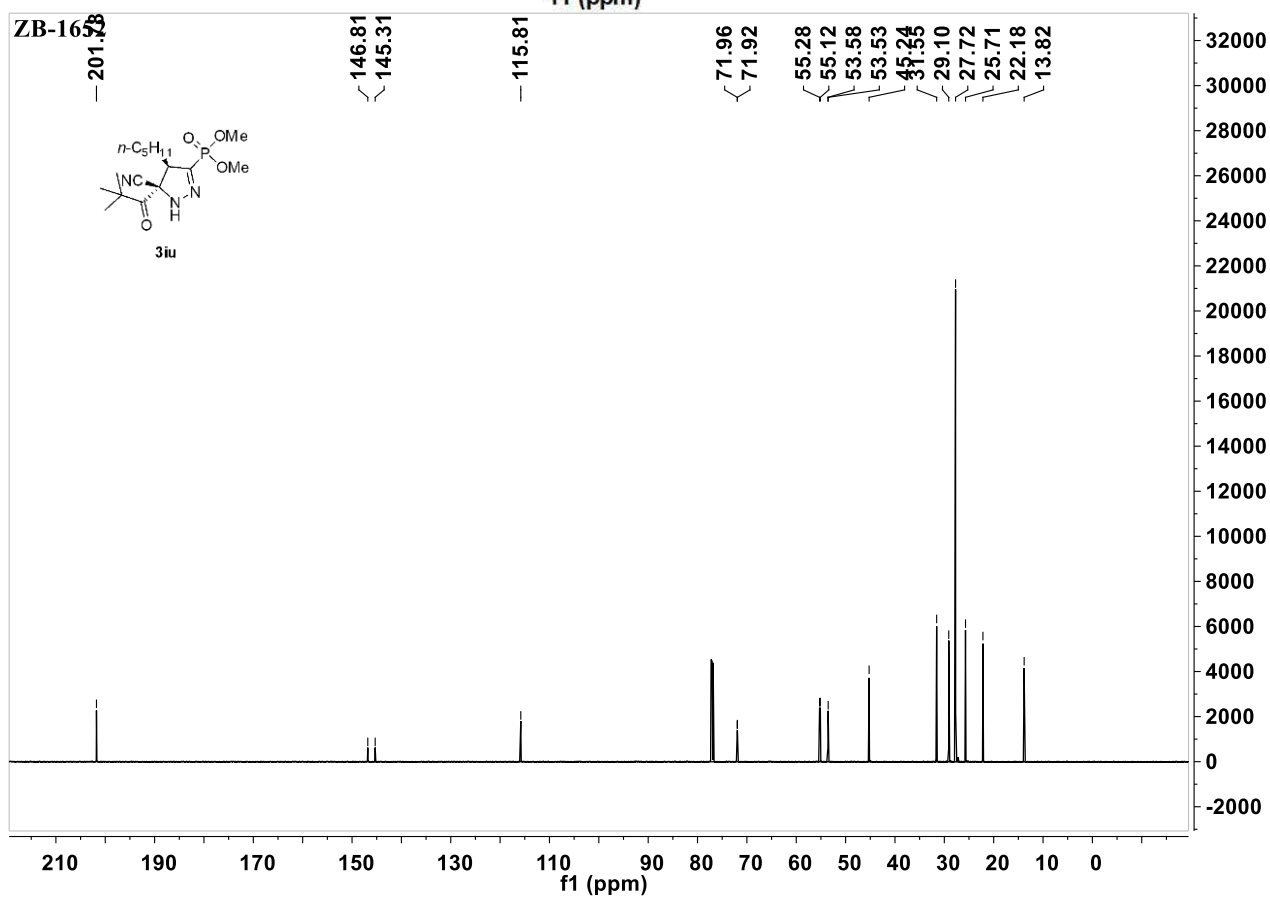
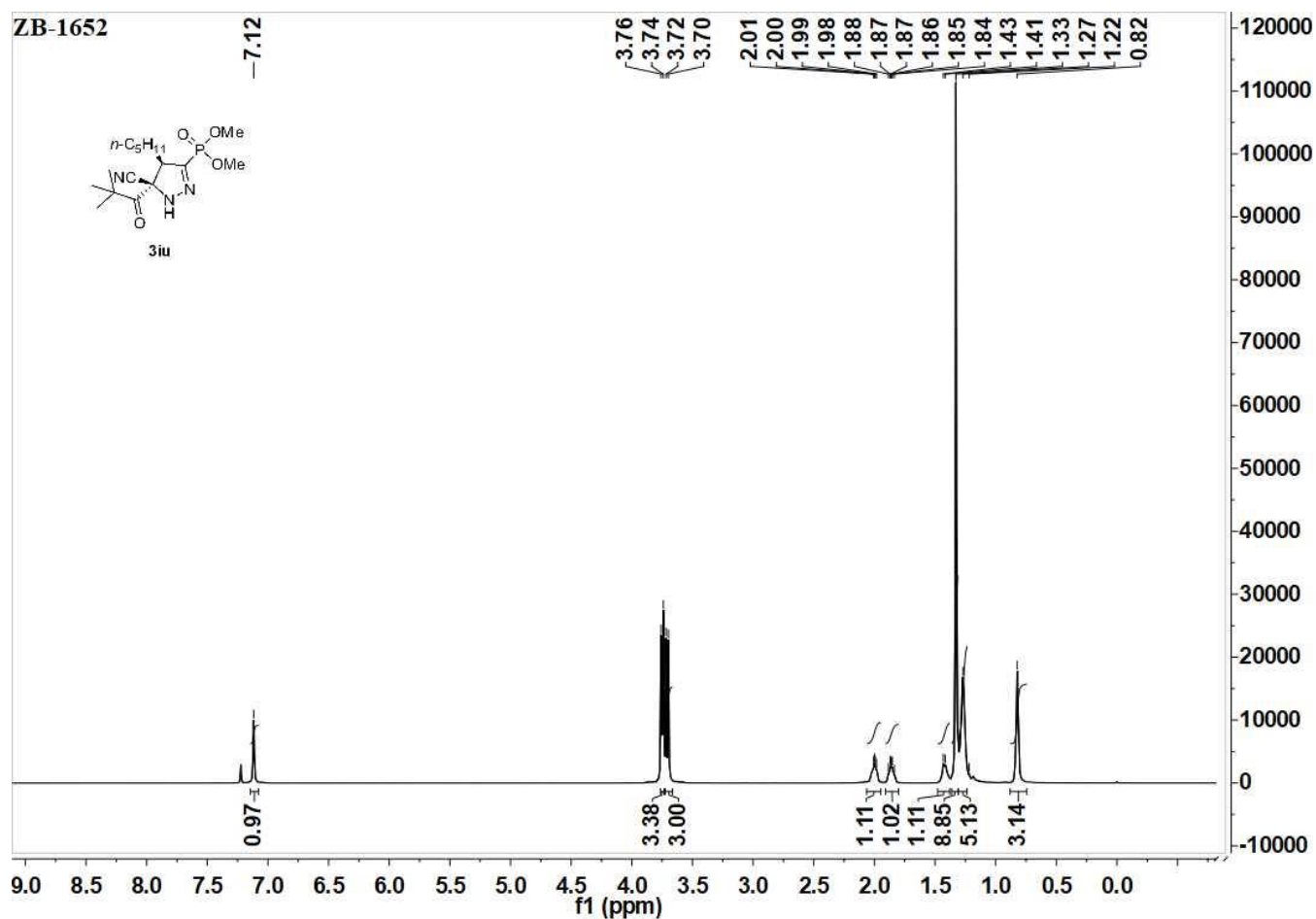


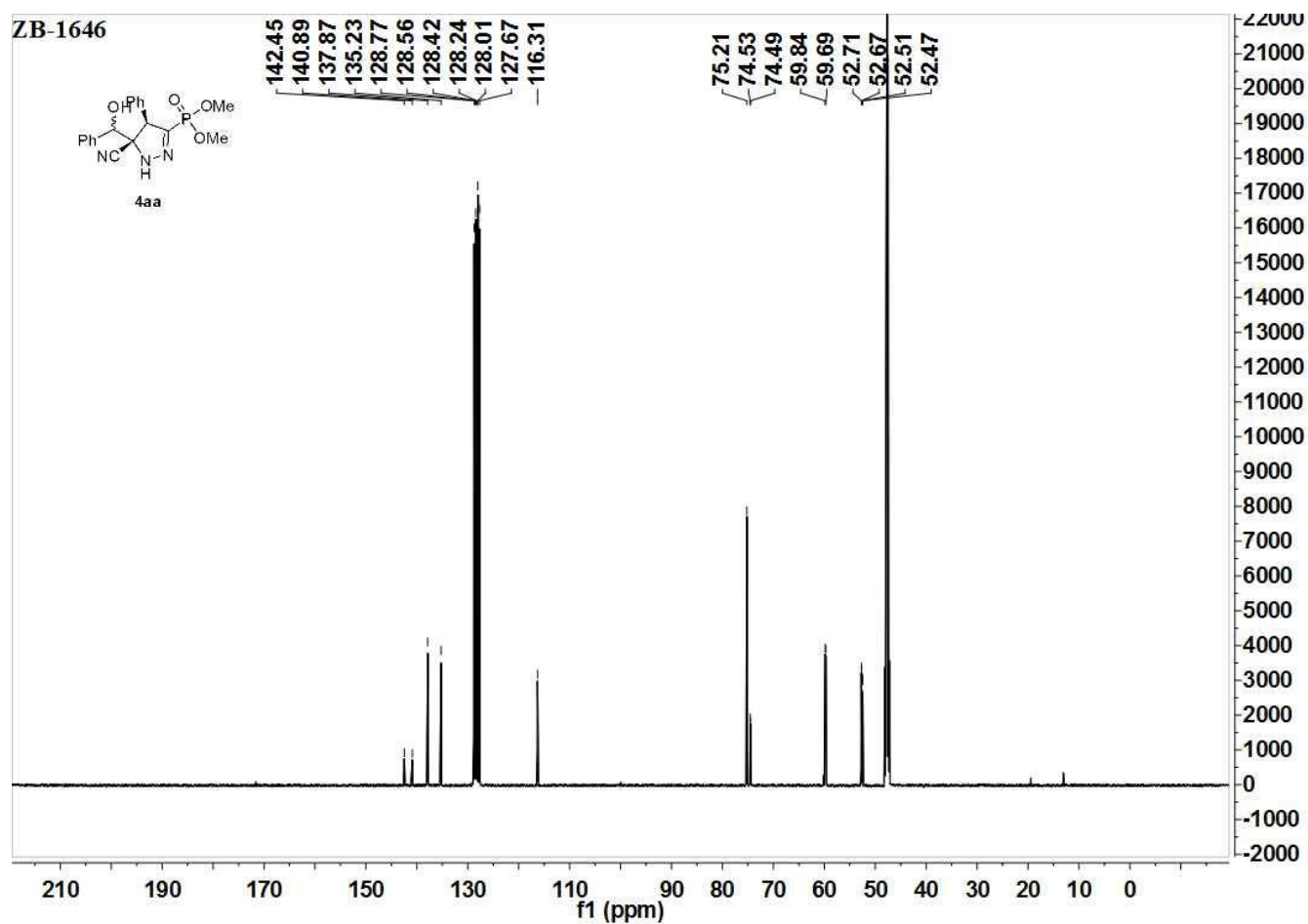
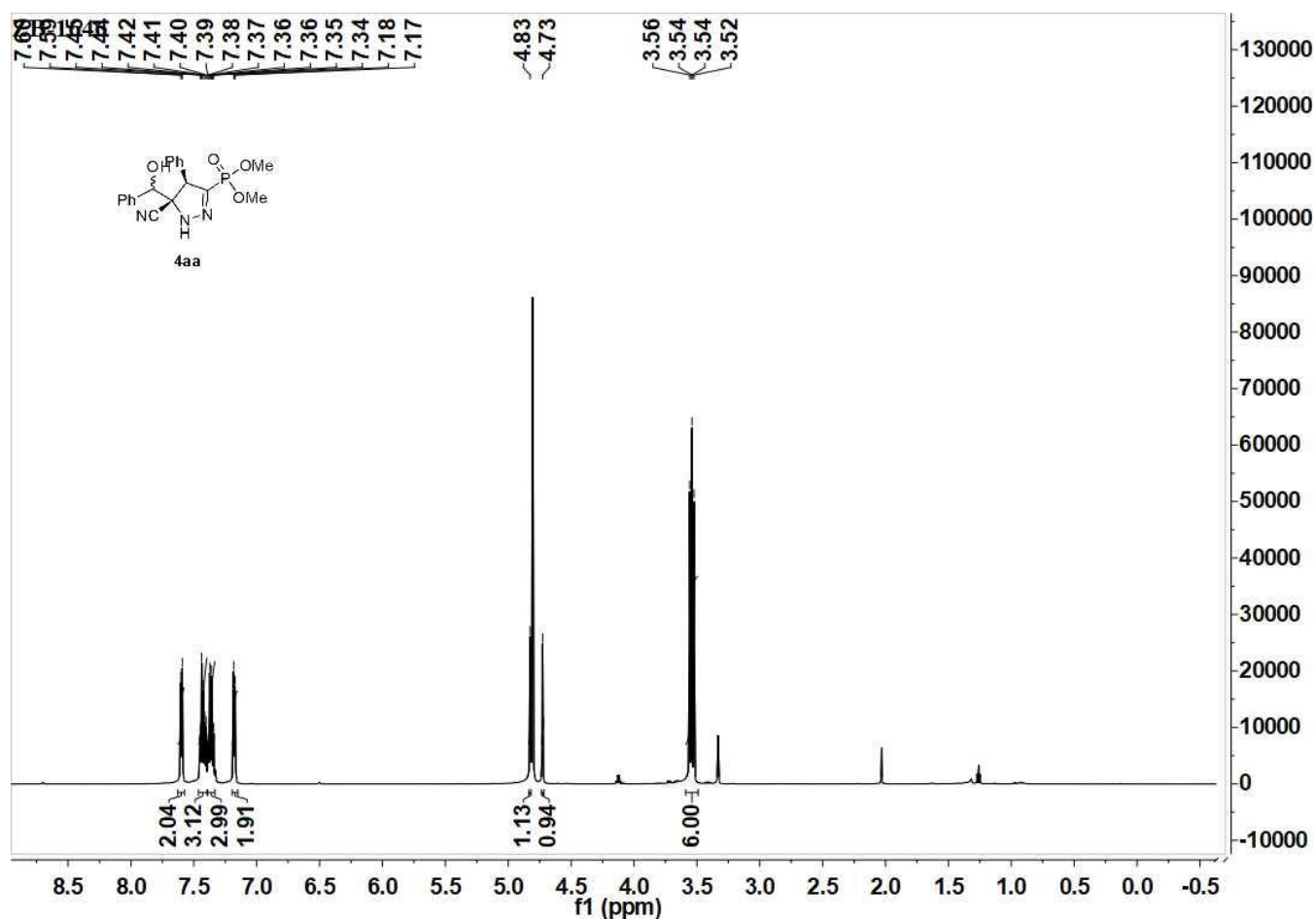


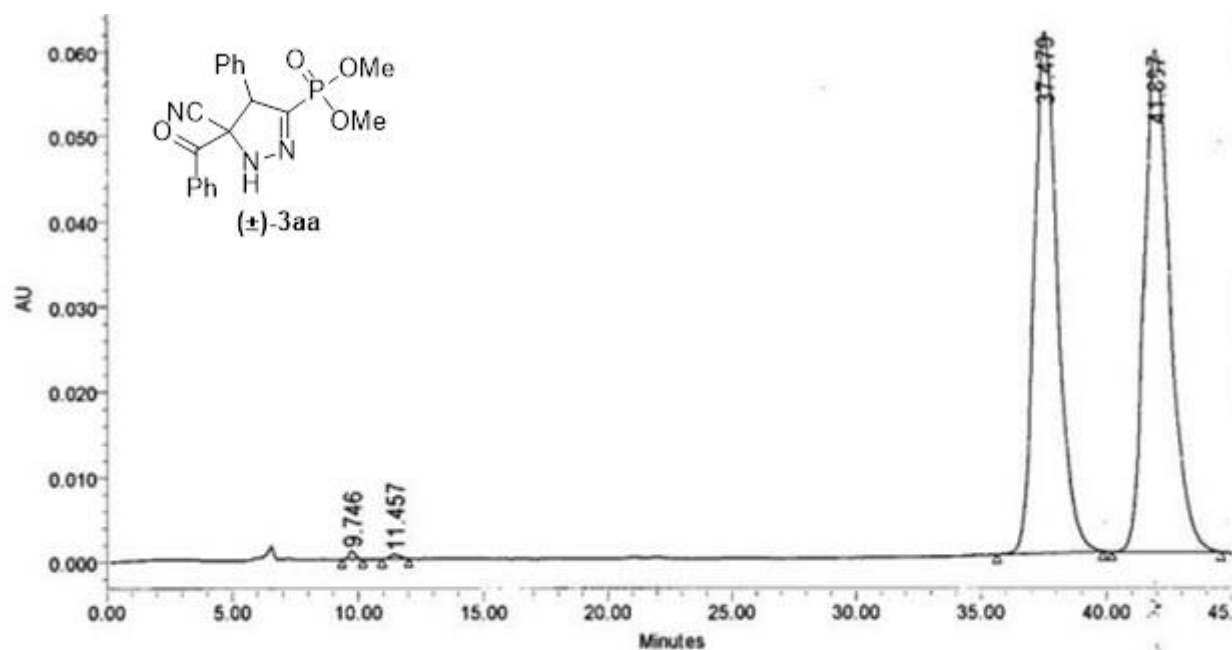




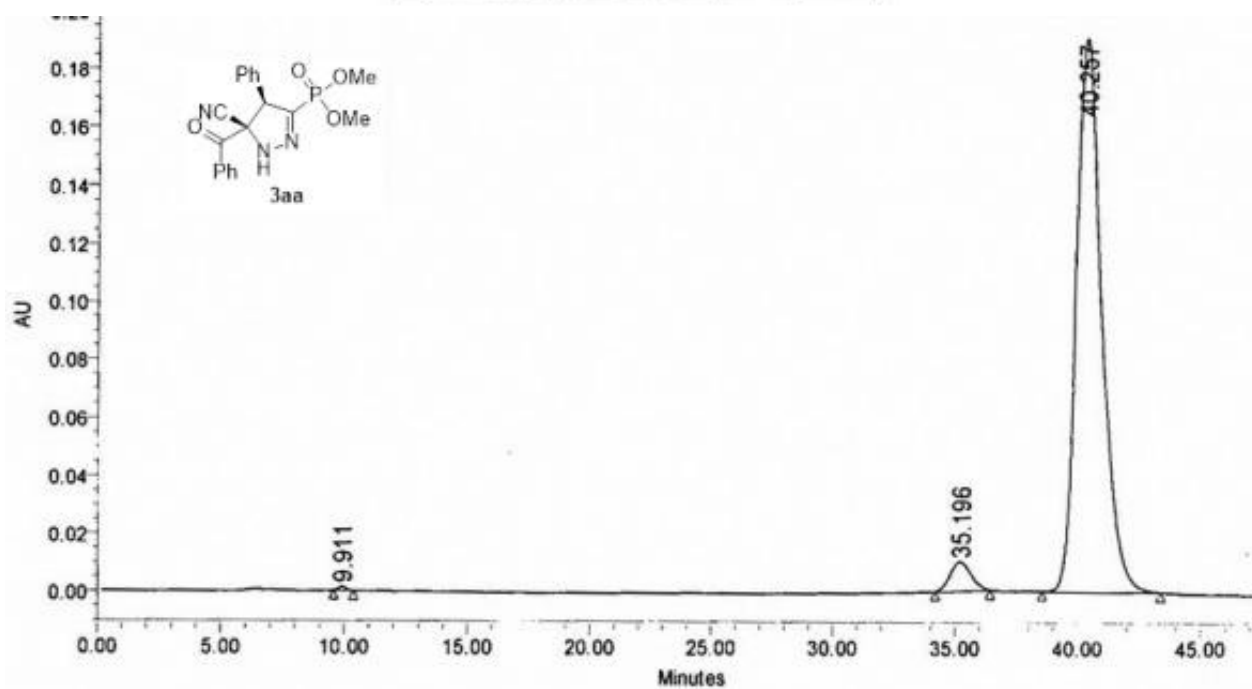




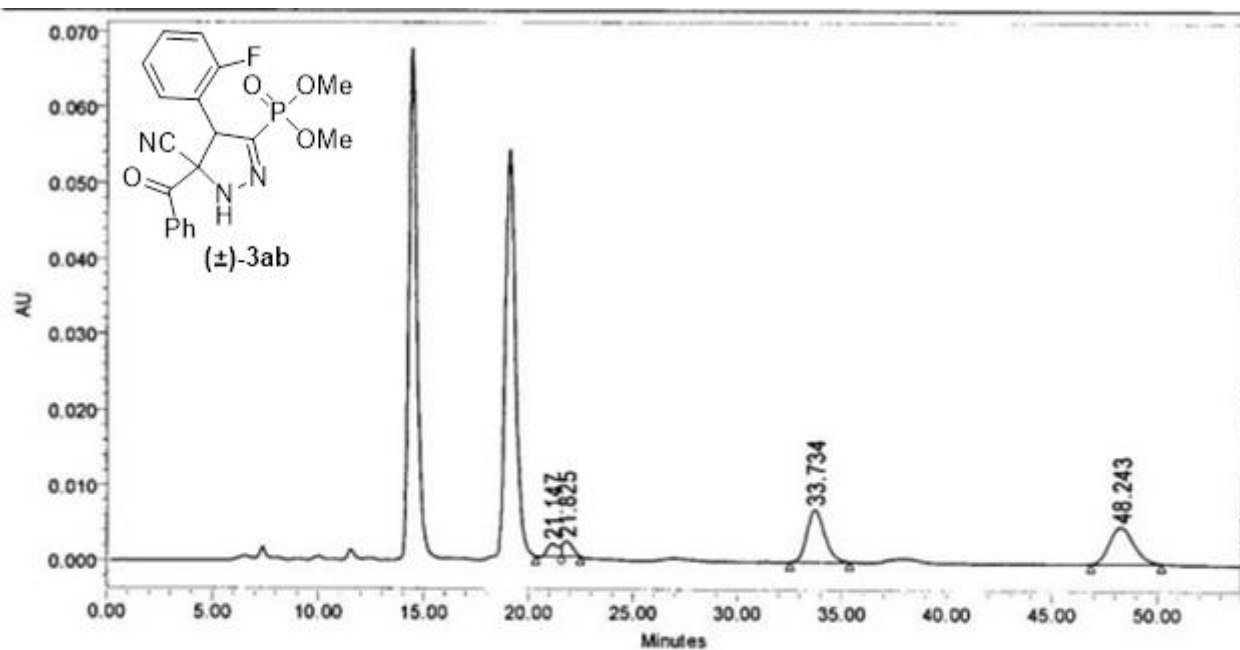




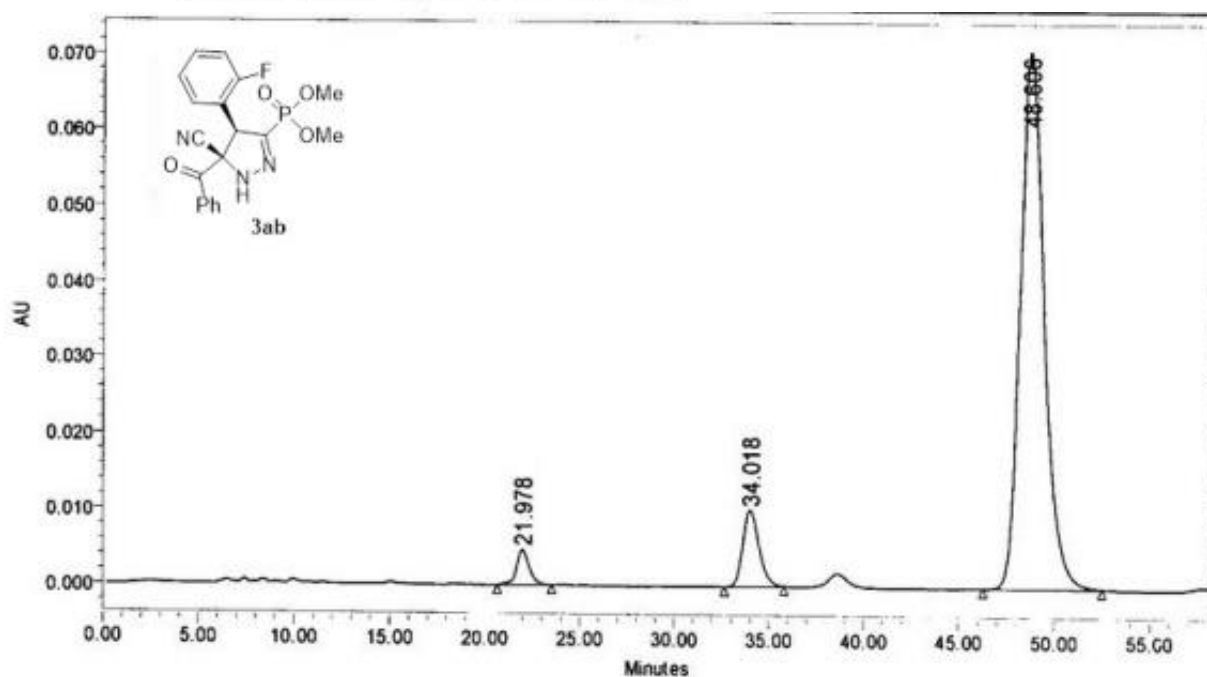
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	9.746	16264	0.20	960	0.79
2	11.457	12937	0.16	491	0.40
3	37.479	3951295	48.24	61329	50.36
4	41.887	4209628	51.40	59006	48.45



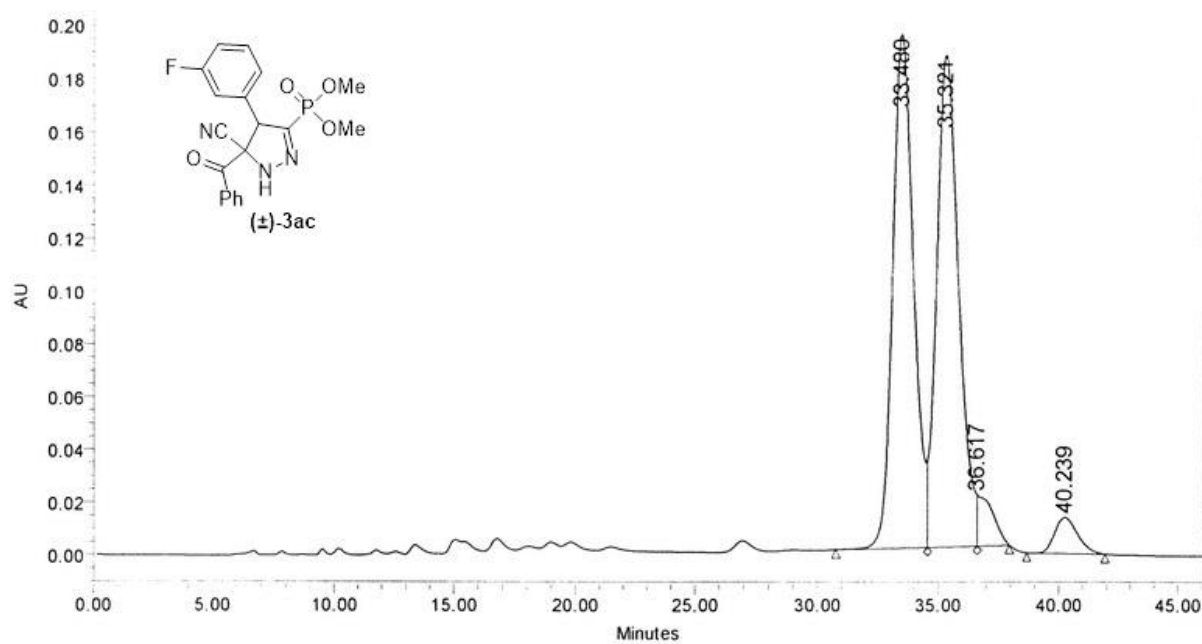
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	9.911	25894	0.18	1301	0.64
2	35.196	588962	4.13	10058	4.98
3	40.257	13652965	95.69	190596	94.38



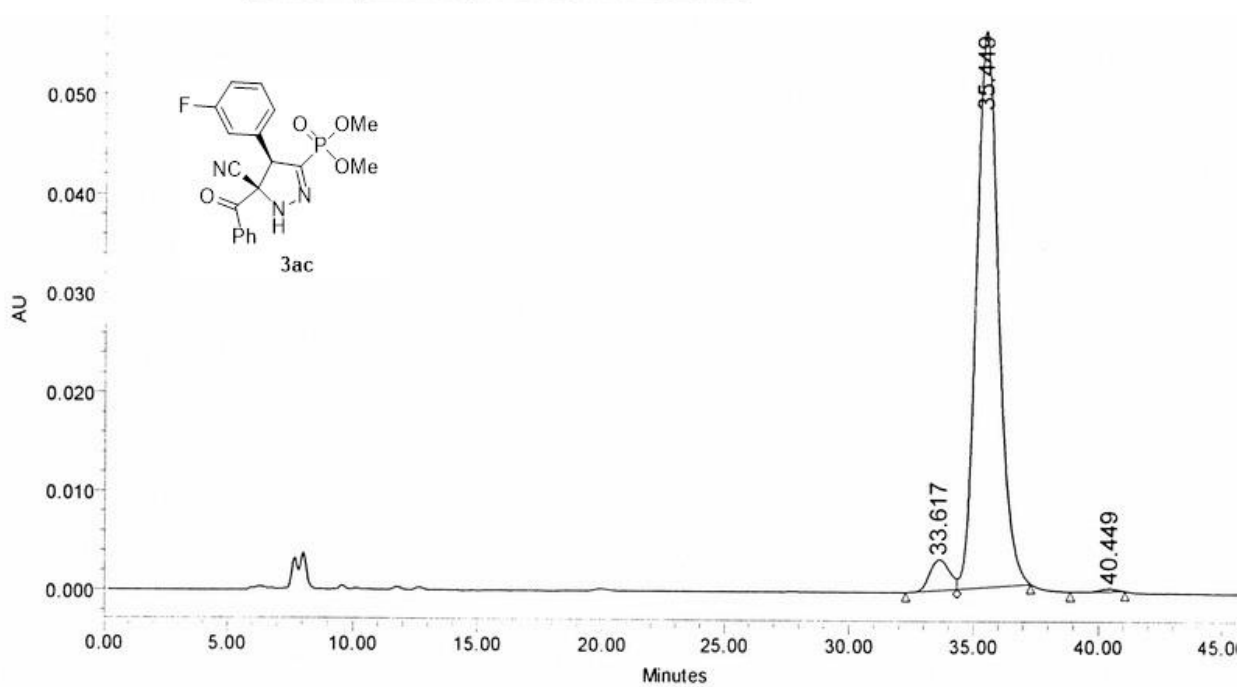
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	21.147	63443	6.88	1663	10.77
2	21.825	64815	7.03	1967	12.74
3	33.734	403415	43.73	6909	44.76
4	48.243	390877	42.37	4895	31.72



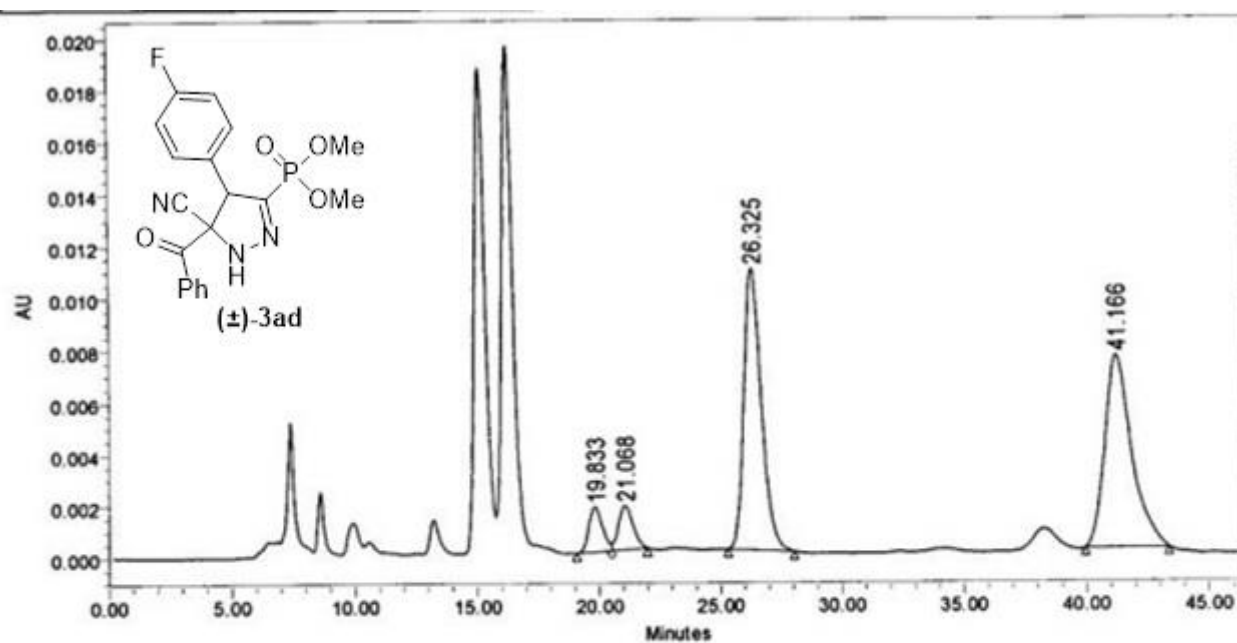
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	21.978	212237	3.07	4592	5.38
2	34.018	600874	8.69	10102	11.83
3	48.606	6102908	88.24	70735	82.80



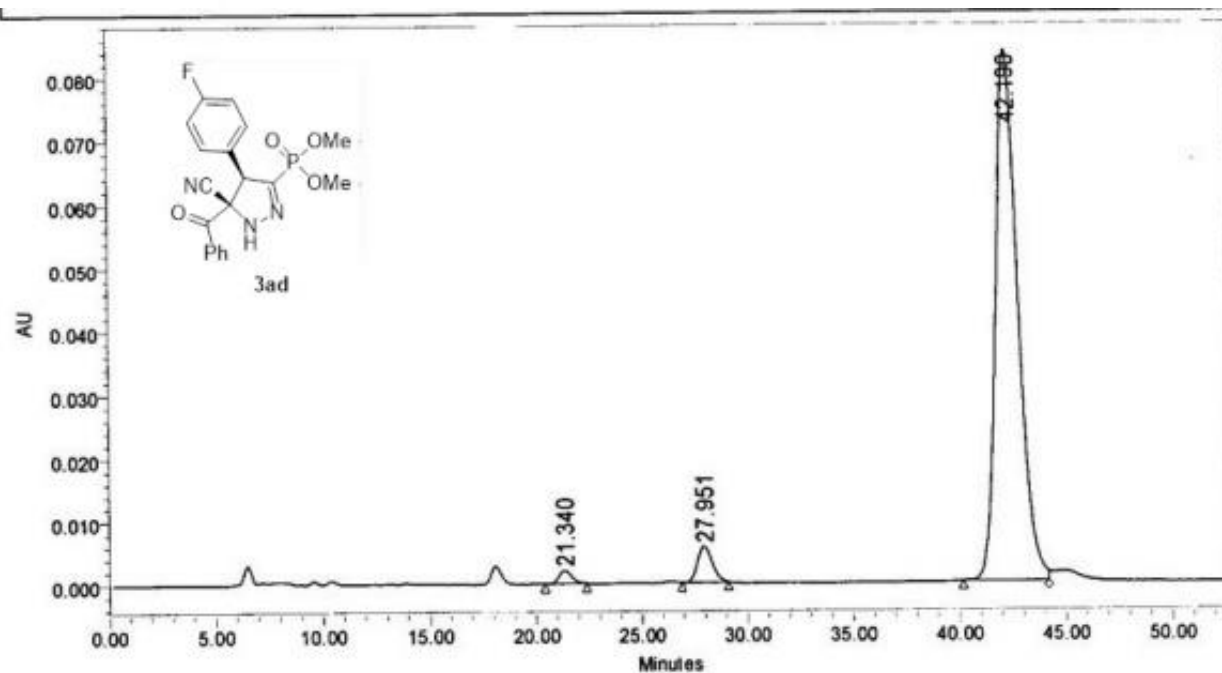
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	33.480	11662632	46.04	194153	47.00
2	35.321	11875644	46.88	185955	45.01
3	36.617	879056	3.47	19359	4.69
4	40.239	914367	3.61	13665	3.31



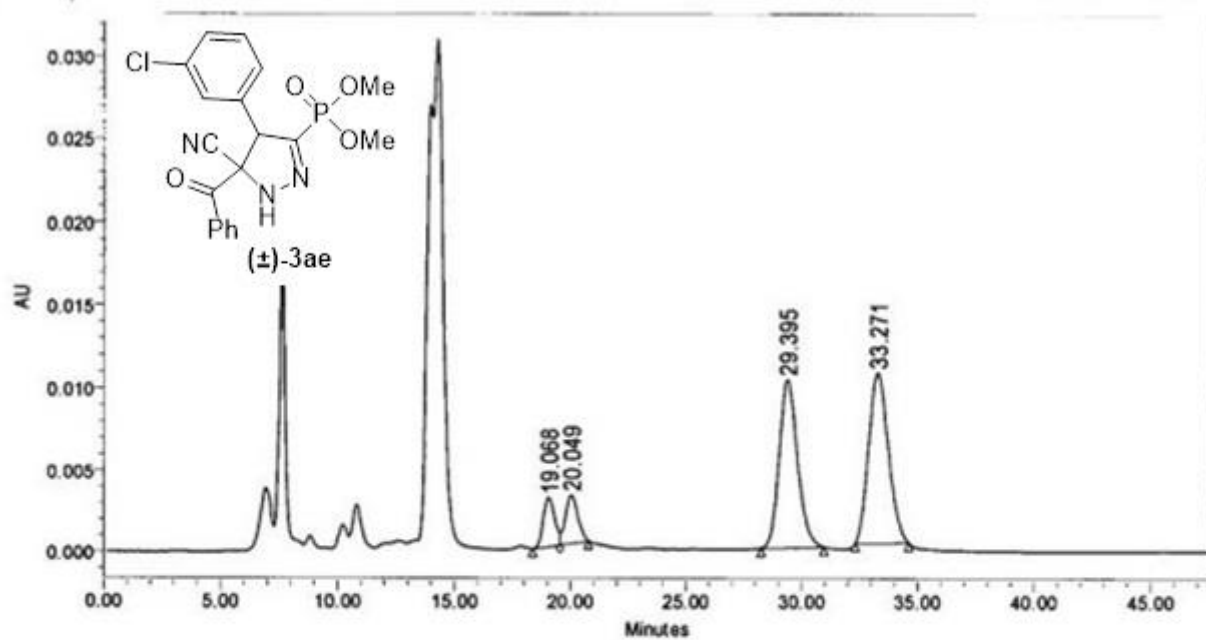
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	33.617	170249	4.65	3106	5.23
2	35.449	3479358	94.96	56049	94.30
3	40.449	14545	0.40	284	0.48



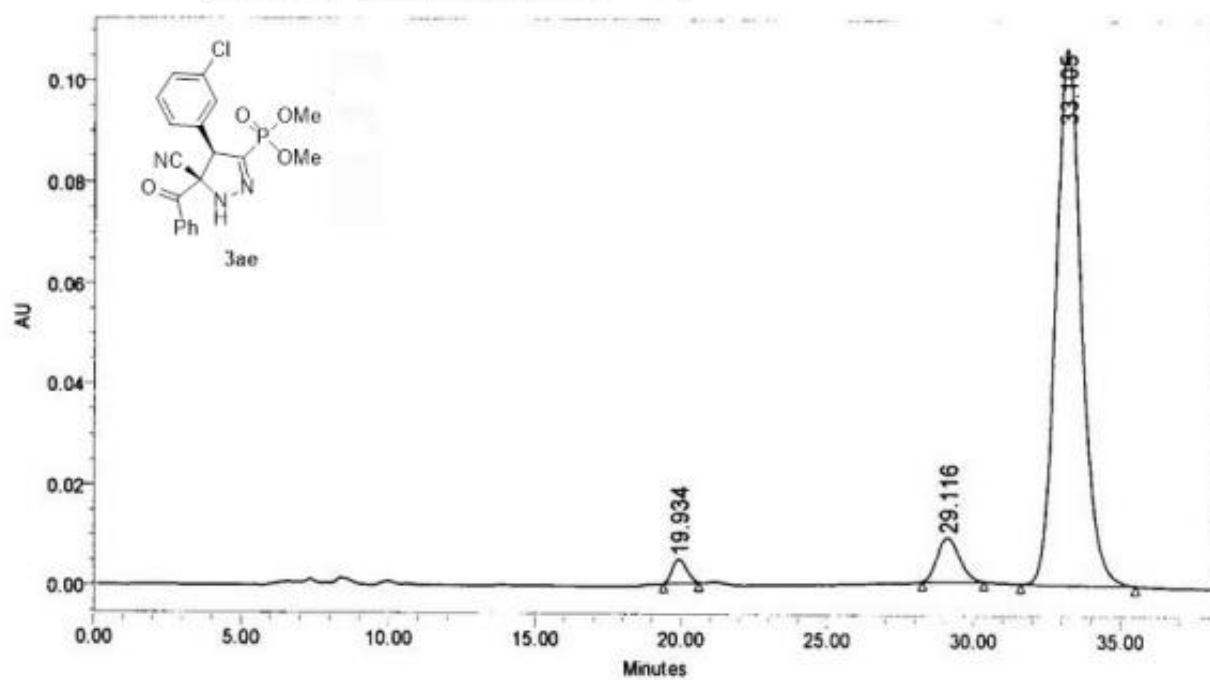
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	19.833	67332	5.43	1729	7.98
2	21.068	70647	5.70	1703	7.86
3	26.325	538197	43.43	10844	50.02
4	41.166	563104	45.44	7404	34.15



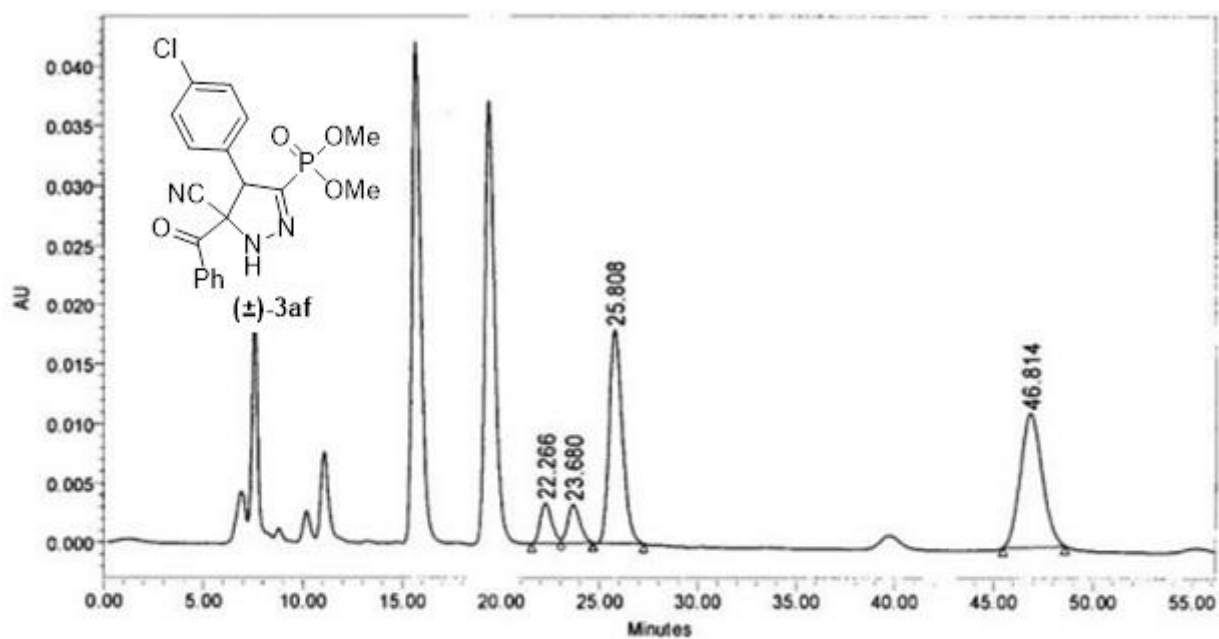
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	21.340	84169	1.32	2062	2.26
2	27.951	272090	4.28	5649	6.18
3	42.190	5999584	94.39	83721	91.57



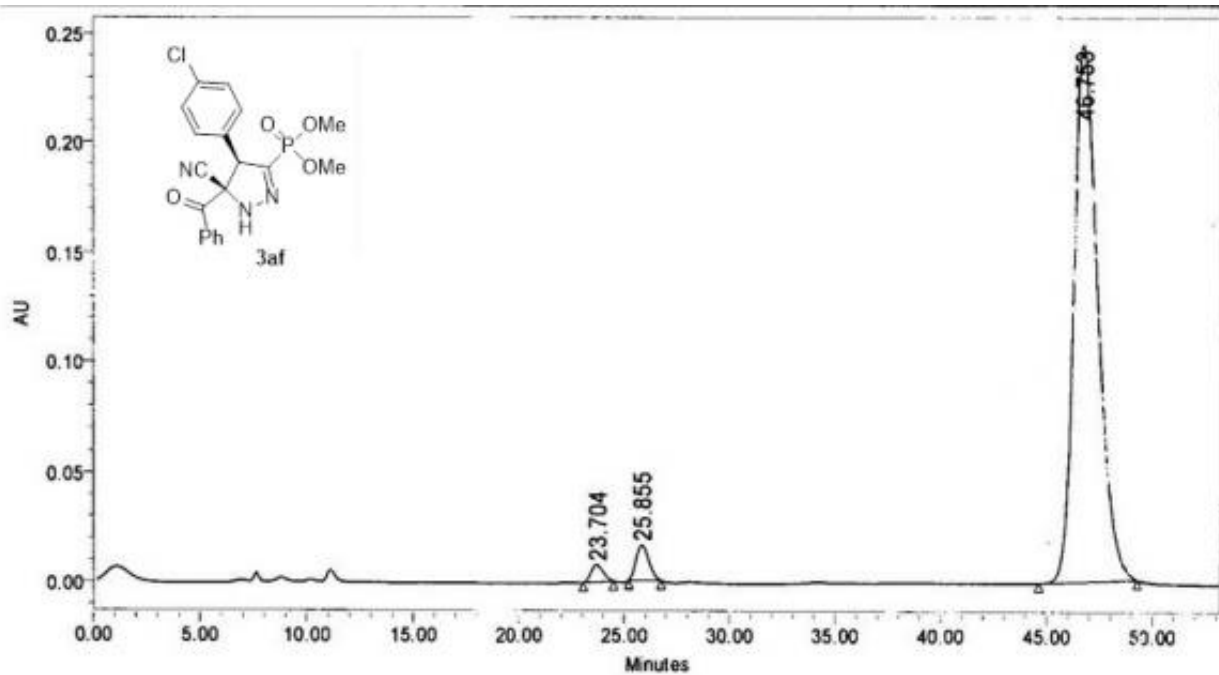
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	19.068	101659	7.30	3007	11.29
2	20.049	109978	7.90	2971	11.15
3	29.395	564332	40.54	10261	38.52
4	33.271	615908	44.25	10397	39.03



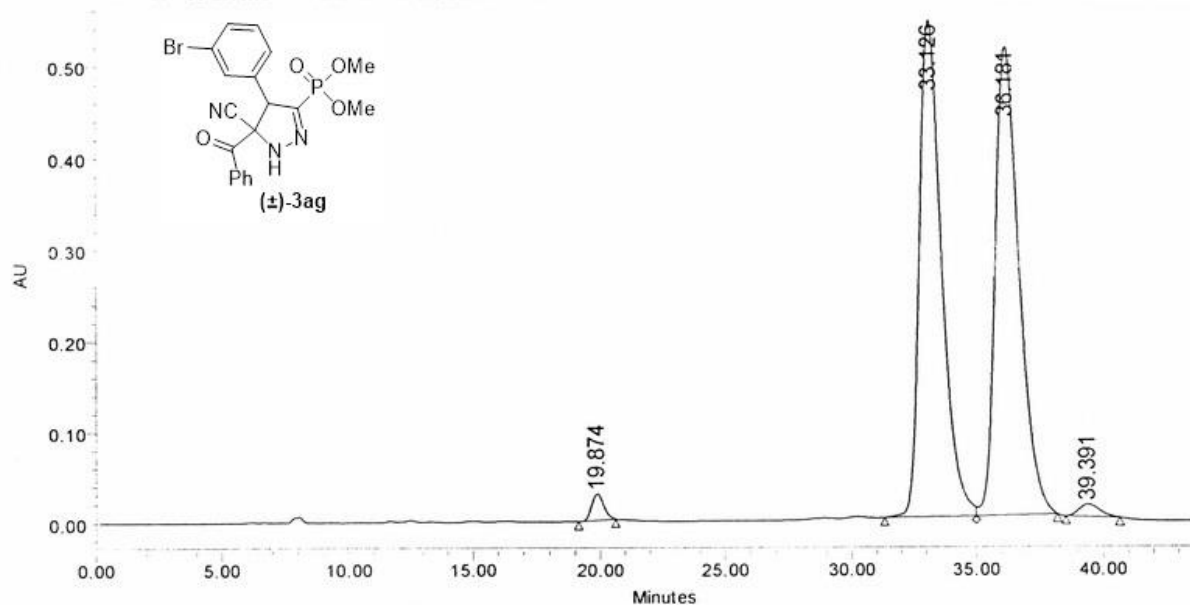
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	19.934	161391	2.29	4707	3.93
2	29.116	457985	6.50	8752	7.31
3	33.105	6426362	91.21	106216	88.75



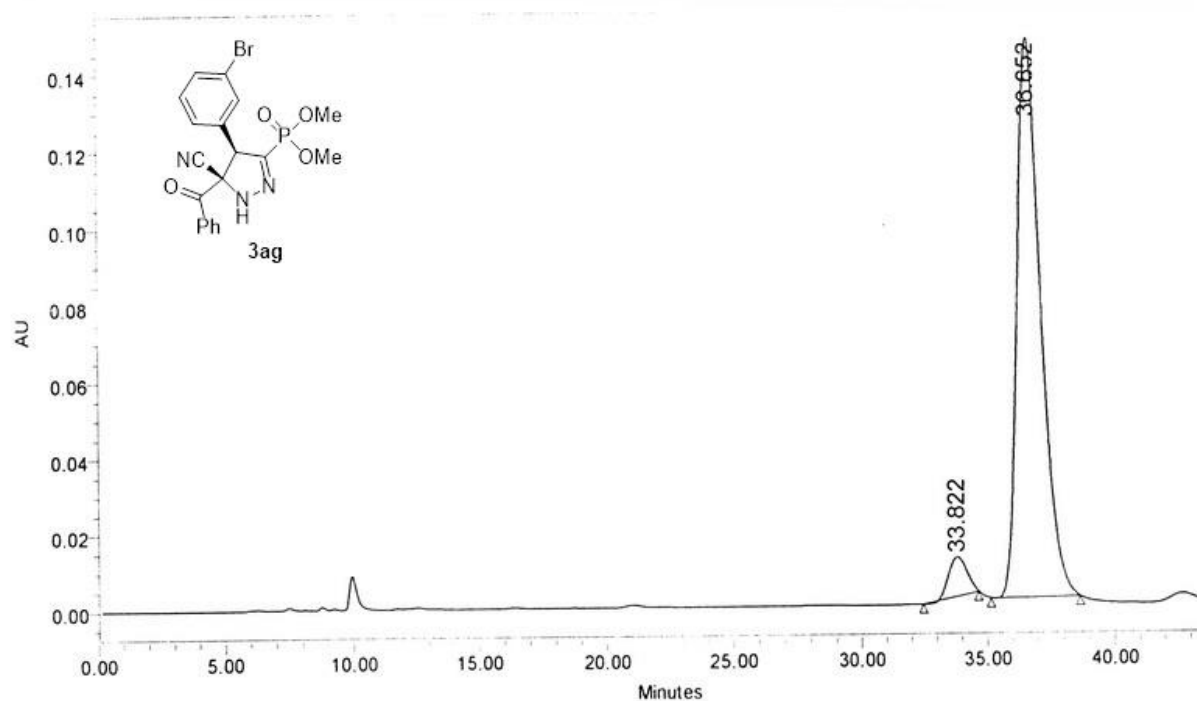
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	22.266	137481	6.99	3395	9.48
2	23.680	139183	7.07	3229	9.02
3	25.808	832691	42.32	17927	50.08
4	46.814	858098	43.61	11244	31.41



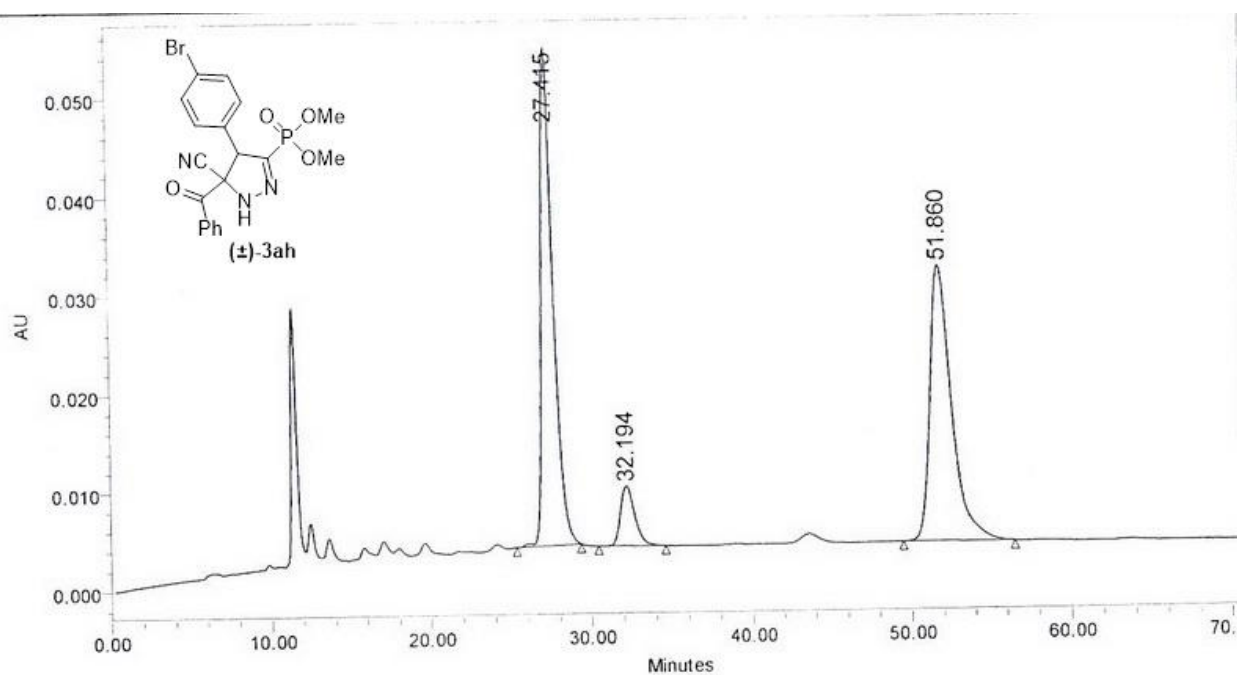
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	23.704	311988	1.55	7784	2.91
2	25.855	676424	3.35	16039	5.99
3	46.753	19195330	95.10	244116	91.11



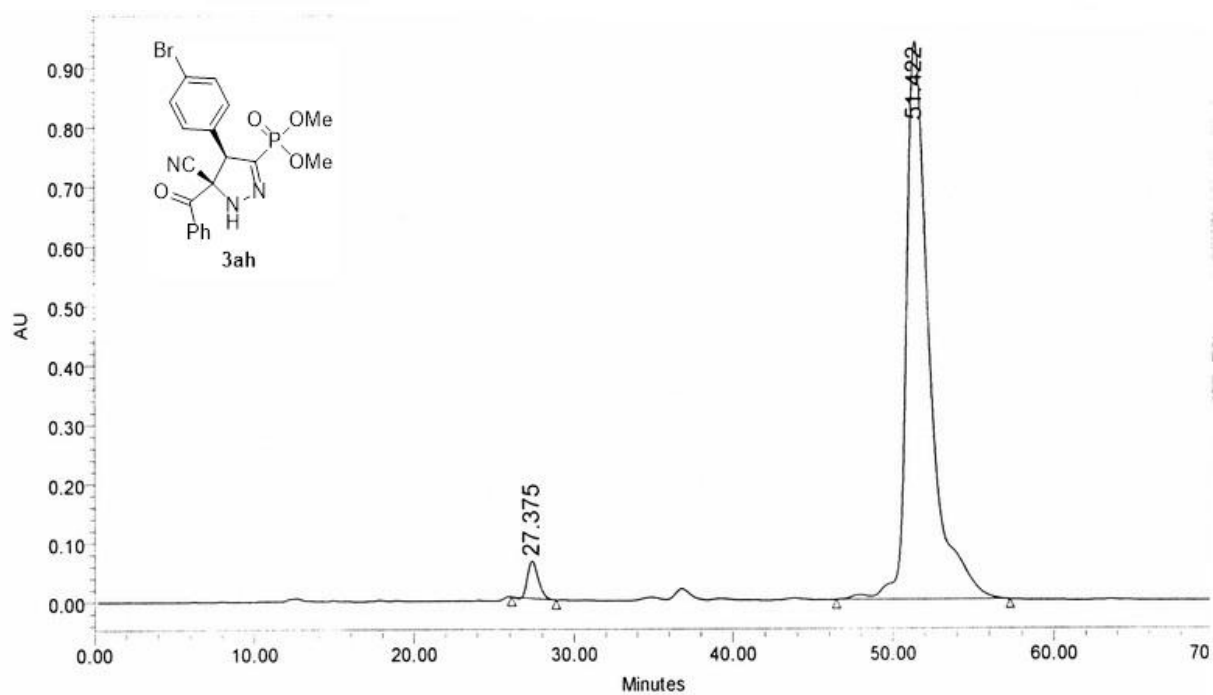
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	19.874	959678	1.39	29034	2.65
2	33.126	33604154	48.71	541814	49.43
3	36.181	33666891	48.80	511783	46.69
4	39.391	761093	1.10	13481	1.23



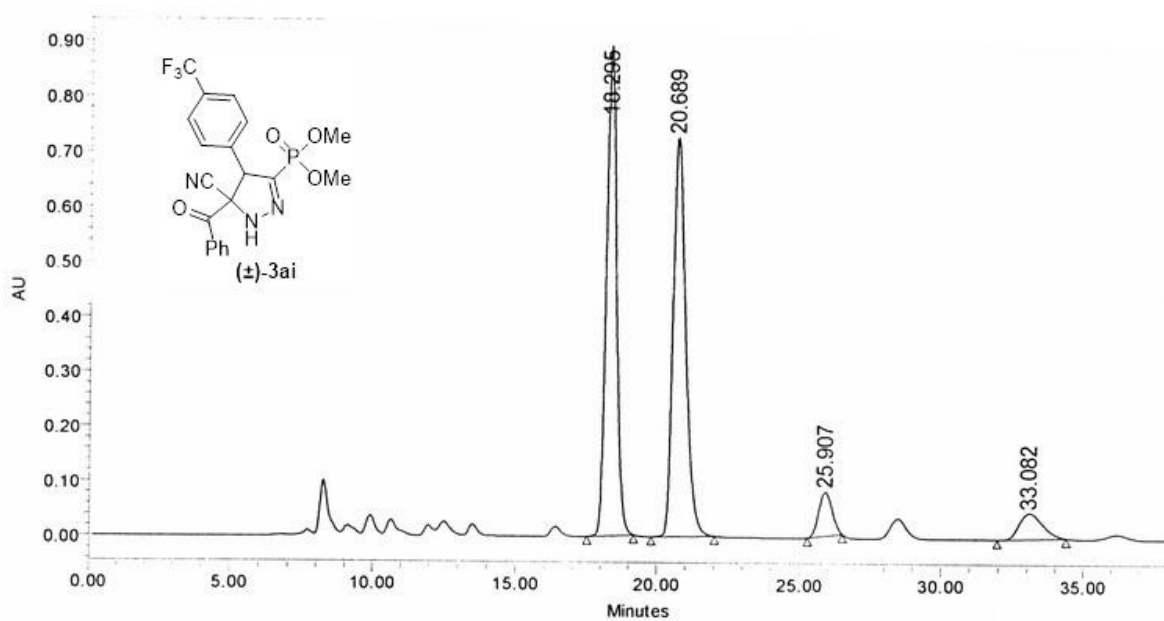
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	33.822	522666	5.33	10277	6.58
2	36.652	9288220	94.67	145986	93.42



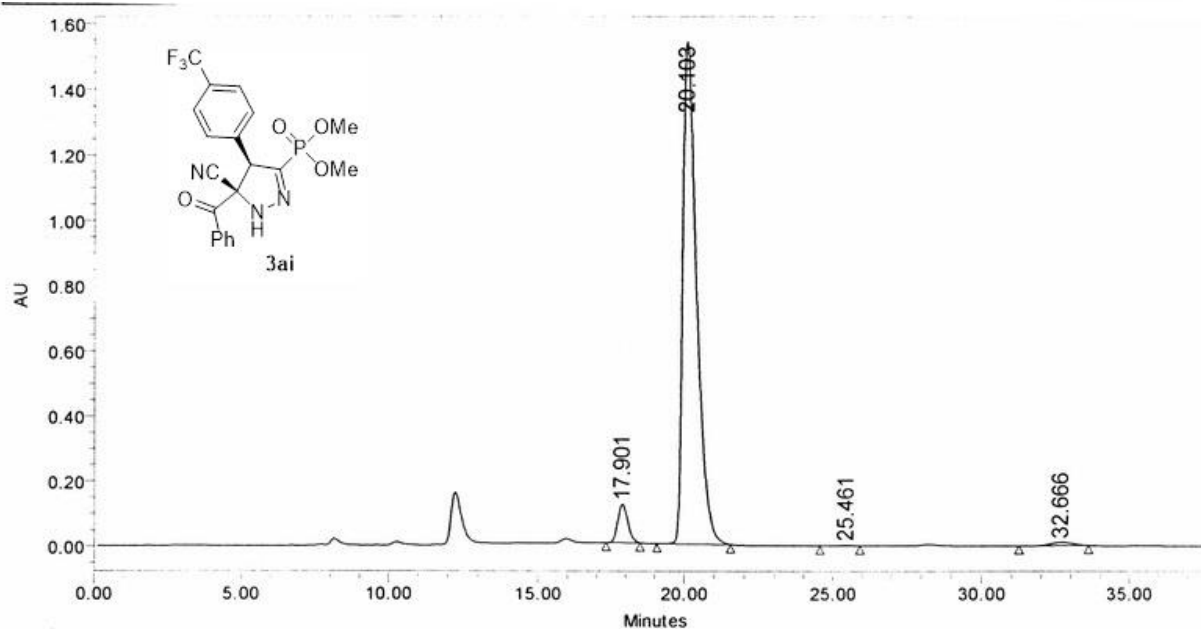
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	27.415	2624953	46.70	50487	59.63
2	32.194	370050	6.58	6110	7.22
3	51.860	2625353	46.71	28069	33.15



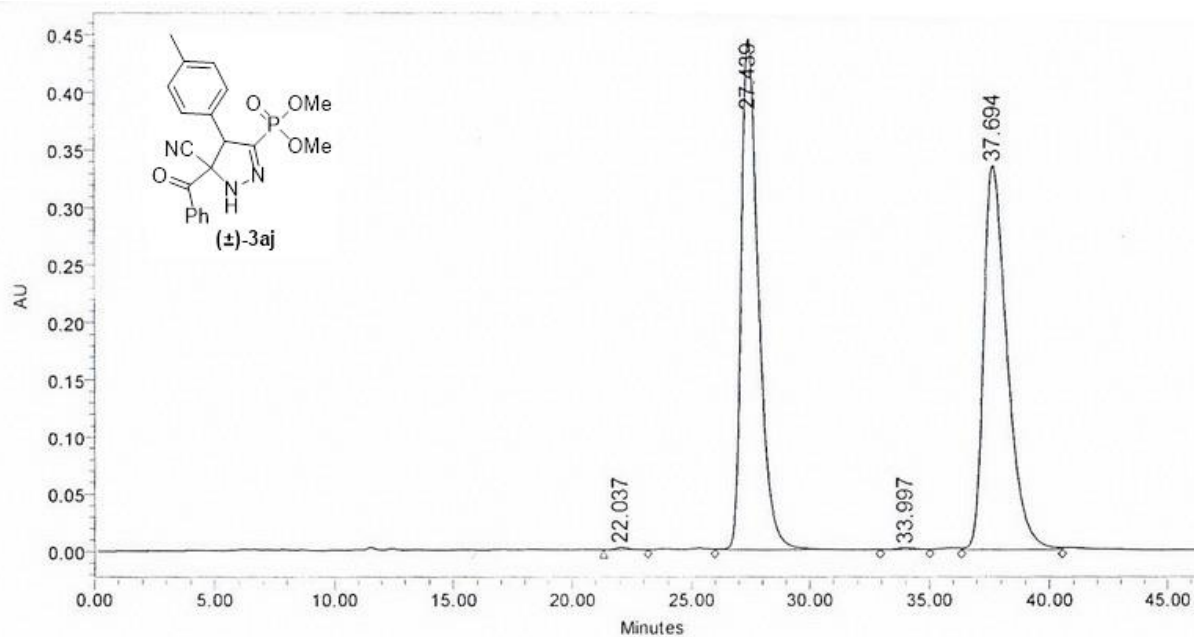
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	27.375	2944669	3.05	62790	6.28
2	51.422	93530121	96.95	937628	93.72



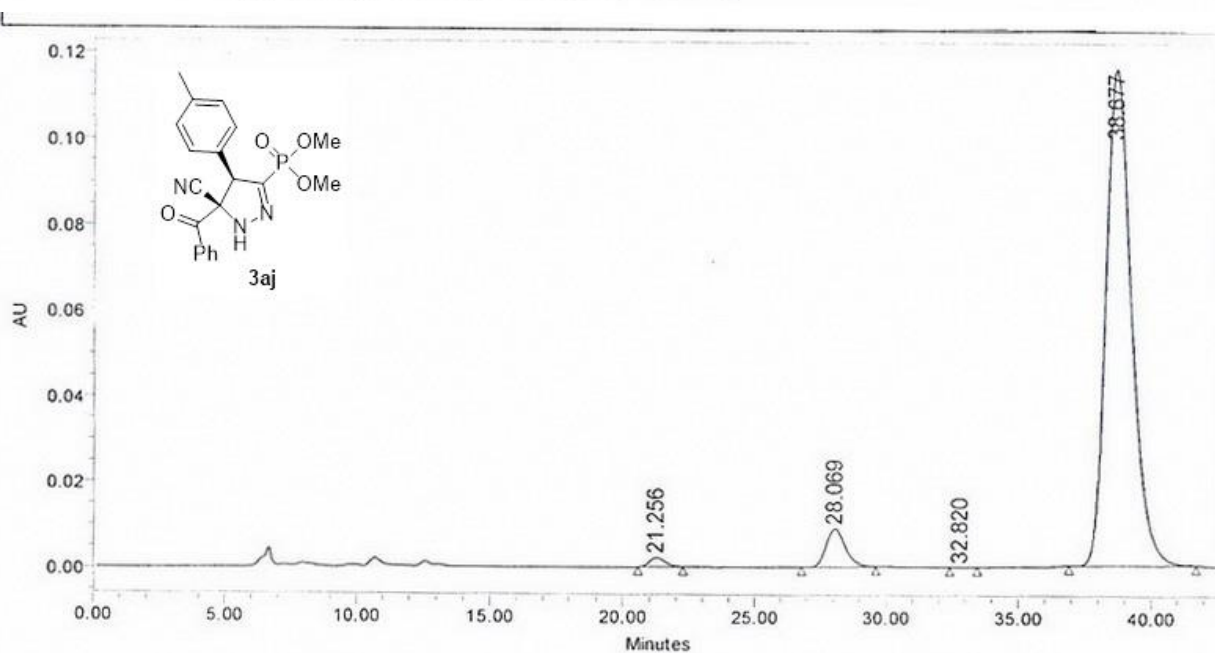
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	18.295	22461919	44.71	891946	51.07
2	20.689	22423017	44.63	726718	41.61
3	25.907	2654339	5.28	80322	4.60
4	33.082	2703287	5.38	47409	2.71



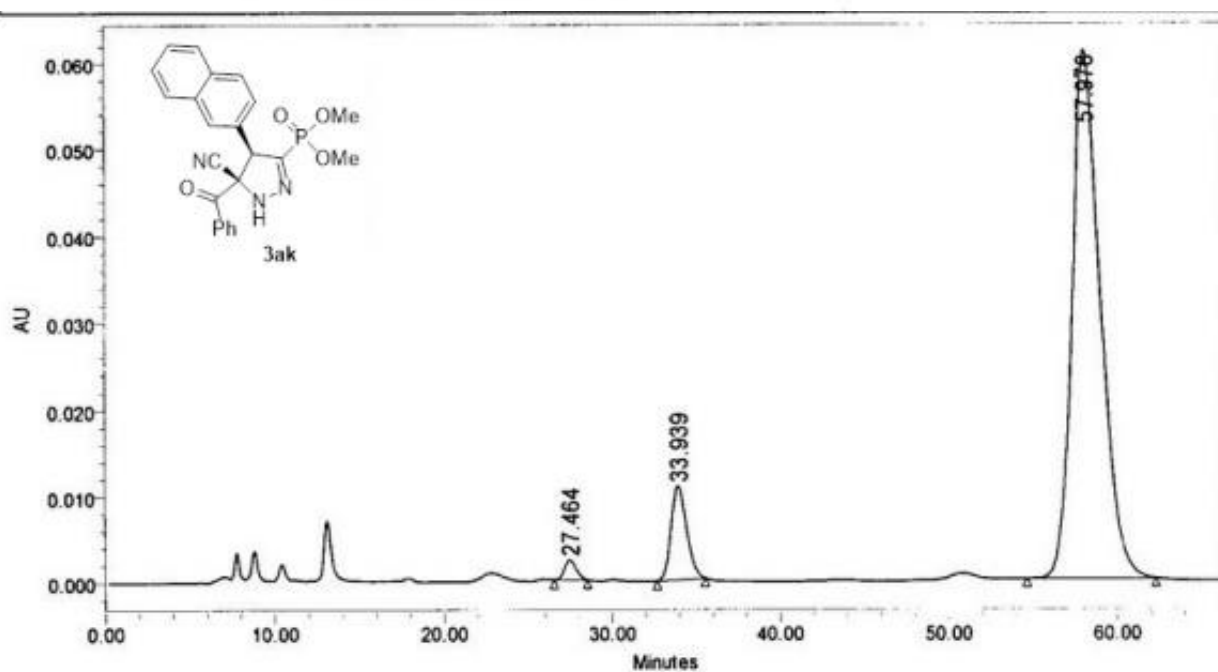
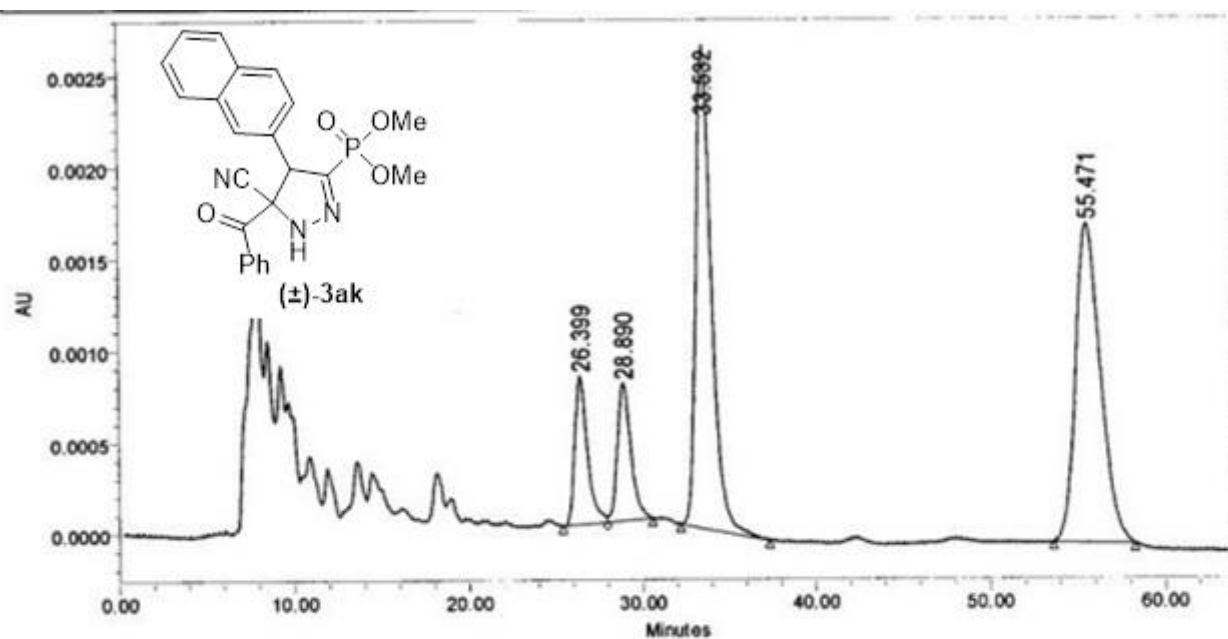
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	17.901	2863358	5.42	118537	7.10
2	20.103	49354778	93.38	1537767	92.13
3	25.461	65919	0.12	2132	0.13
4	32.666	571478	1.08	10741	0.64



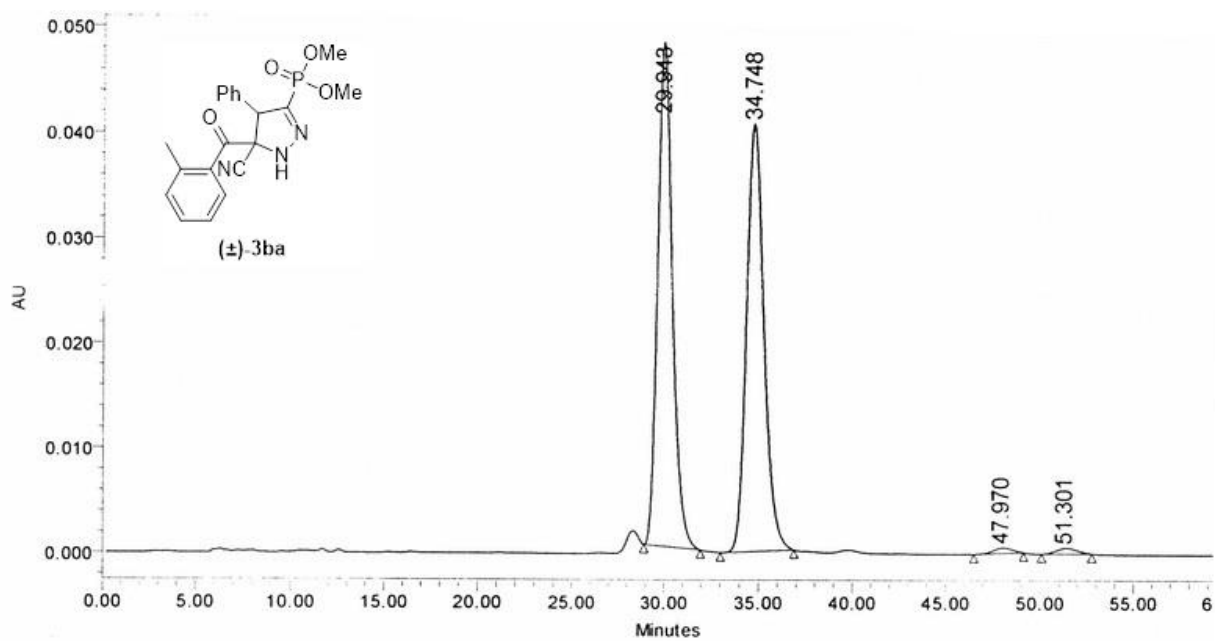
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	22.037	80178	0.18	1842	0.24
2	27.439	22564301	49.83	445003	56.82
3	33.997	91027	0.20	1509	0.19
4	37.694	22548729	49.79	334777	42.75



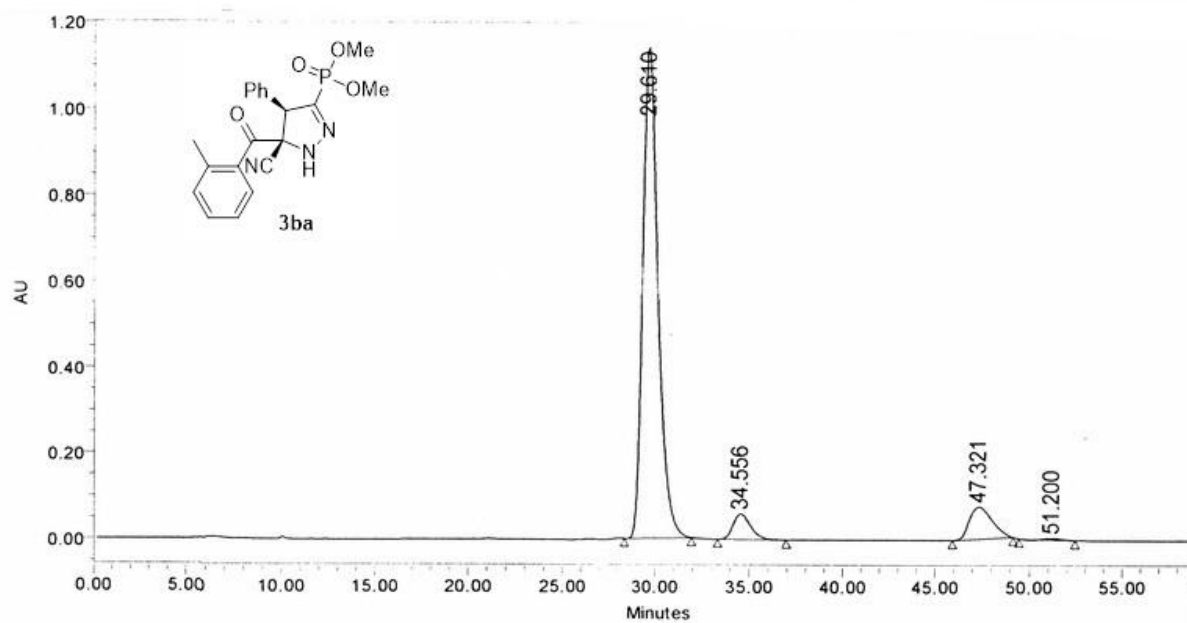
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	21.256	88578	1.07	2156	1.70
2	28.069	445345	5.39	8872	7.00
3	32.820	224	0.00	17	0.01
4	38.677	7725734	93.53	115685	91.28



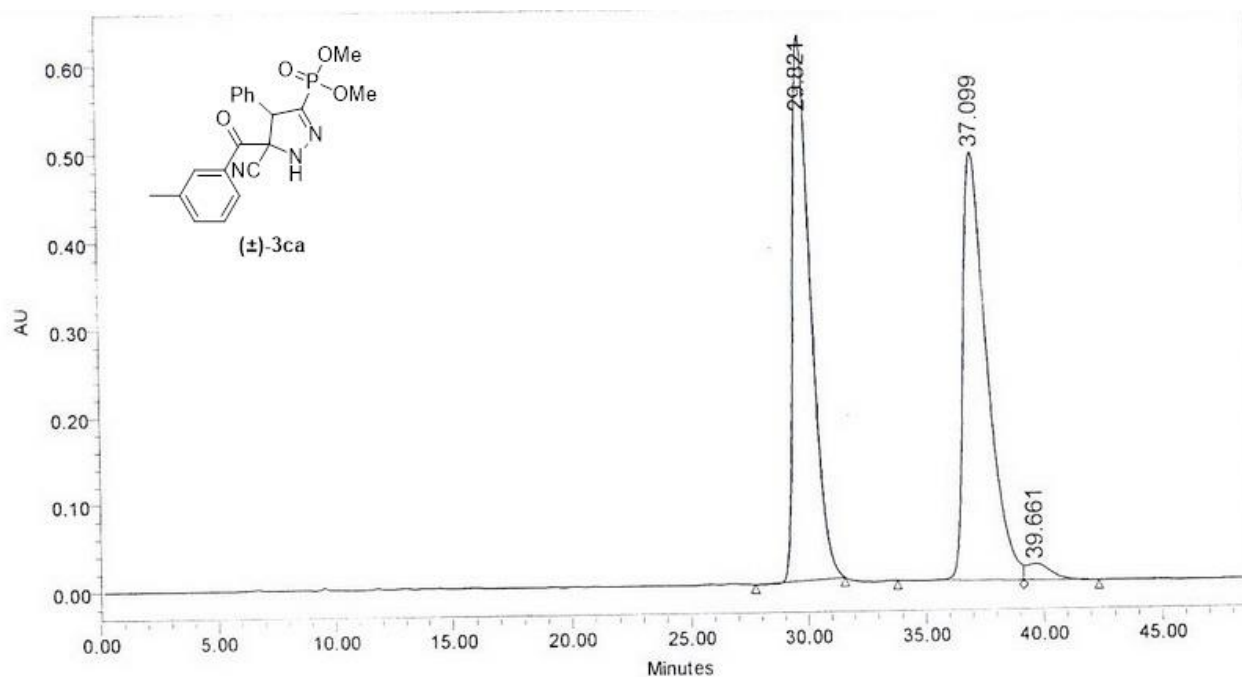
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	27.464	112001	1.43	2289	3.08
2	33.939	700714	8.94	10924	14.72
3	57.976	7027041	89.63	60998	82.20



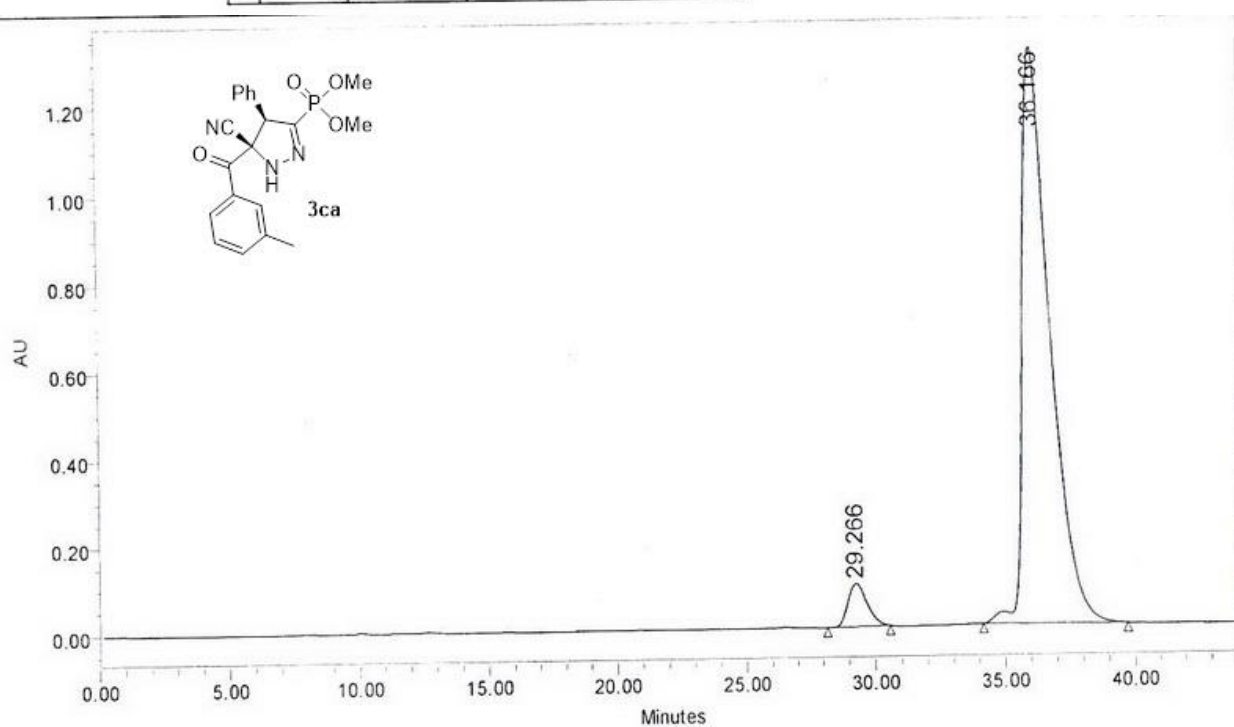
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	29.943	2642753	49.81	47907	53.42
2	34.748	2581457	48.66	40686	45.37
3	47.970	37423	0.71	527	0.59
4	51.301	43731	0.82	559	0.62



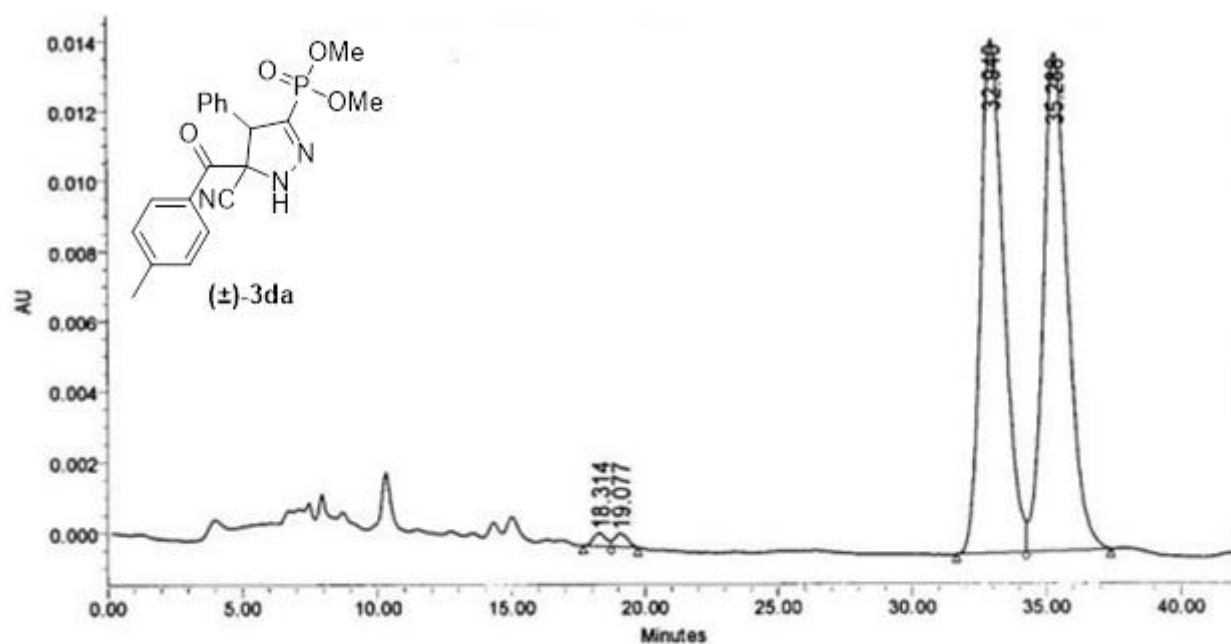
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	29.610	64838880	86.25	1140520	89.21
2	34.556	3790498	5.04	59569	4.66
3	47.321	6261192	8.33	74973	5.86
4	51.200	285011	0.38	3403	0.27



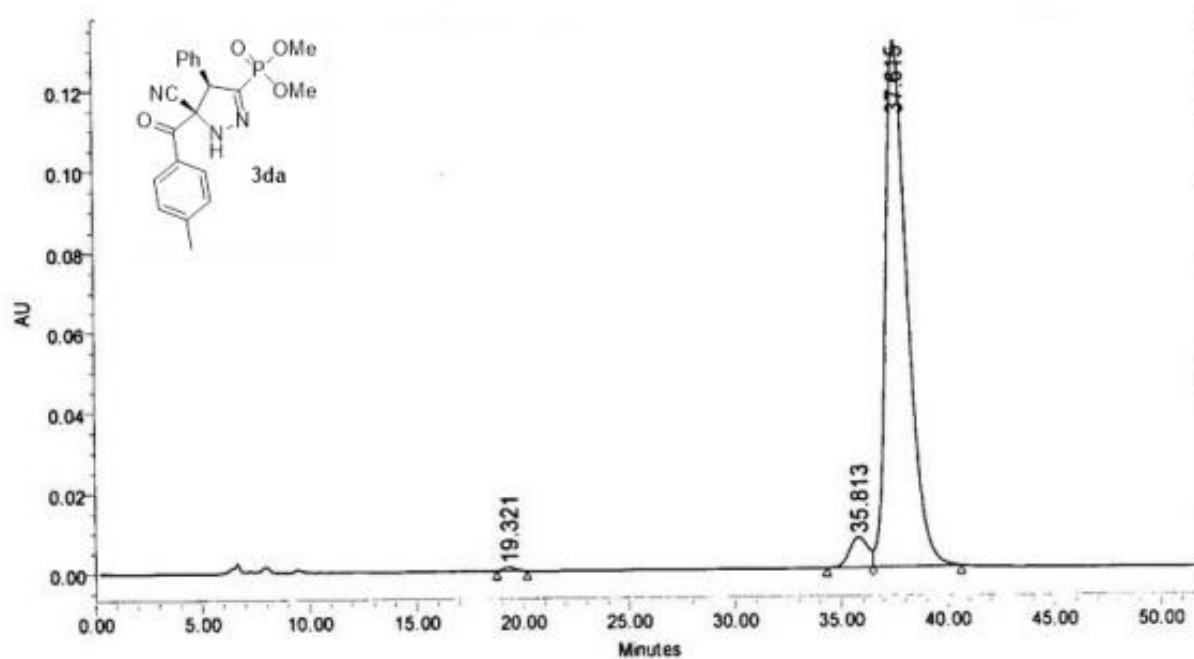
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	29.821	33165828	48.05	622629	55.09
2	37.099	34521273	50.01	489131	43.28
3	39.661	1341134	1.94	18477	1.63



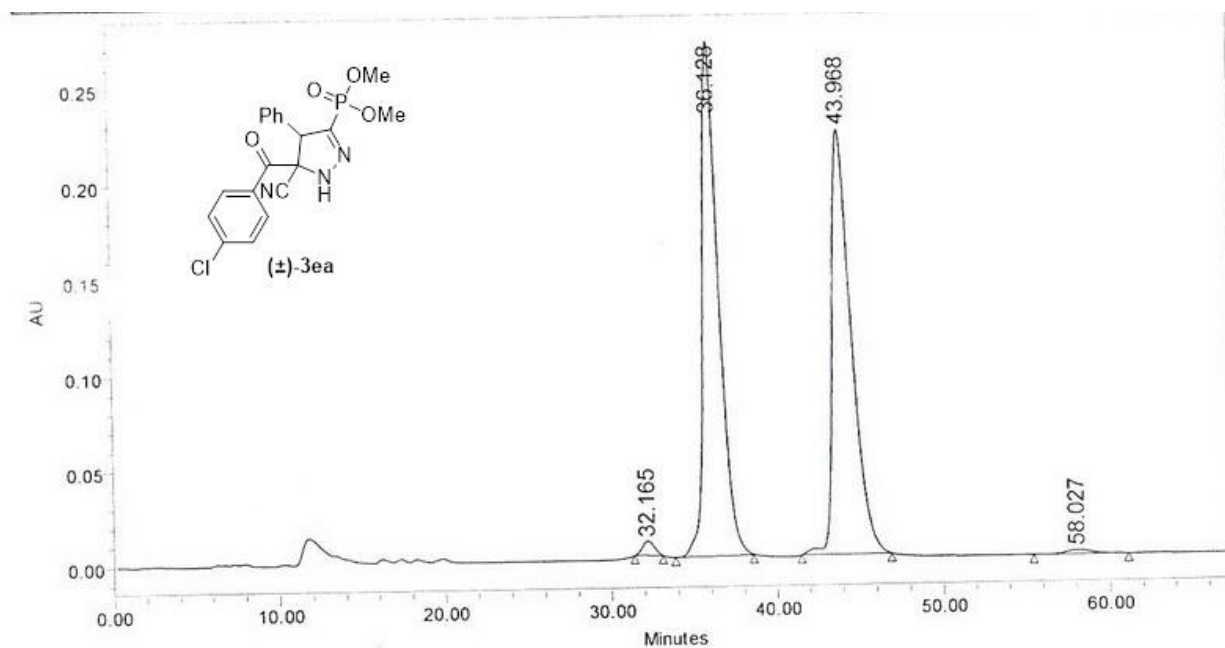
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	29.266	5022983	4.96	98120	6.95
2	36.166	96319751	95.04	1312747	93.05



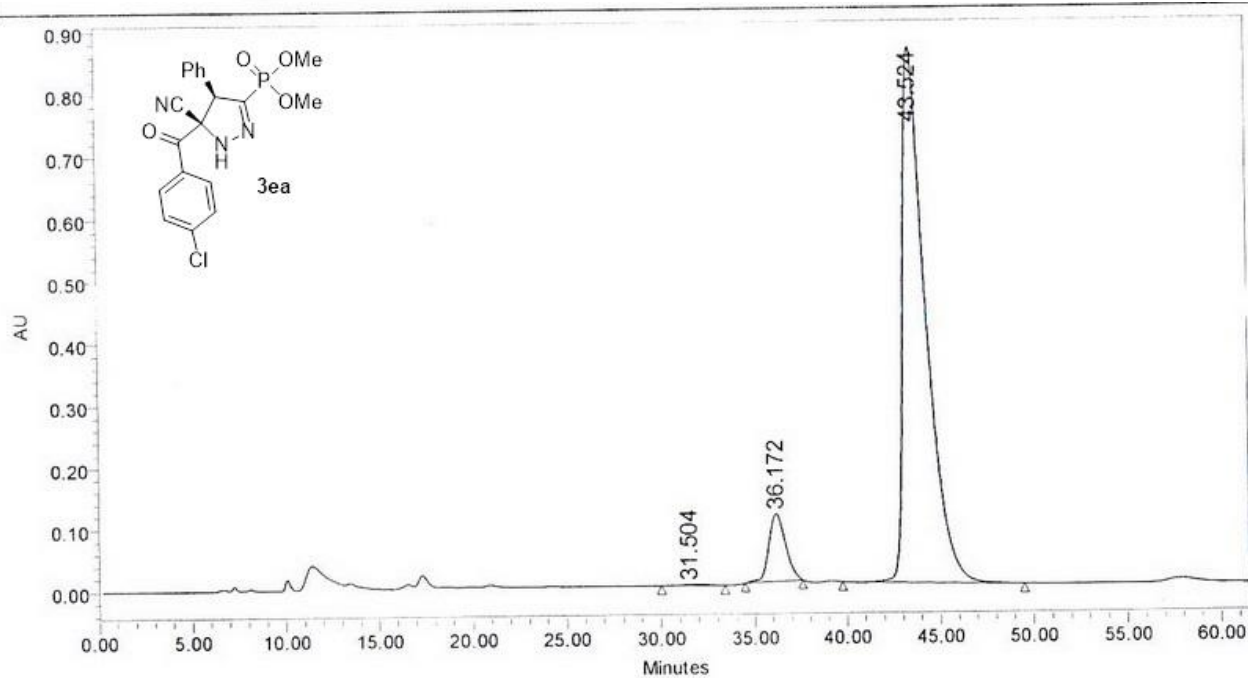
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	18.314	11822	0.67	363	1.23
2	19.077	12434	0.70	366	1.24
3	32.940	864570	48.72	14586	49.53
4	35.288	885582	49.91	14136	48.00



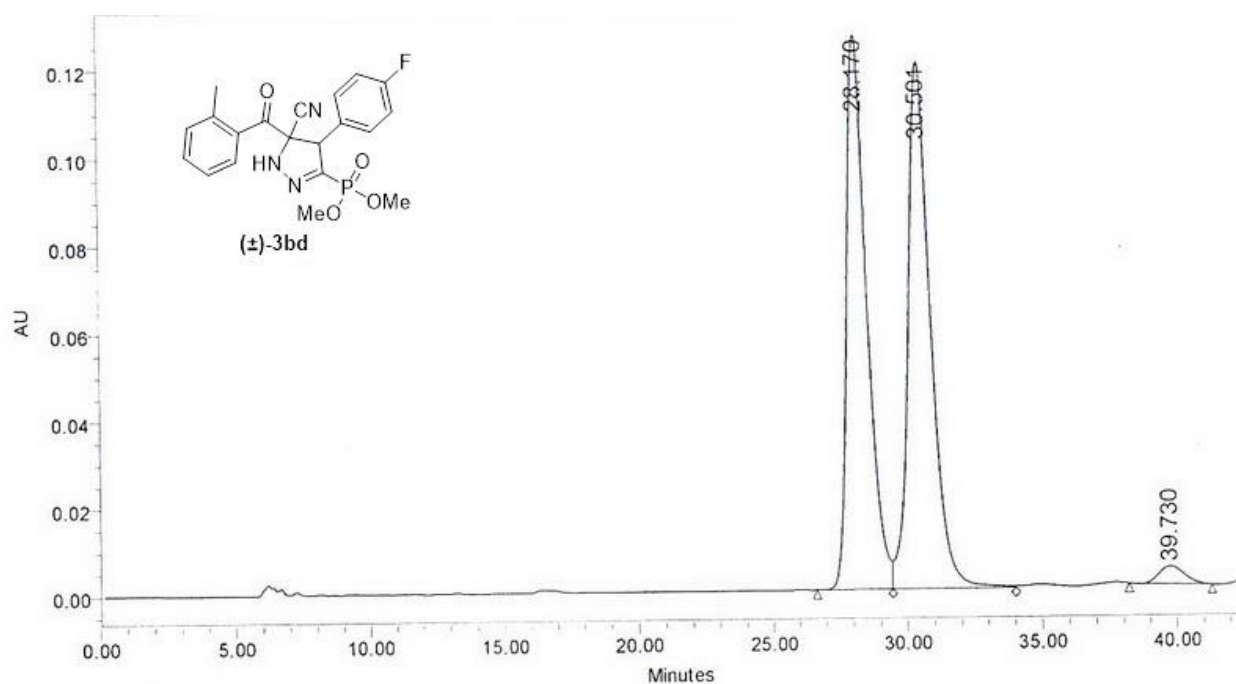
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	19.321	35235	0.36	933	0.67
2	35.813	447456	4.63	7462	5.37
3	37.615	9181045	95.01	130671	93.96



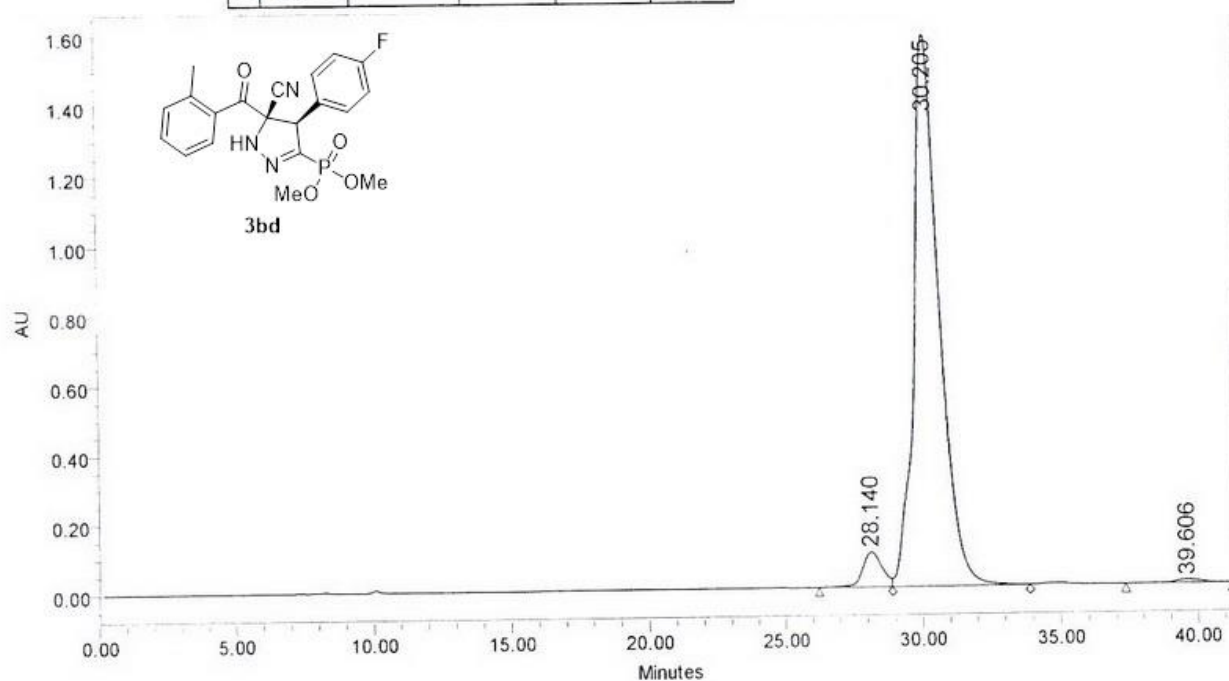
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	32.165	383578	1.04	7583	1.51
2	36.128	18297060	49.82	269656	53.69
3	43.968	17799774	48.46	222685	44.34
4	58.027	248296	0.68	2324	0.46



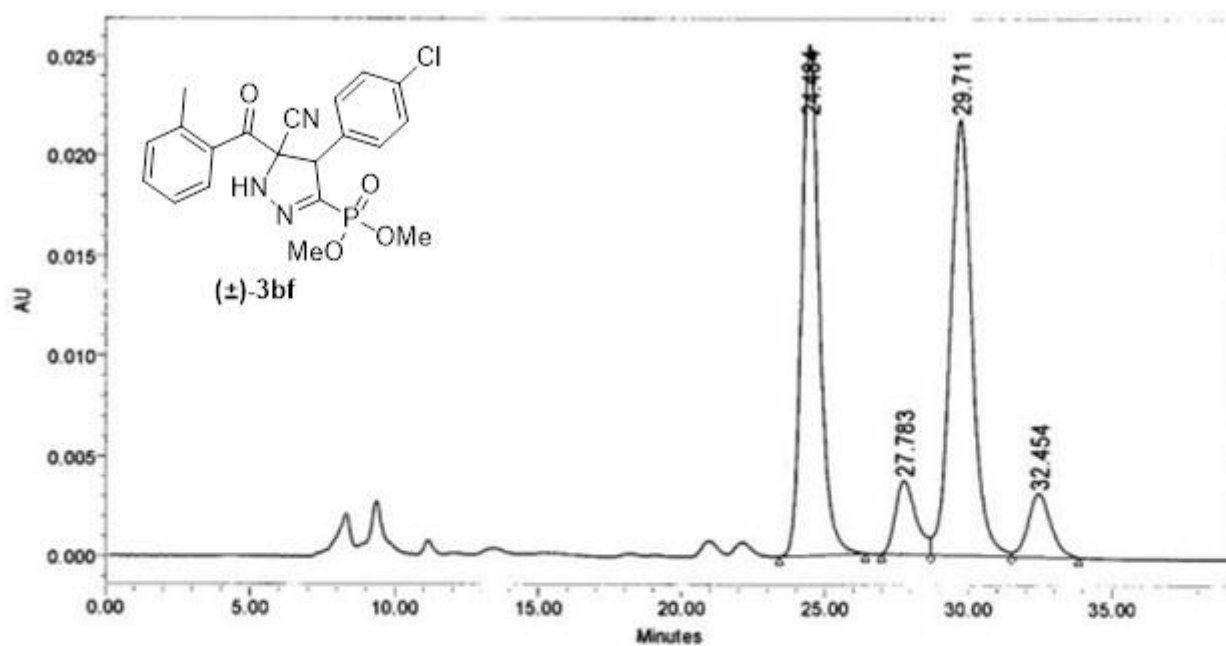
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	31.504	128546	0.16	1763	0.18
2	36.172	6907949	8.56	108851	11.20
3	43.524	73708884	91.29	861122	88.62



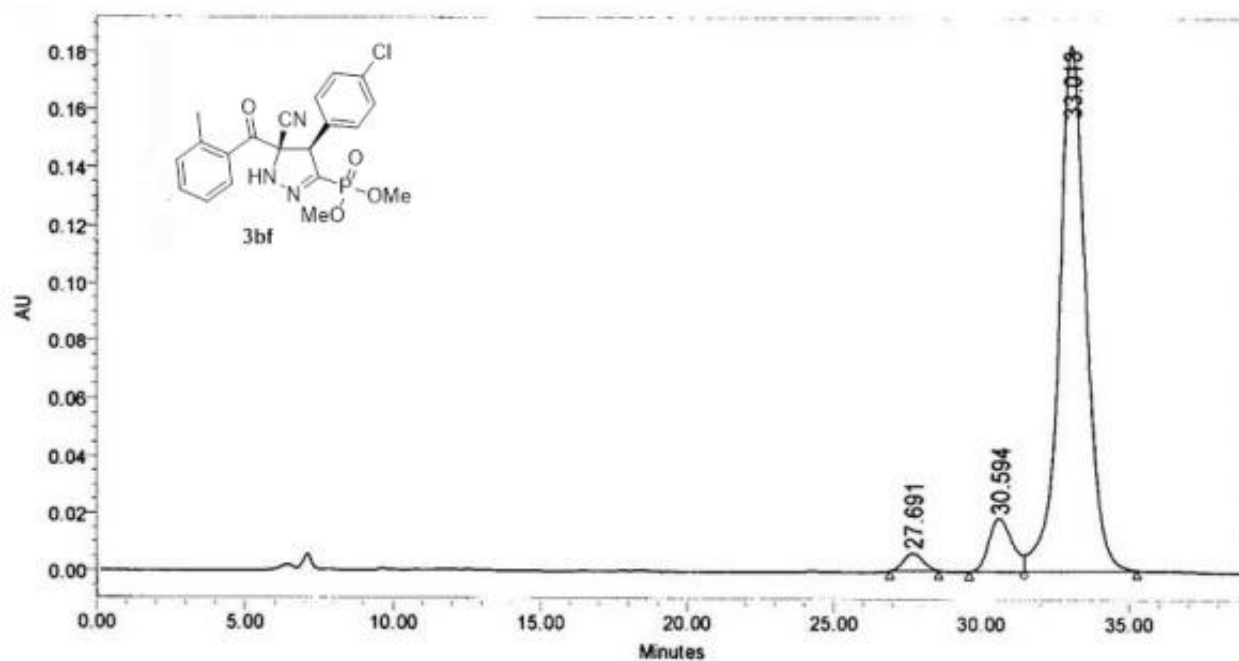
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	28.170	6507402	47.38	126506	50.44
2	30.501	6960375	50.67	120263	47.95
3	39.730	267618	1.95	4057	1.62



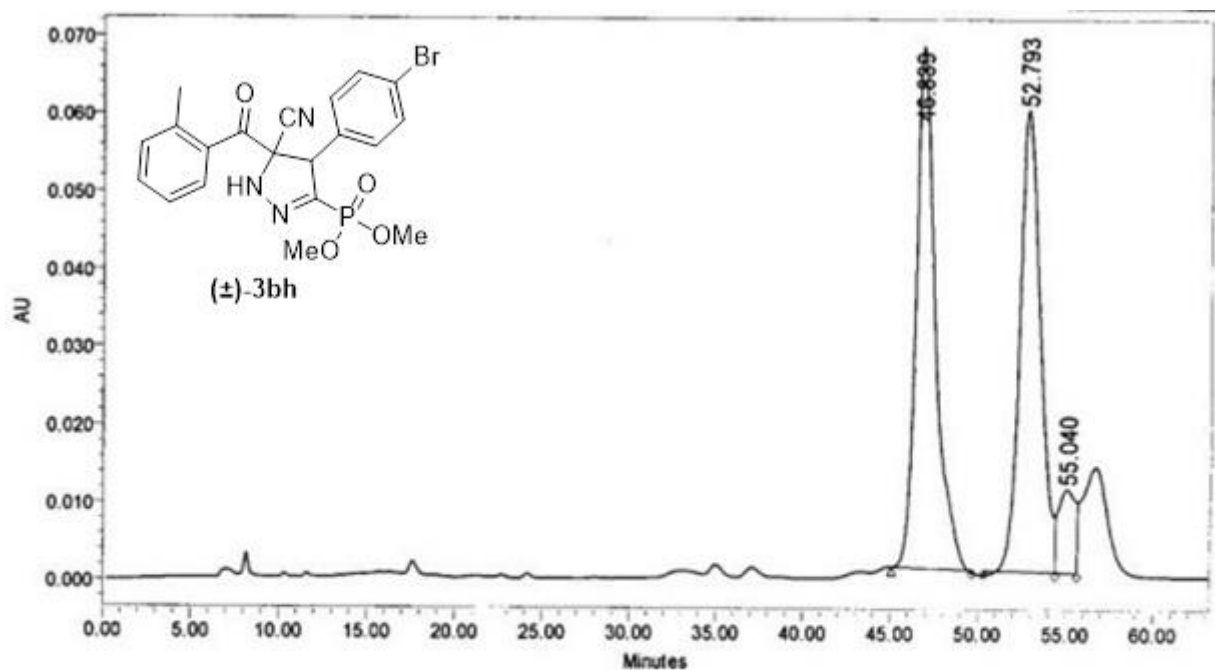
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	28.140	4958373	4.66	100360	5.93
2	30.205	100687627	94.71	1580888	93.48
3	39.606	667135	0.63	9886	0.58



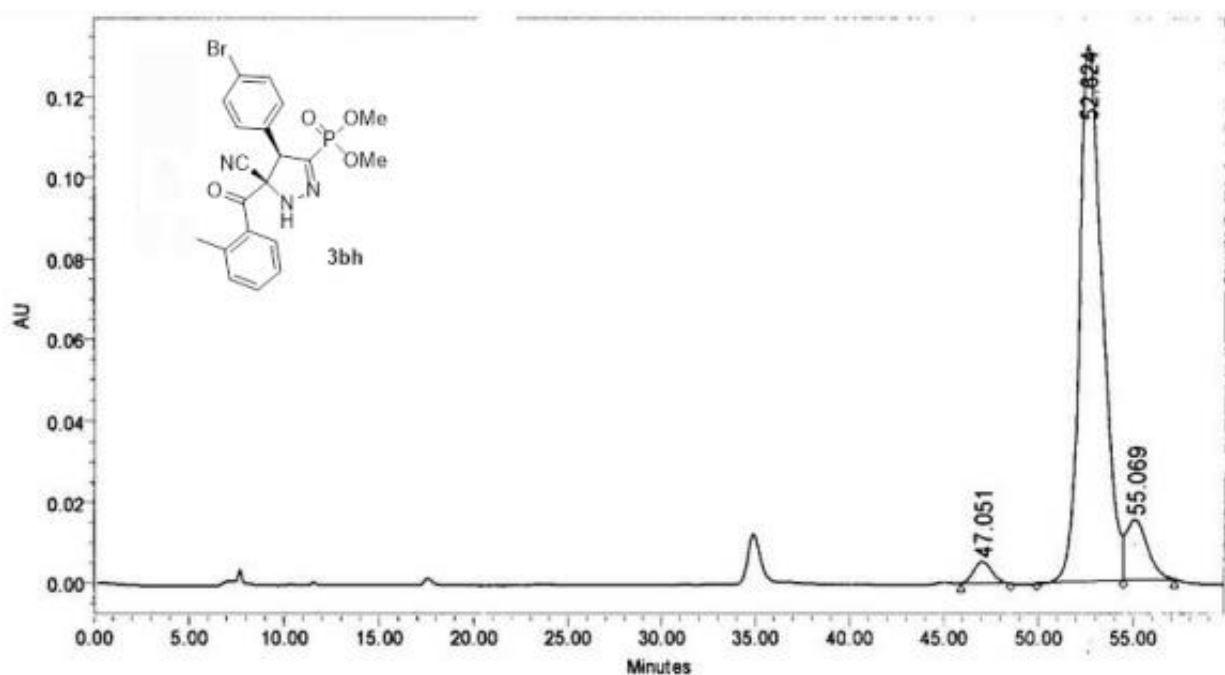
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	24.484	1093232	42.36	25532	47.19
2	27.783	184449	7.15	3703	6.84
3	29.711	1132519	43.88	21720	40.15
4	32.454	170477	6.61	3147	5.82



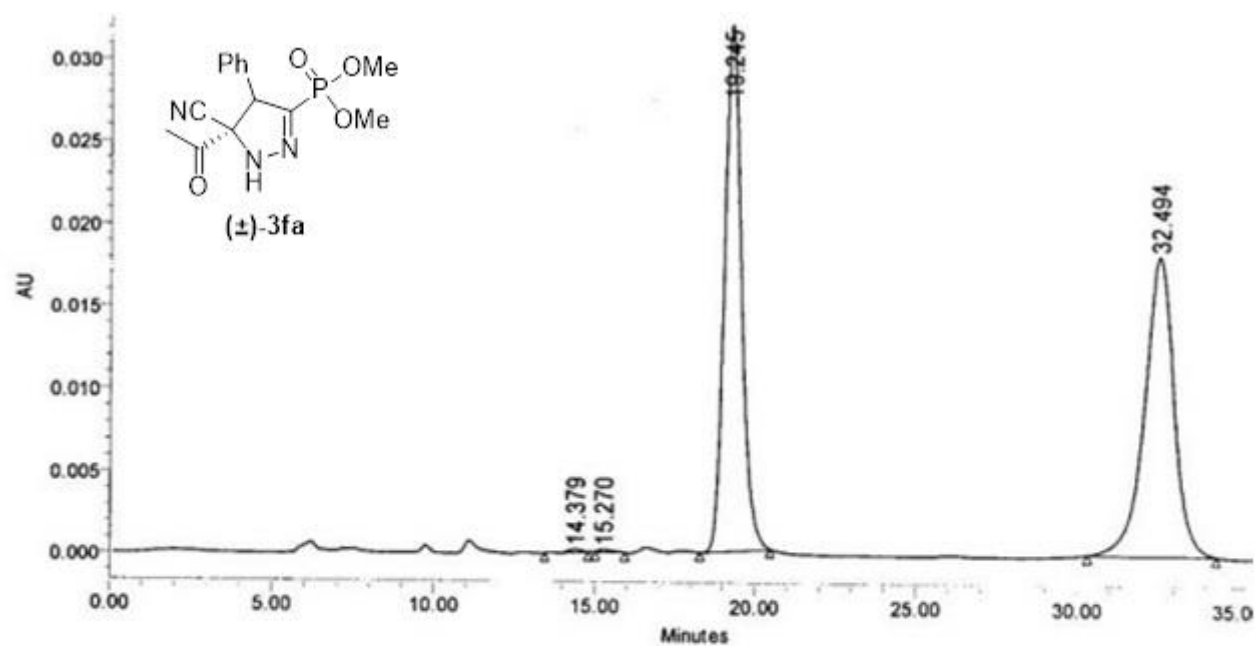
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	27.691	275524	2.19	6031	2.92
2	30.594	1004998	7.99	18486	8.95
3	33.013	11304088	89.82	182119	88.14



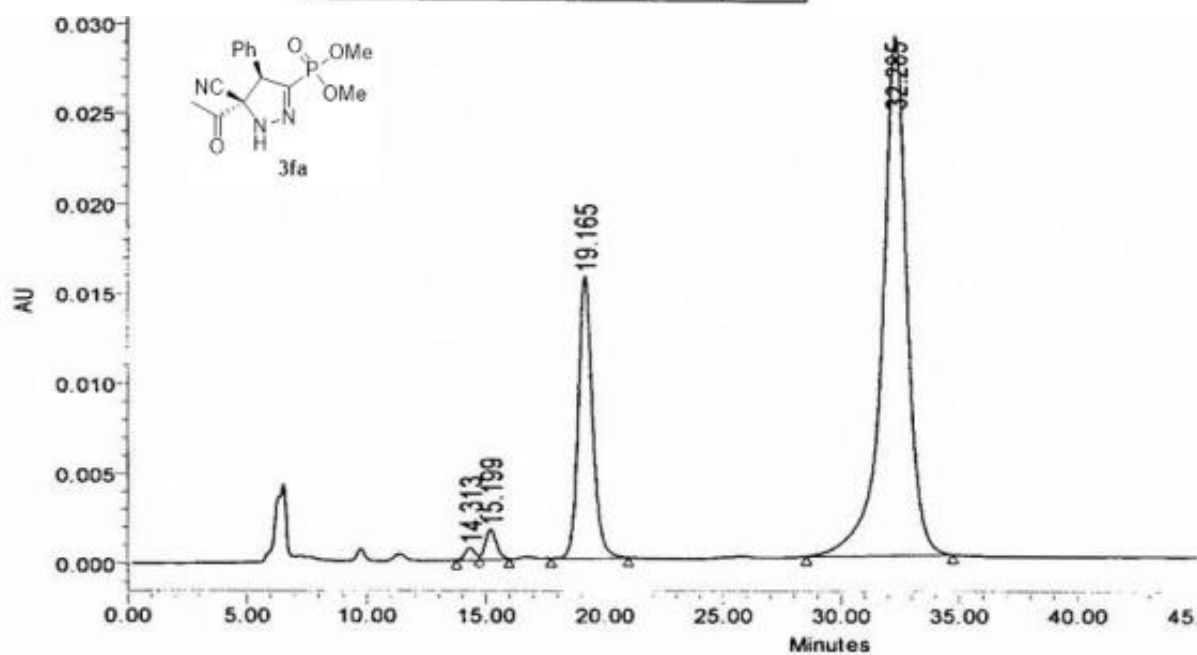
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	46.839	5125209	48.08	67012	48.91
2	52.793	4822082	45.24	59261	43.25
3	55.040	711394	6.67	10741	7.84



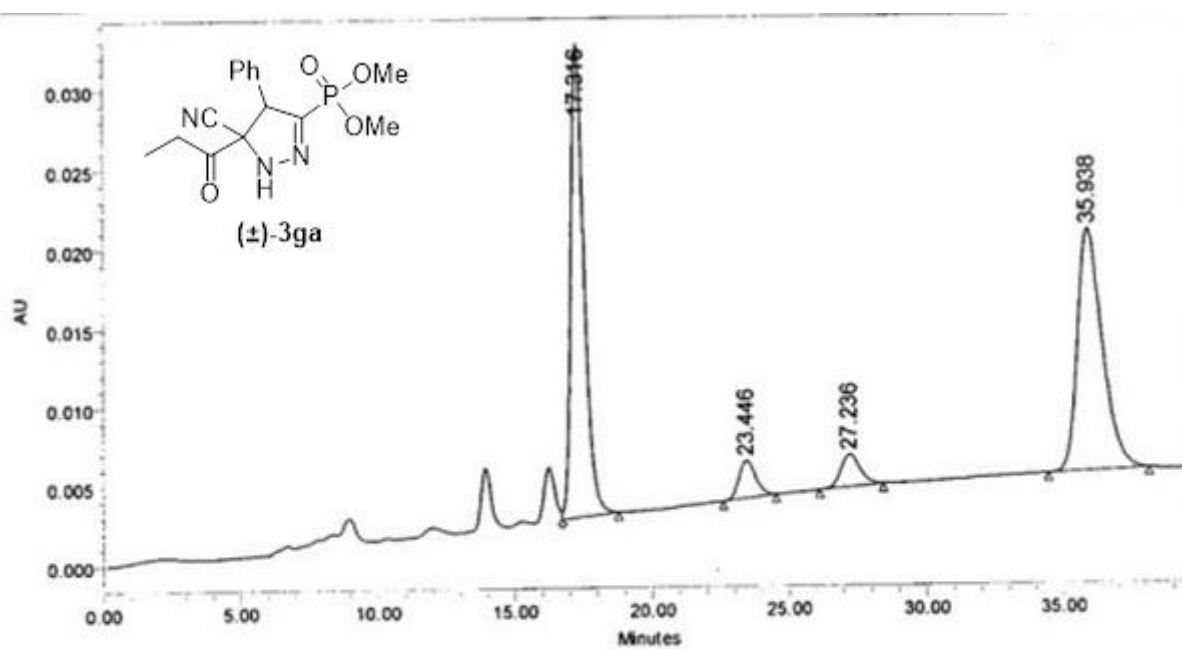
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	47.051	337459	2.69	5207	3.41
2	52.624	11032806	87.99	132371	86.73
3	55.069	1168724	9.32	15040	9.85



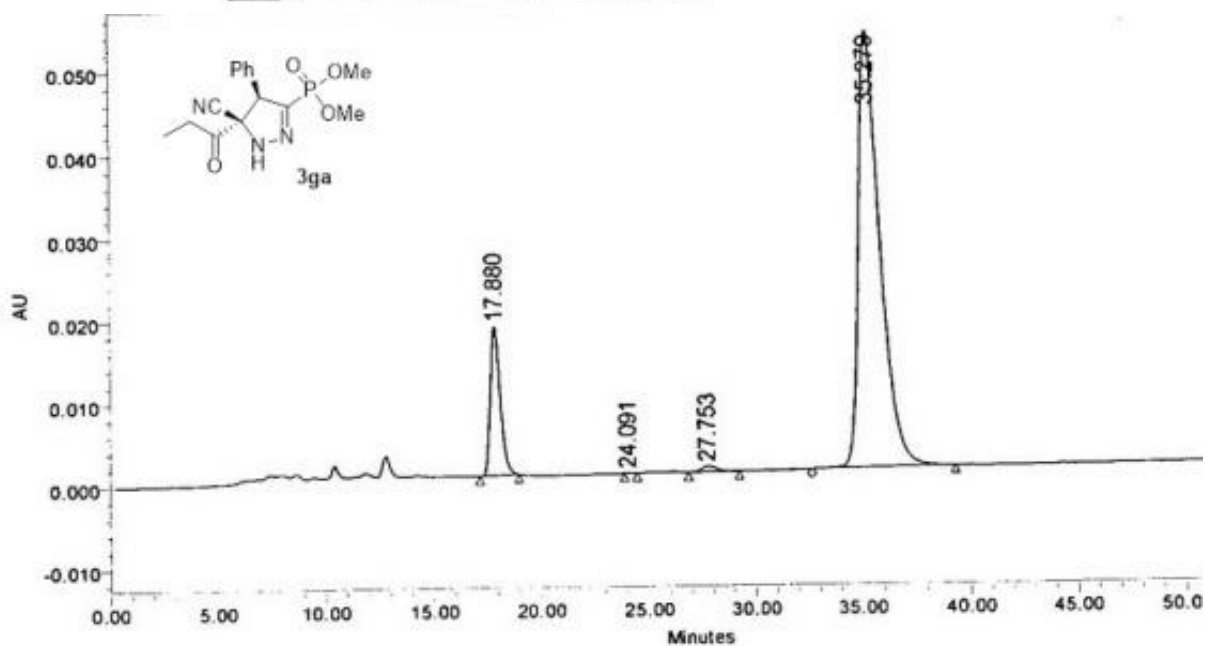
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	14.379	5482	0.23	205	0.41
2	15.270	4671	0.20	171	0.34
3	19.245	1177321	50.35	32000	63.24
4	32.494	1150777	49.22	18223	36.01



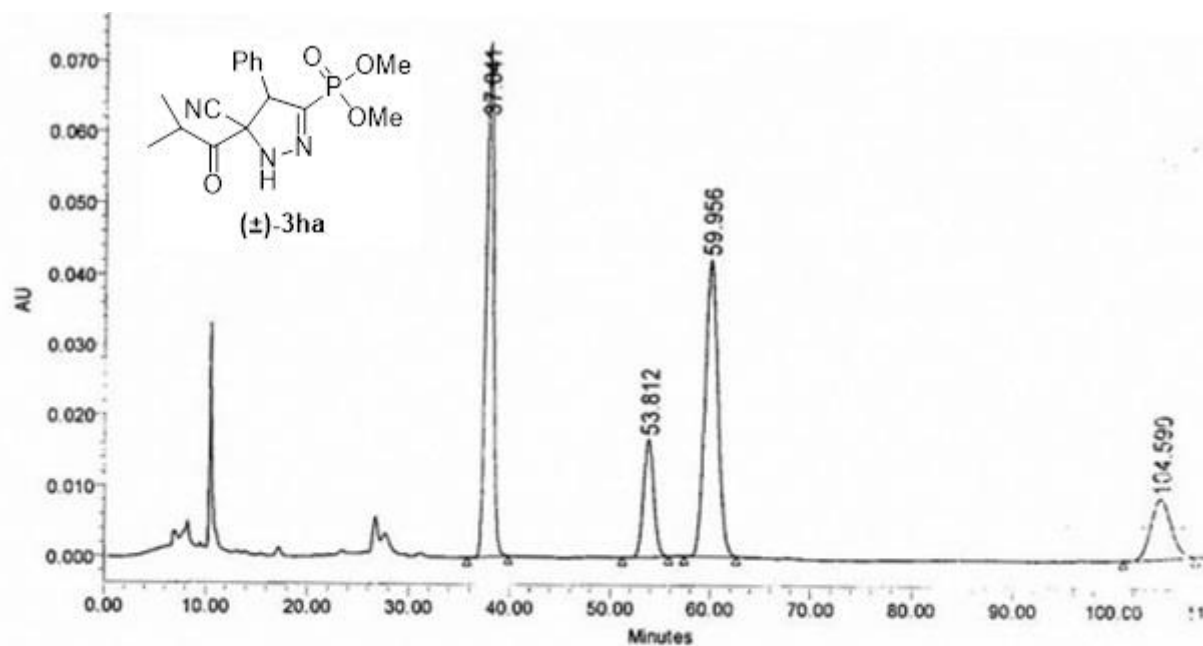
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	14.313	18951	0.67	643	1.38
2	15.199	52568	1.87	1648	3.52
3	19.165	643962	22.90	15658	33.49
4	32.285	2096481	74.56	28806	61.61



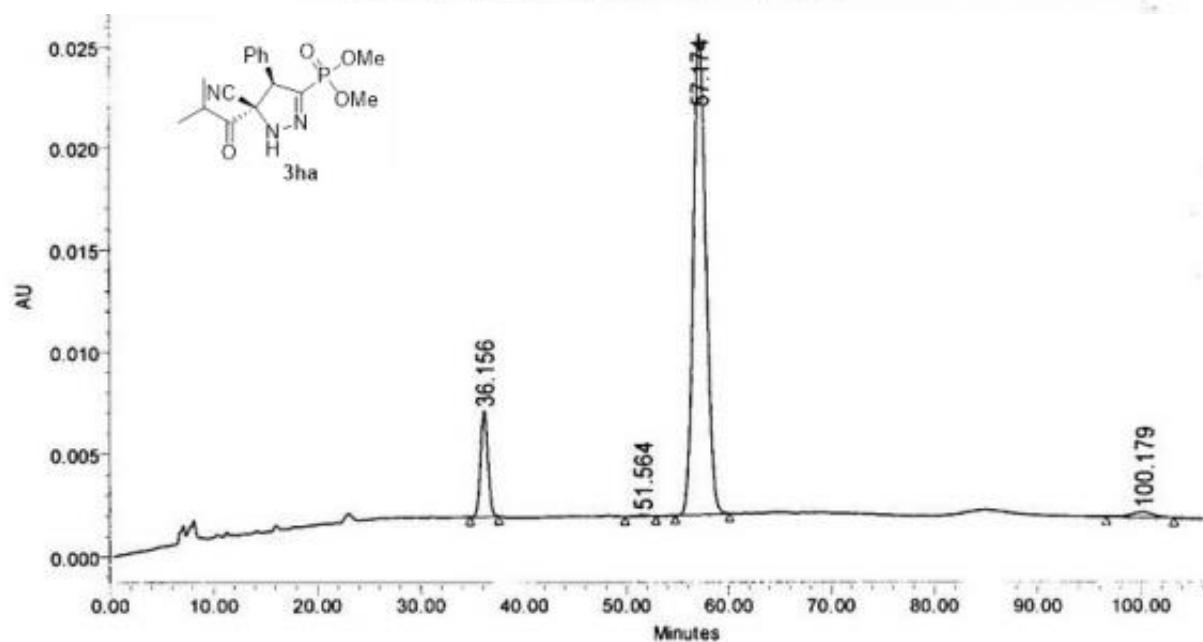
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.316	988469	45.98	29857	60.18
2	23.446	101201	4.71	2398	4.83
3	27.236	98109	4.56	2049	4.13
4	35.938	962029	44.75	15311	30.86



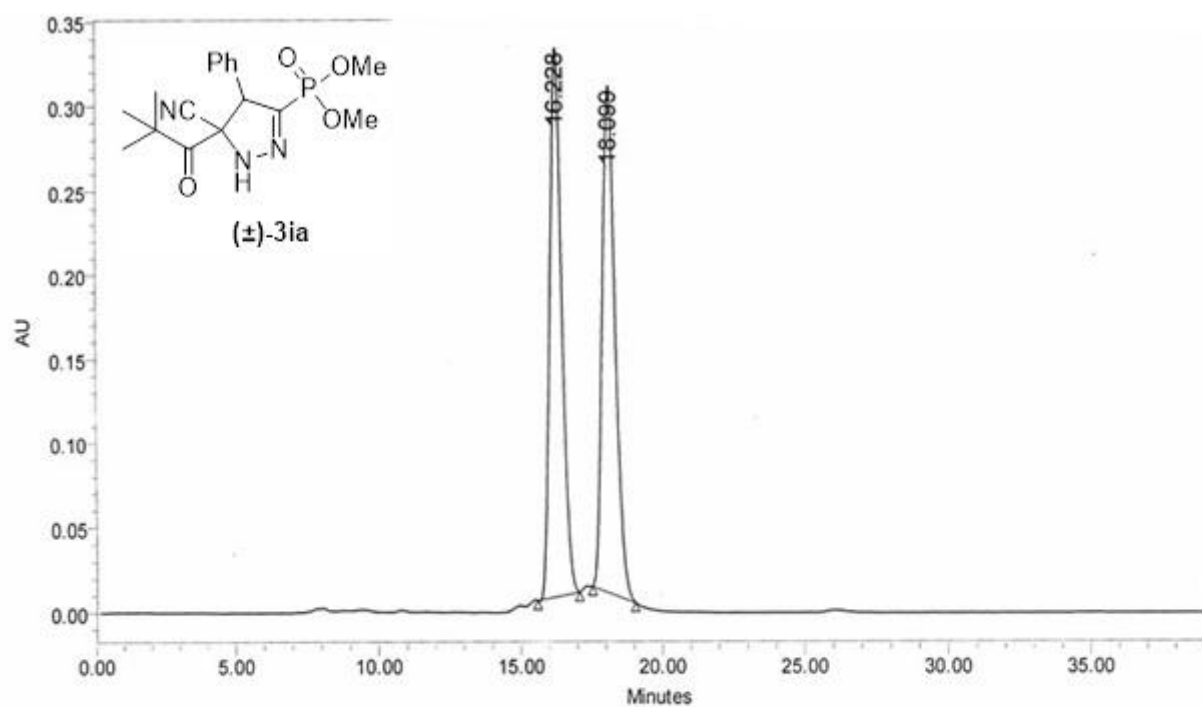
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.880	579393	13.49	18122	25.36
2	24.091	1431	0.03	68	0.10
3	27.753	34211	0.80	708	0.99
4	35.279	3679731	85.68	52574	73.56



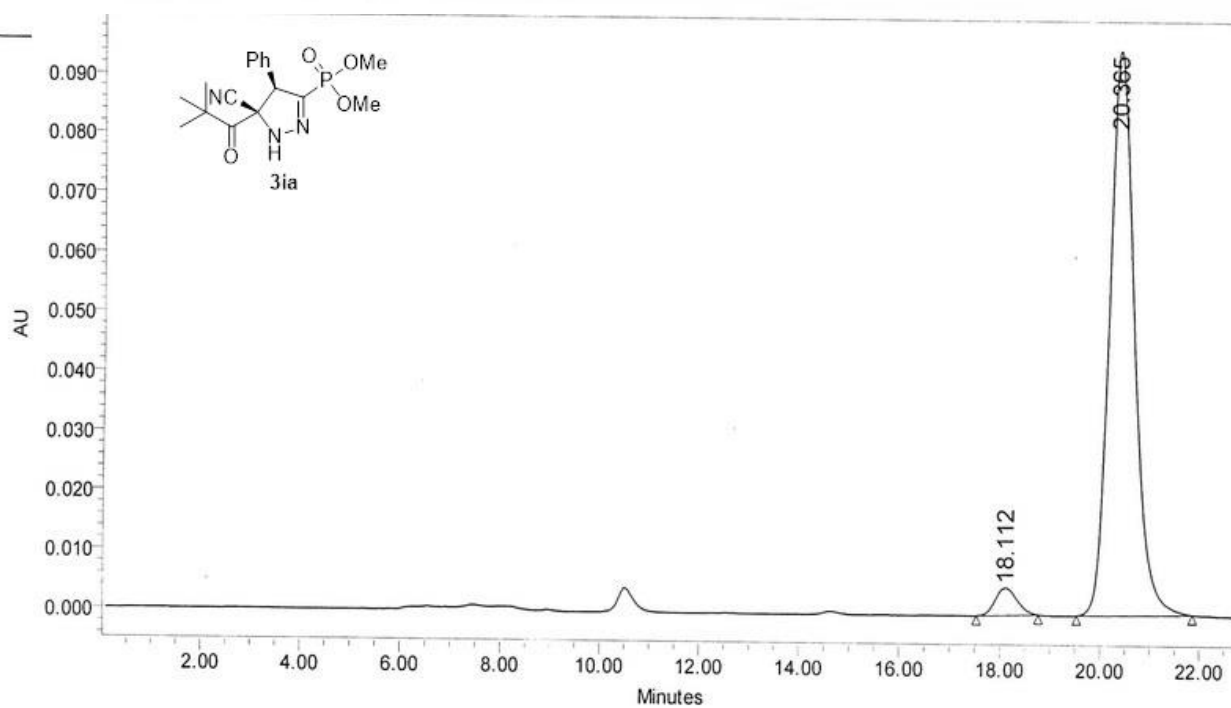
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	37.841	3755526	38.01	72681	51.98
2	53.812	1185113	11.99	16616	11.88
3	59.956	3761313	38.07	42066	30.08
4	104.590	1179258	11.93	8474	6.06



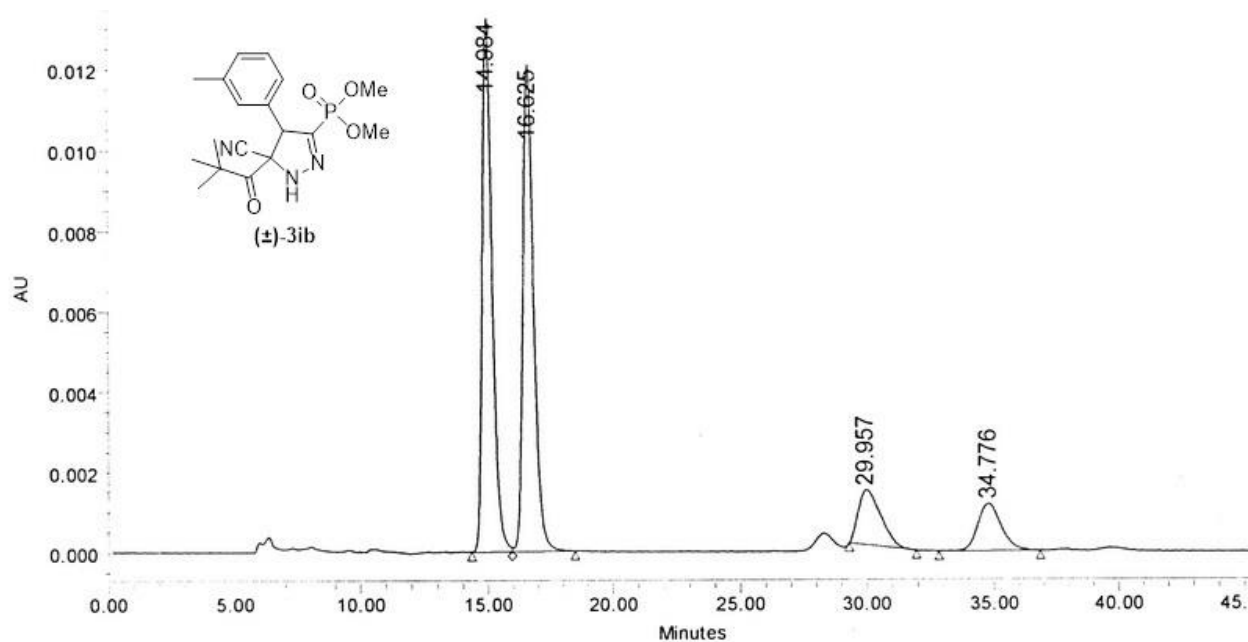
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	36.156	253567	11.05	5126	17.67
2	51.564	4188	0.18	81	0.28
3	57.174	2000174	87.20	23551	81.17
4	100.179	35899	1.57	255	0.88



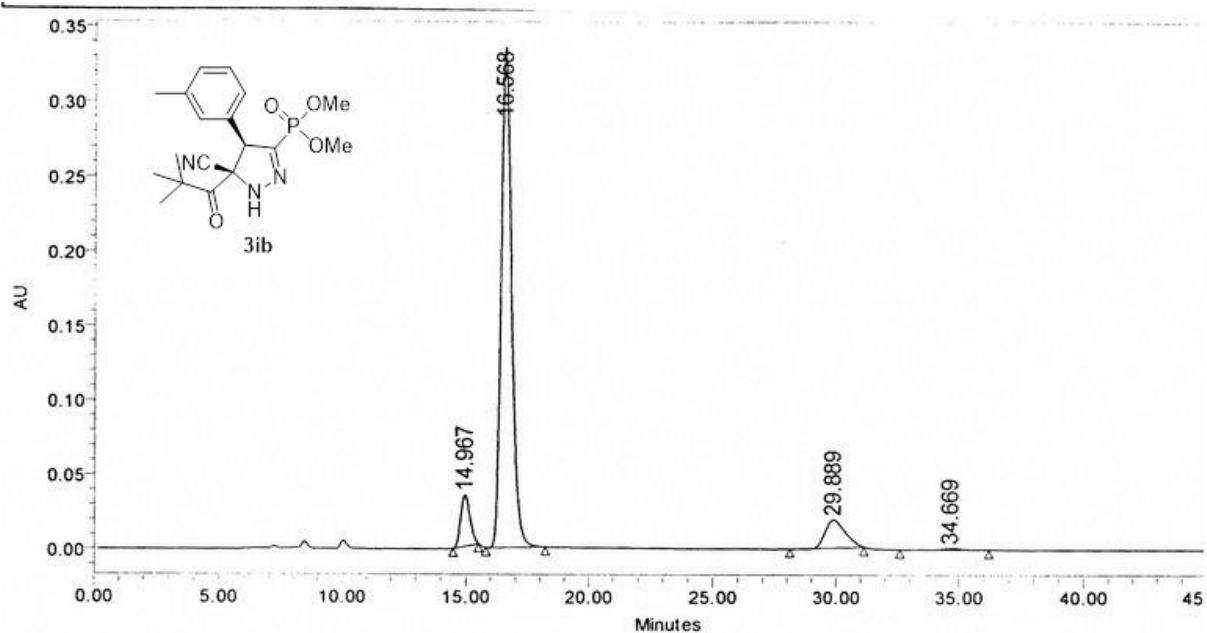
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	16.228	9452954	49.84	325262	52.02
2	18.099	9511756	50.16	299969	47.98



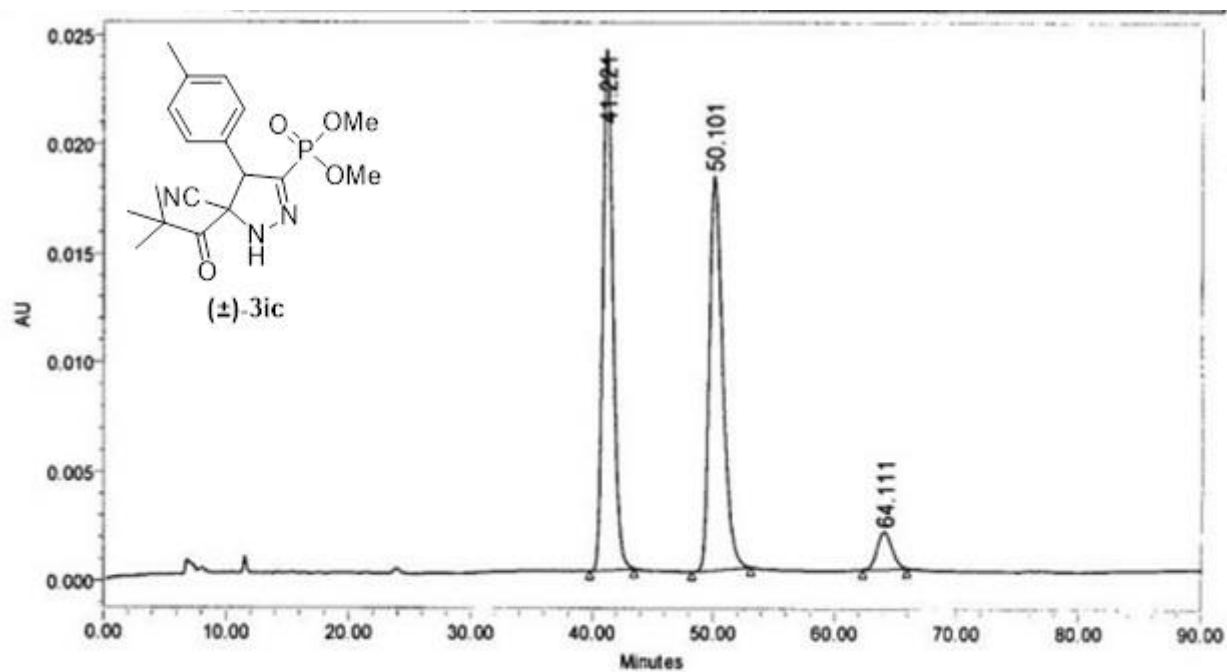
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	18.112	138901	4.05	4620	4.64
2	20.365	3292211	95.95	94938	95.36



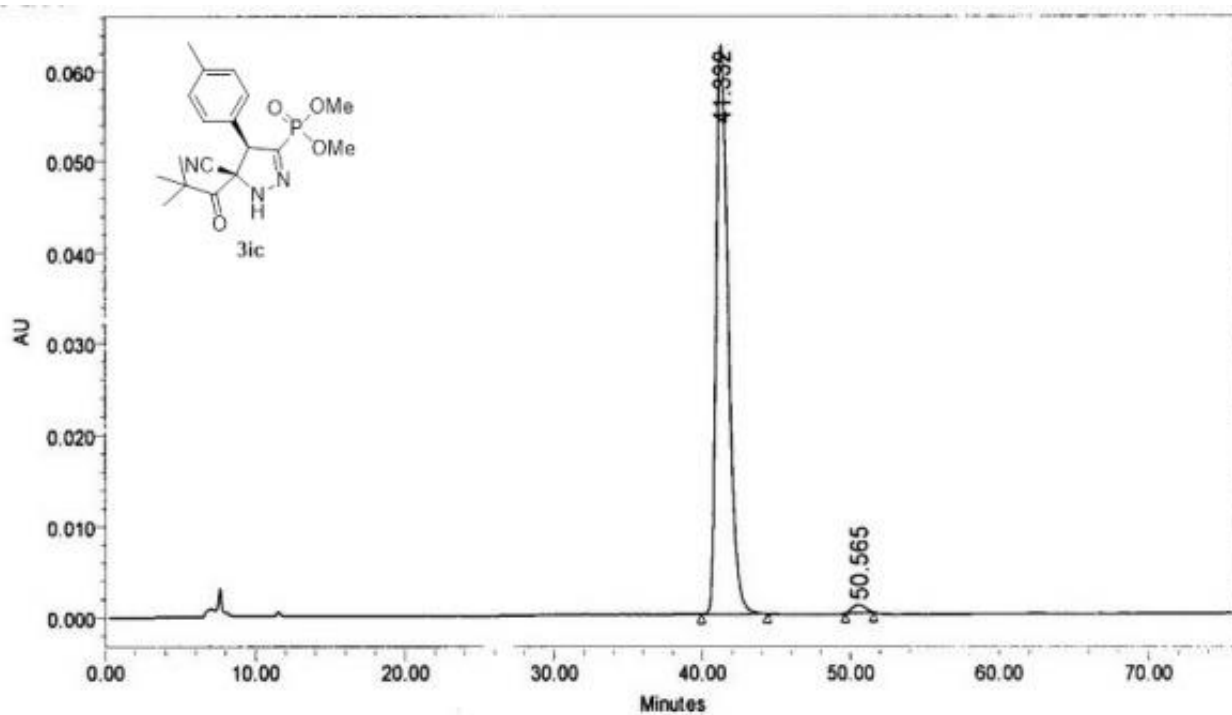
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	14.984	362407	41.18	13237	47.52
2	16.625	359394	40.83	12088	43.39
3	29.957	82929	9.42	1359	4.88
4	34.776	75404	8.57	1172	4.21



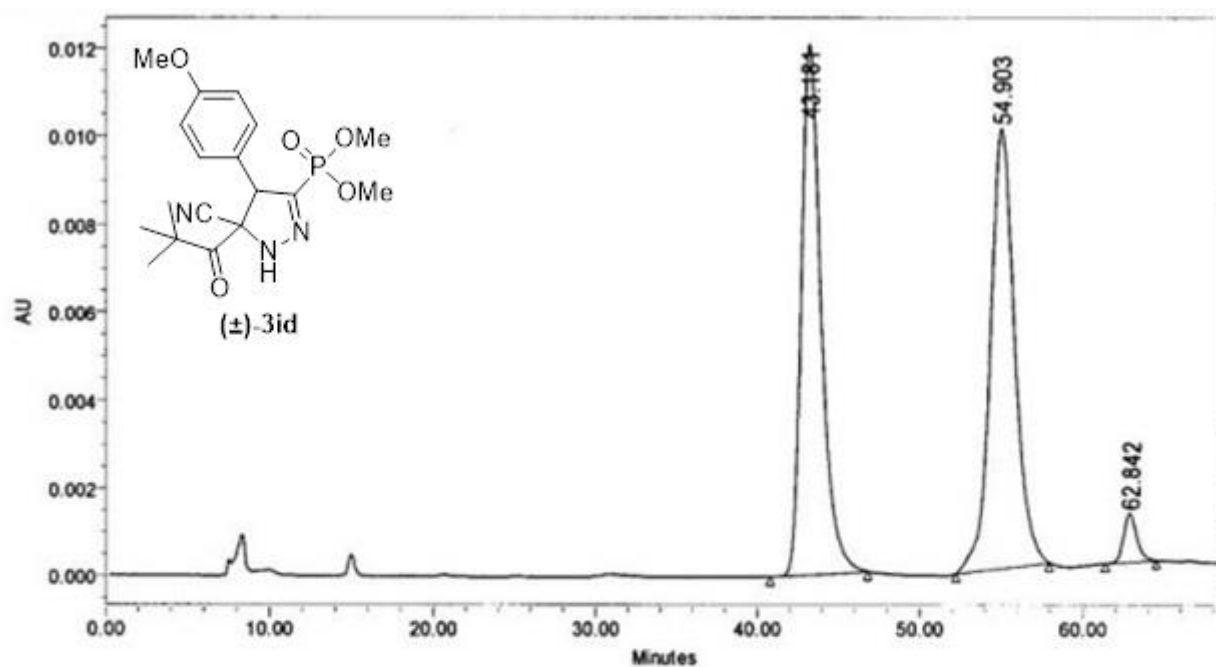
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	14.967	879079	7.40	34437	8.84
2	16.568	9850412	82.96	335323	86.09
3	29.889	1084142	9.13	18787	4.82
4	34.669	59921	0.50	953	0.24



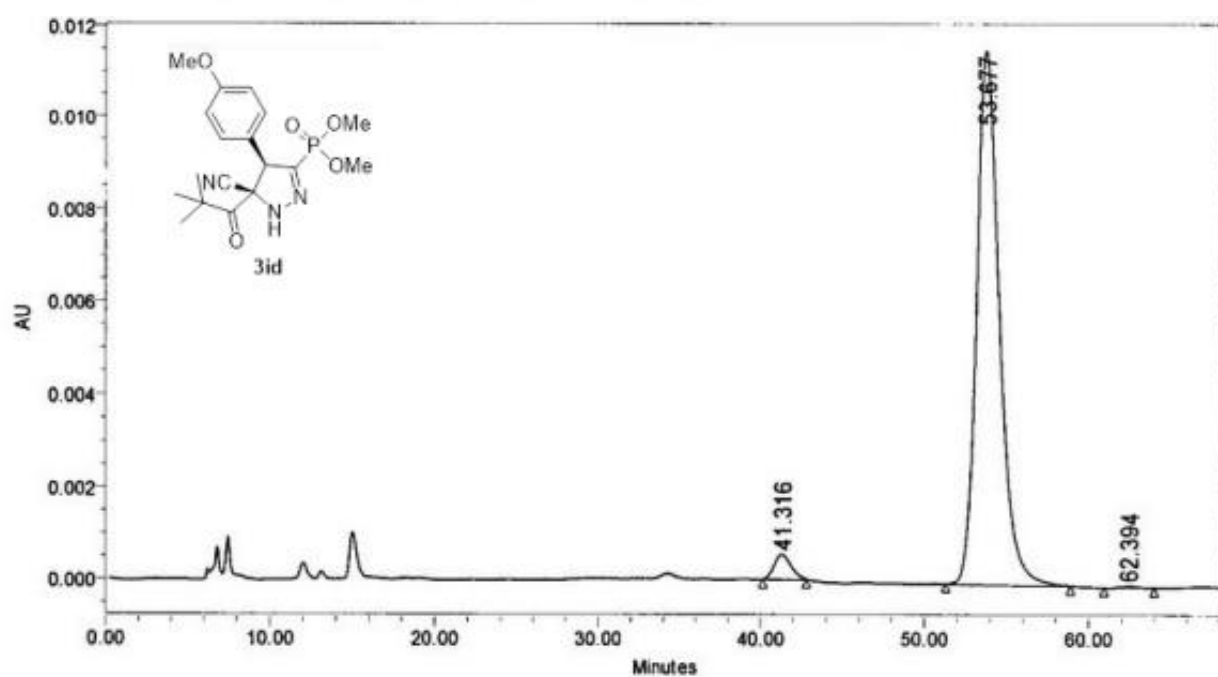
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	41.221	1384136	47.59	23864	54.71
2	50.101	1379773	47.44	18043	41.36
3	64.111	144380	4.96	1715	3.93



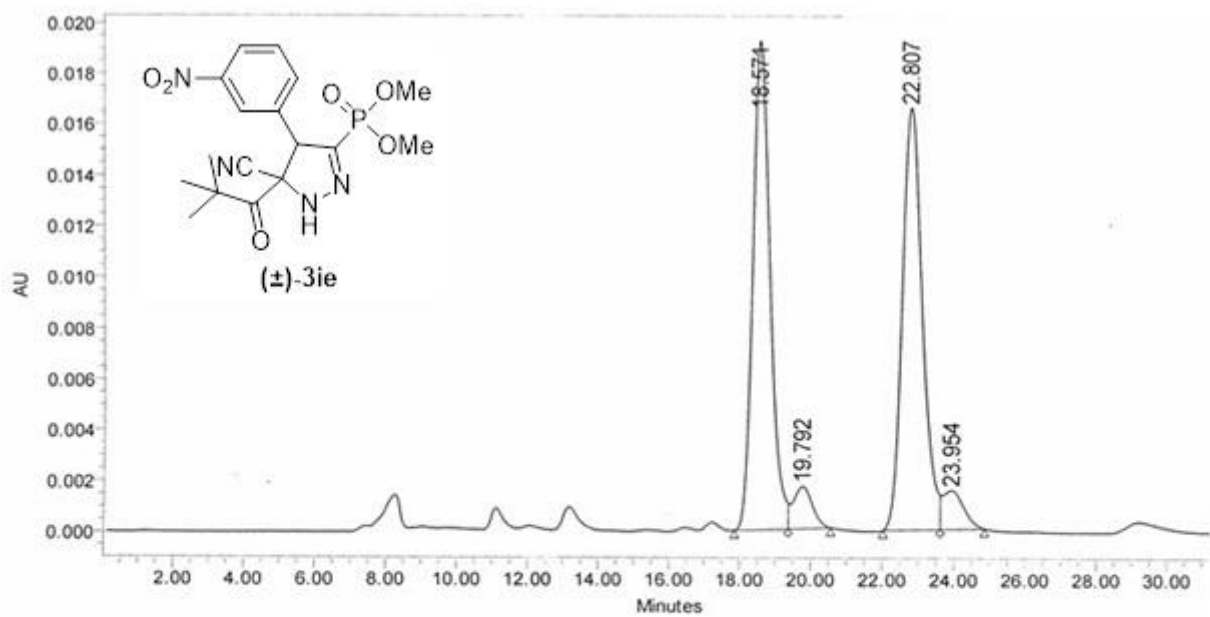
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	41.332	3549997	98.55	62553	98.63
2	50.565	52242	1.45	866	1.37



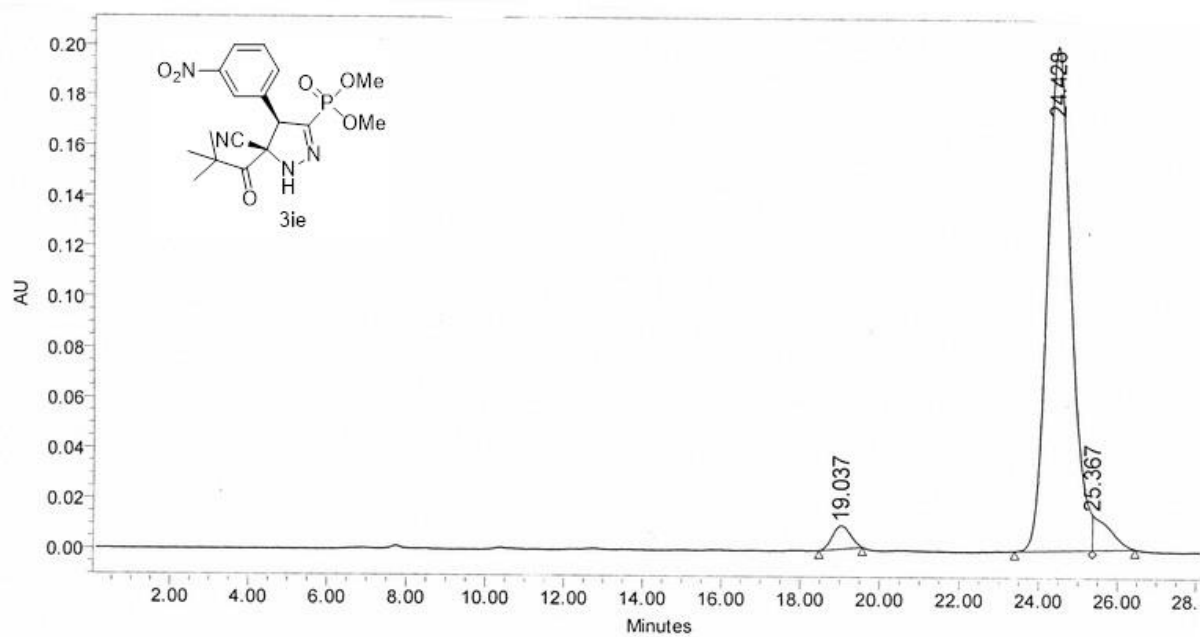
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	43.181	1018297	48.33	12065	52.08
2	54.903	1027503	48.76	9996	43.15
3	62.842	61317	2.91	1104	4.77



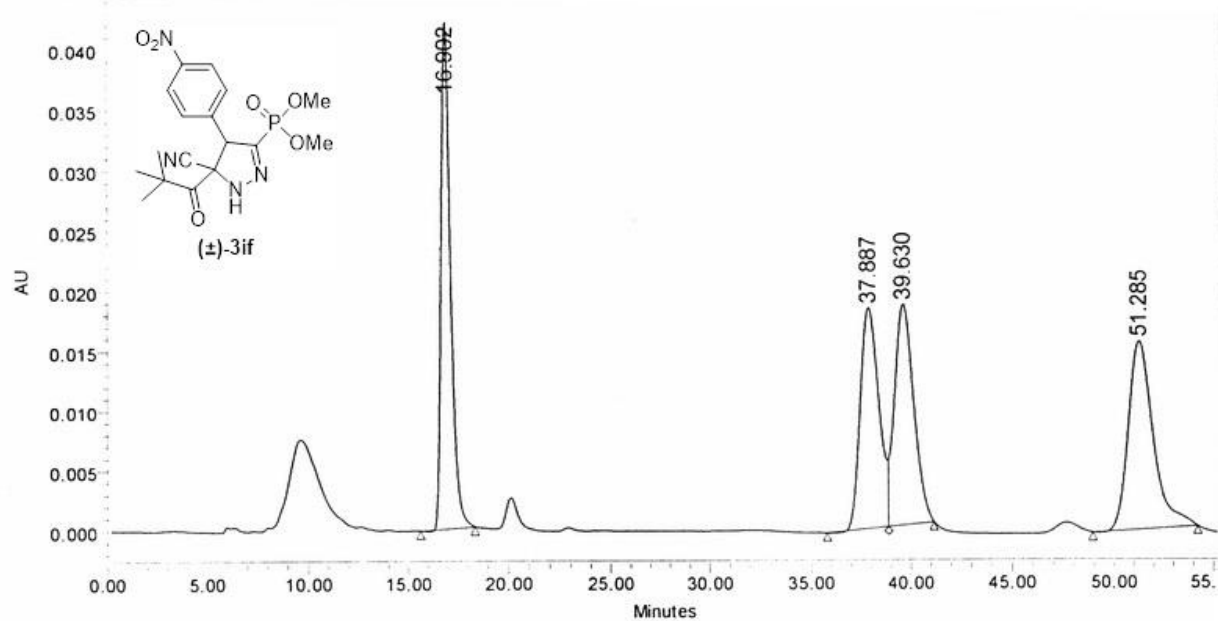
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	41.316	39017	3.39	545	4.48
2	53.677	1110661	96.38	11577	95.15
3	62.394	2716	0.24	45	0.37



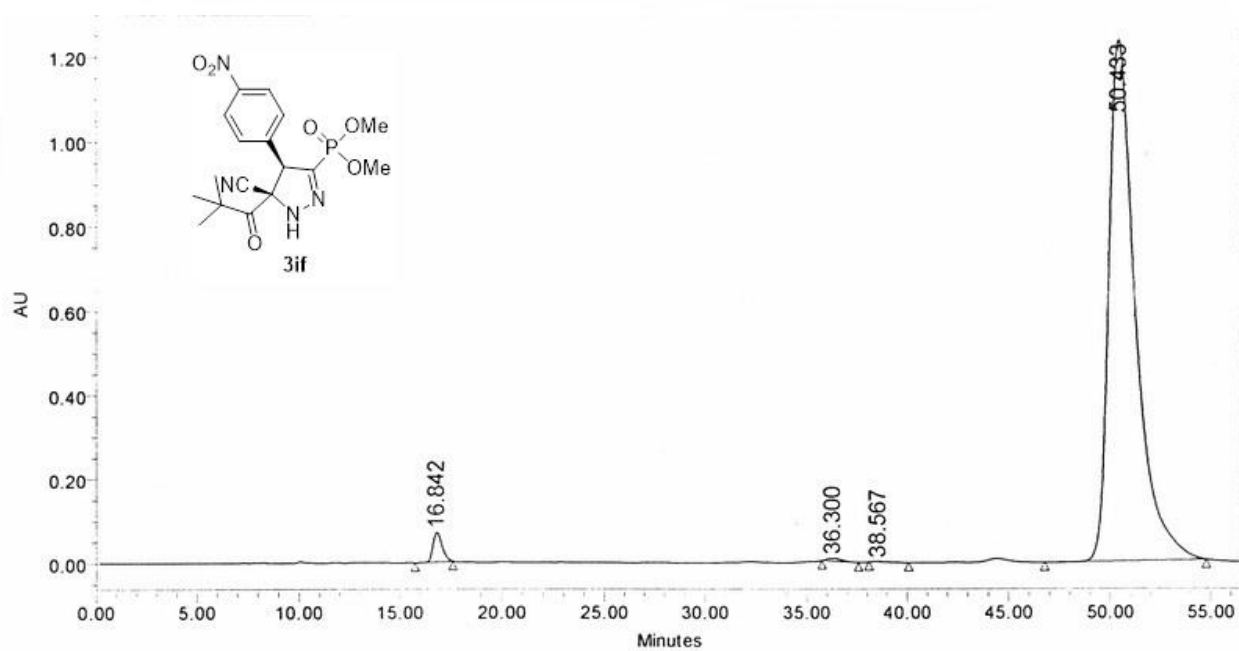
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	18.571	647326	45.67	19214	49.36
2	19.792	62407	4.40	1646	4.23
3	22.807	645115	45.51	16555	42.53
4	23.954	62558	4.41	1513	3.89



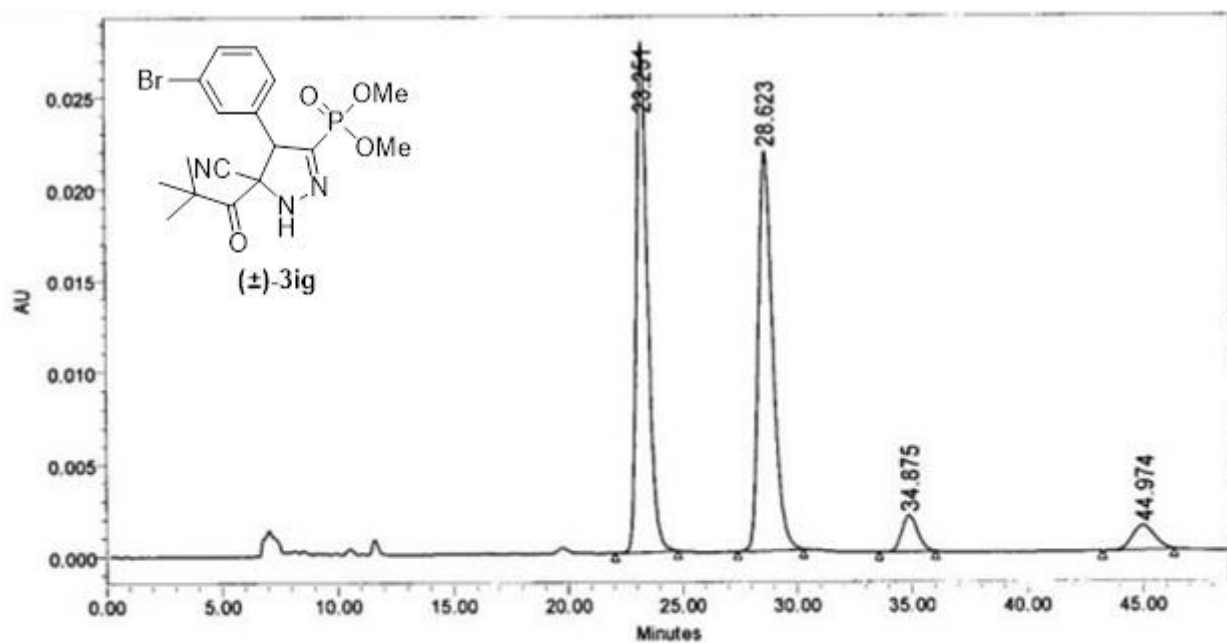
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	19.037	284900	3.12	9176	4.10
2	24.428	8433078	92.31	200682	89.66
3	25.367	417399	4.57	13970	6.24



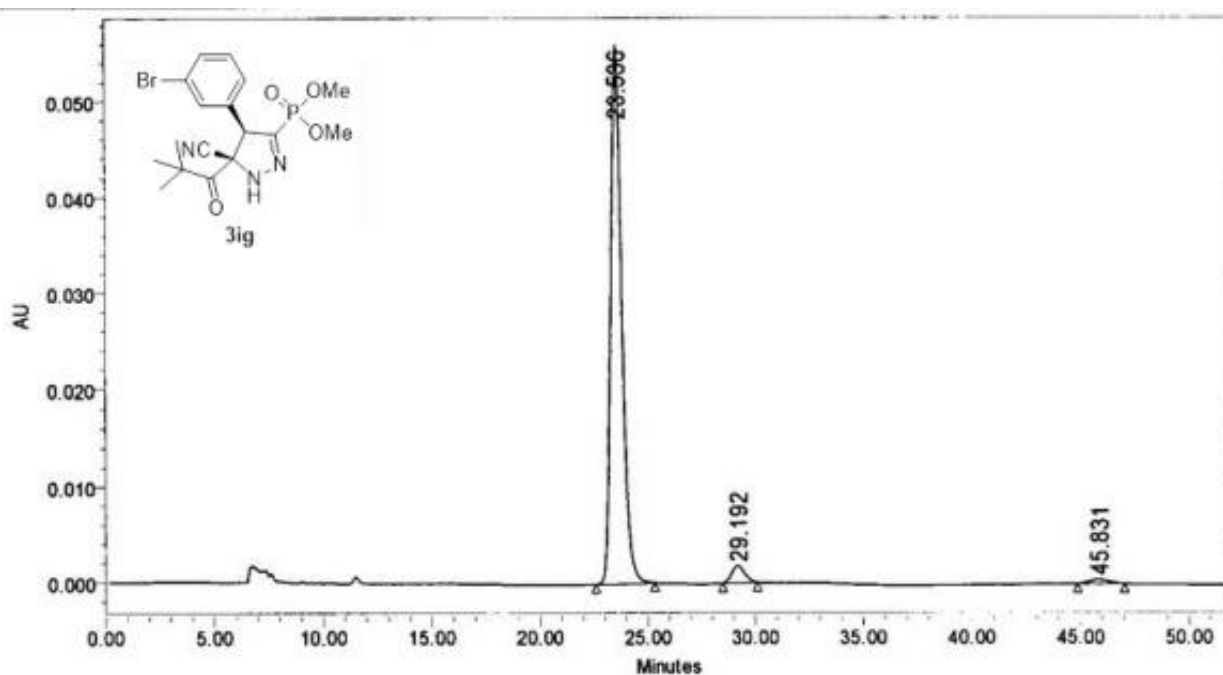
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	16.902	1395483	26.76	42156	44.48
2	37.887	1208119	23.16	18445	19.46
3	39.630	1242960	23.83	18444	19.46
4	51.285	1369020	26.25	15723	16.59



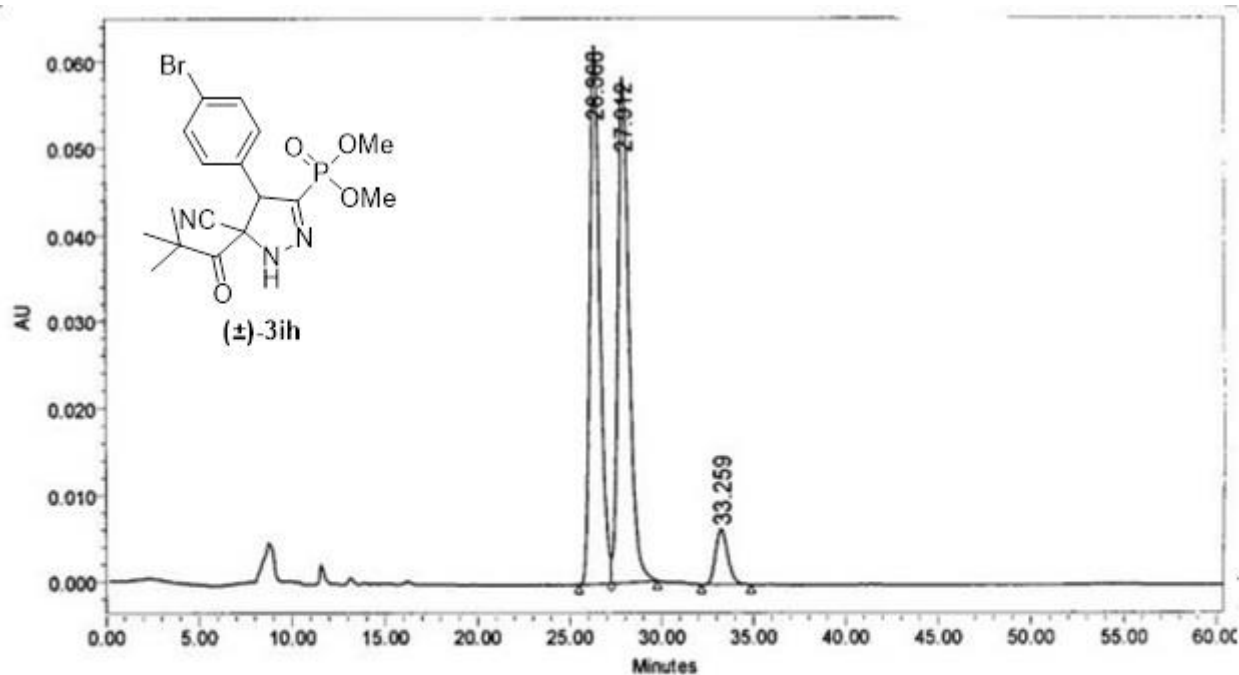
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	16.842	2208931	1.90	70686	5.38
2	36.300	325928	0.28	6743	0.51
3	38.567	72120	0.06	1569	0.12
4	50.433	113919147	97.76	1234436	93.99



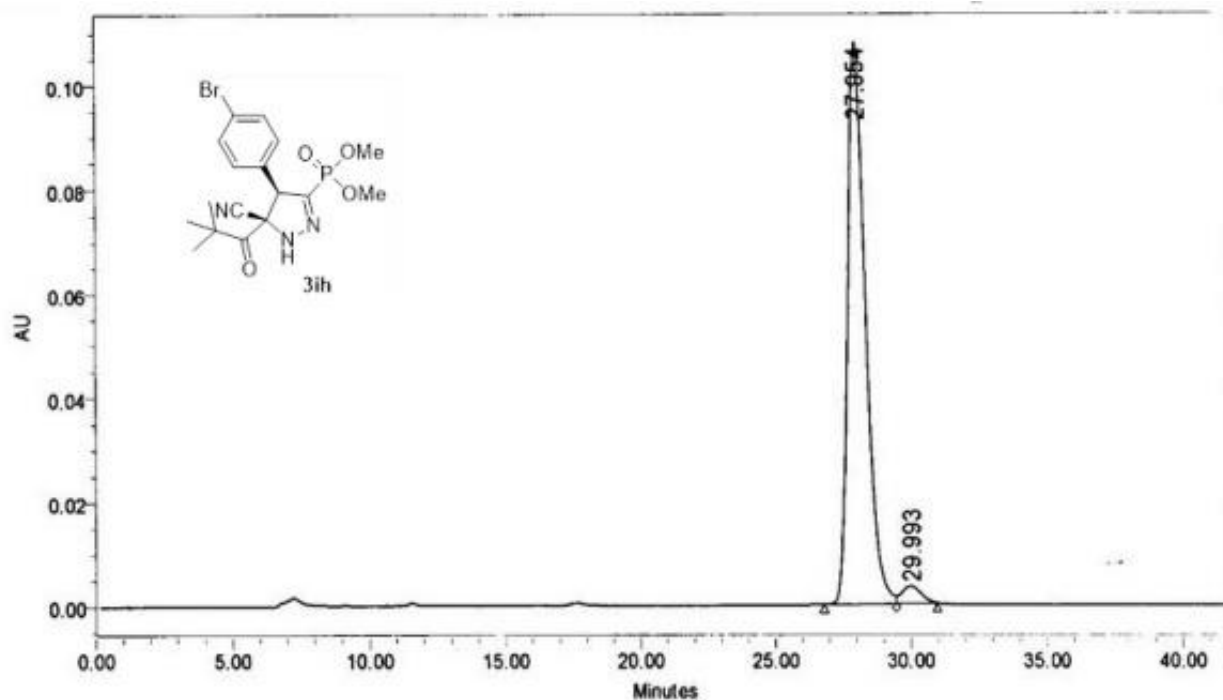
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	23.251	949332	45.77	27759	52.65
2	28.623	944165	45.52	21696	41.15
3	34.875	93257	4.50	1953	3.70
4	44.974	87578	4.22	1313	2.49



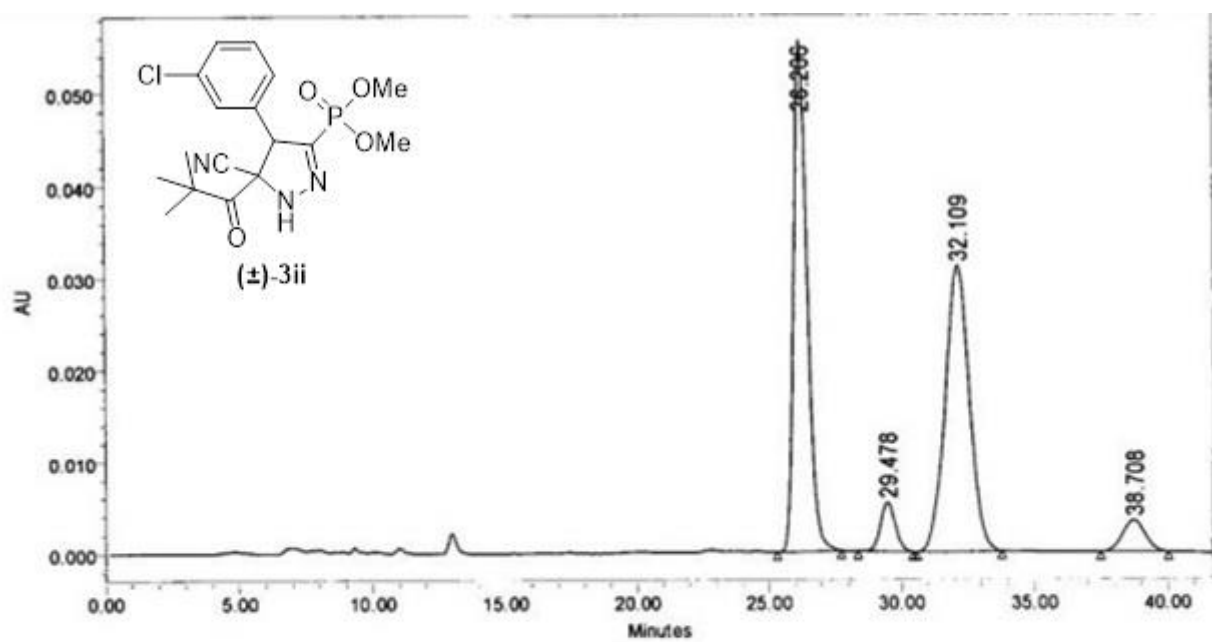
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	23.536	1994184	95.07	56117	96.20
2	29.192	74478	3.55	1765	3.03
3	45.831	29042	1.38	453	0.78



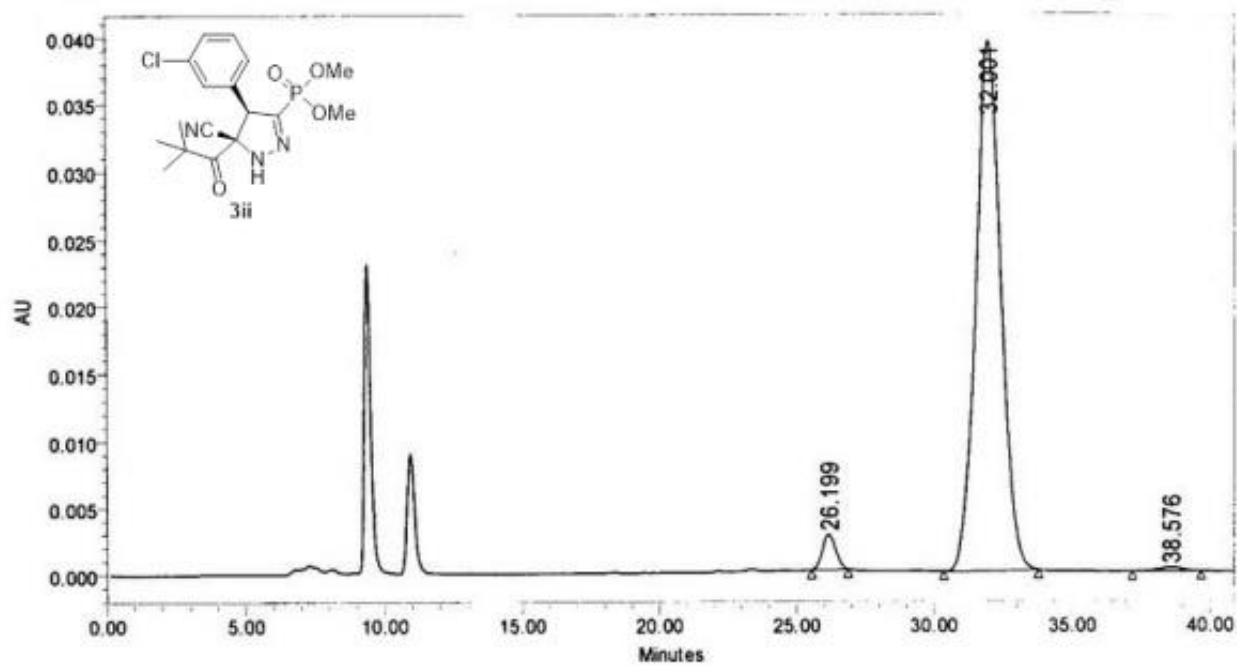
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	26.368	2373053	46.26	62173	48.98
2	27.912	2460954	47.97	58329	45.96
3	33.259	296097	5.77	6424	5.06



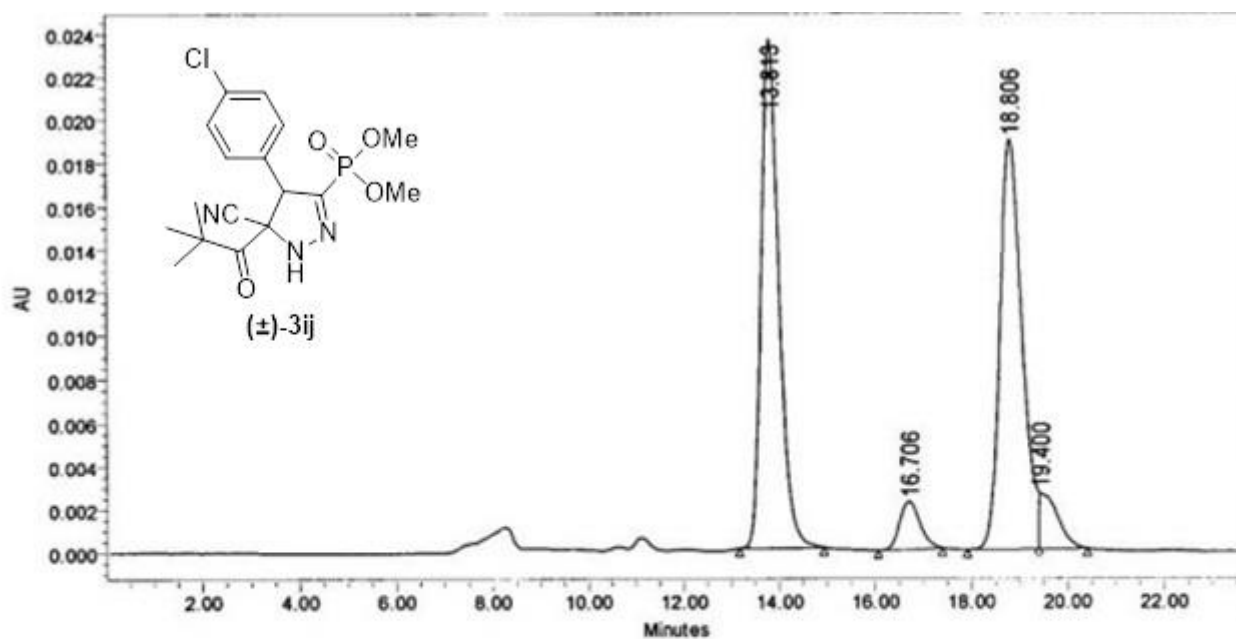
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	27.954	4864963	96.85	107763	97.05
2	29.993	158398	3.15	3277	2.95



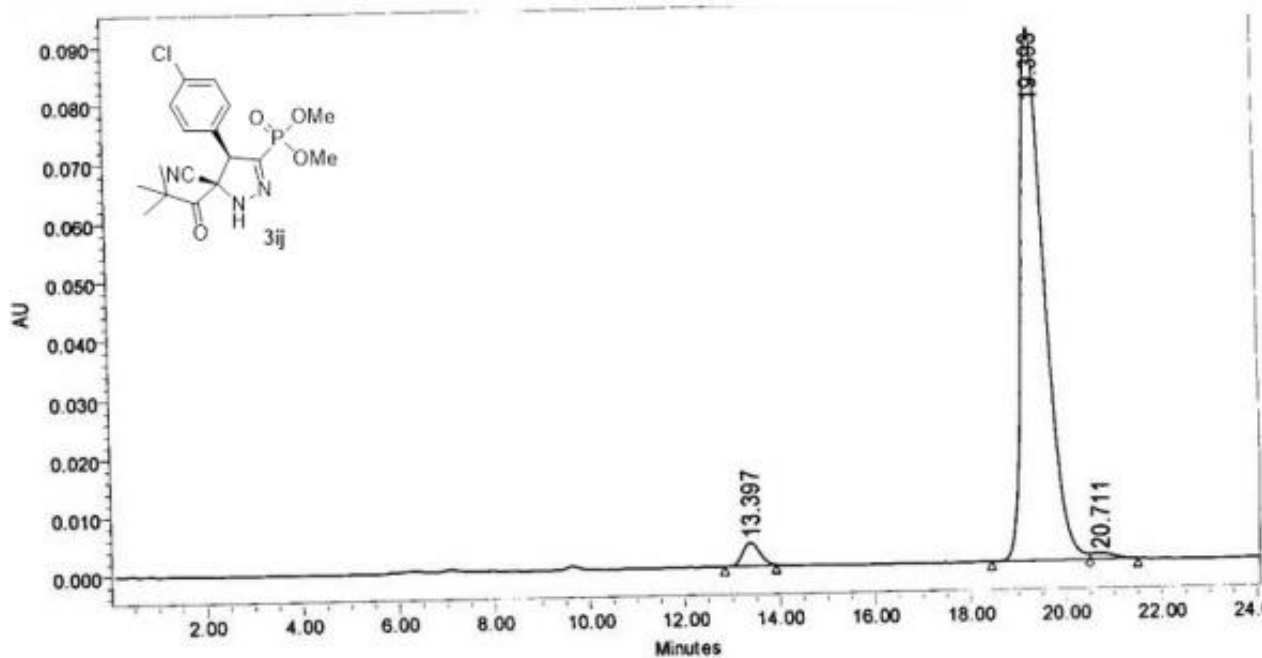
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	26.206	1957901	45.40	55428	58.17
2	29.478	203828	4.73	5324	5.59
3	32.109	1950485	45.23	31129	32.67
4	38.708	200281	4.64	3410	3.58



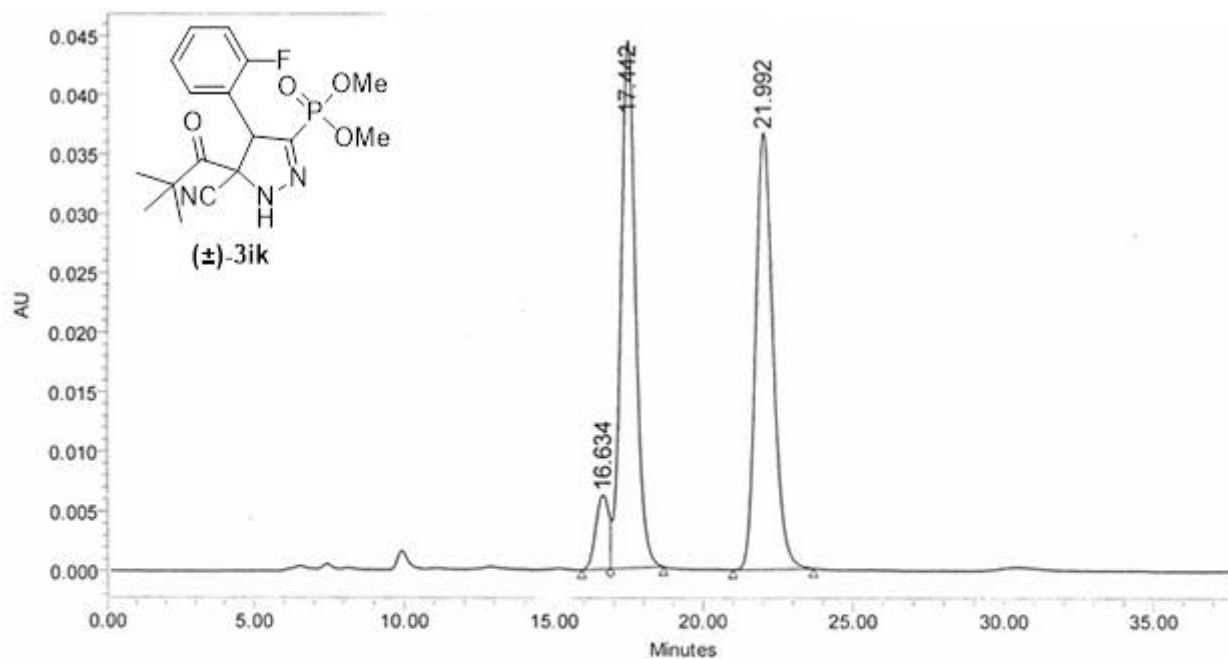
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	26.199	86891	3.38	2604	6.16
2	32.001	2466115	95.98	39405	93.22
3	38.576	16455	0.64	264	0.62



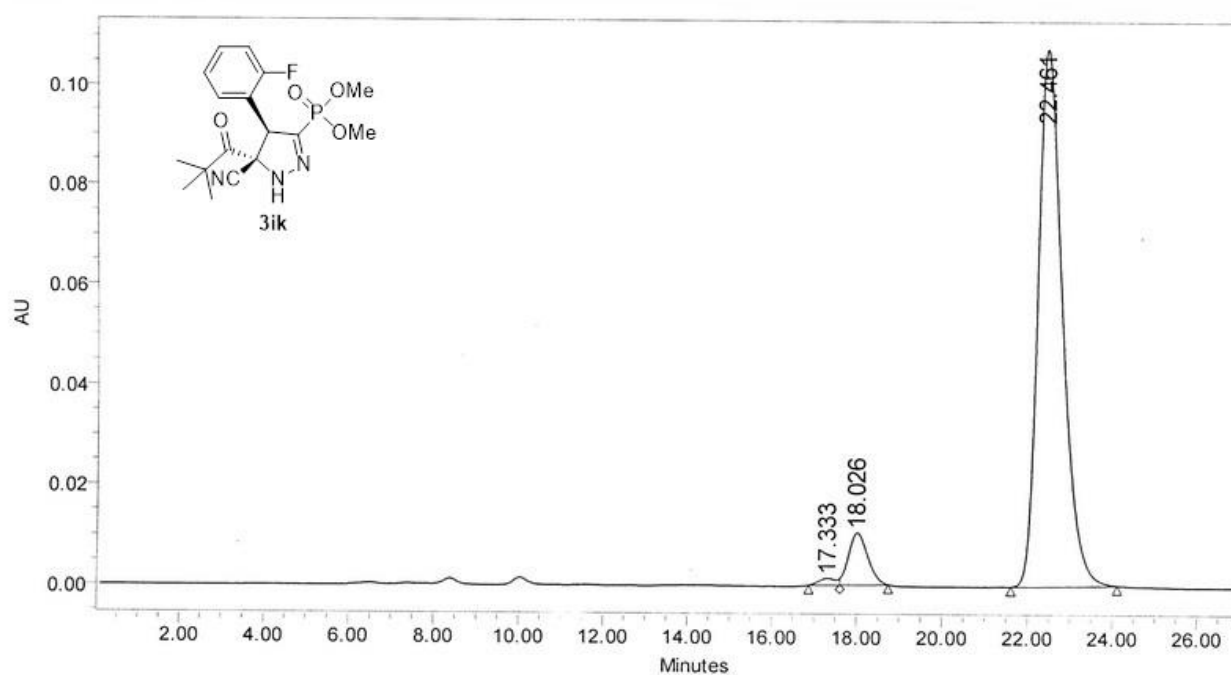
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	13.813	601772	45.16	23525	49.81
2	16.706	63428	4.76	2207	4.67
3	18.806	599793	45.01	18903	40.03
4	19.400	67499	5.07	2592	5.49



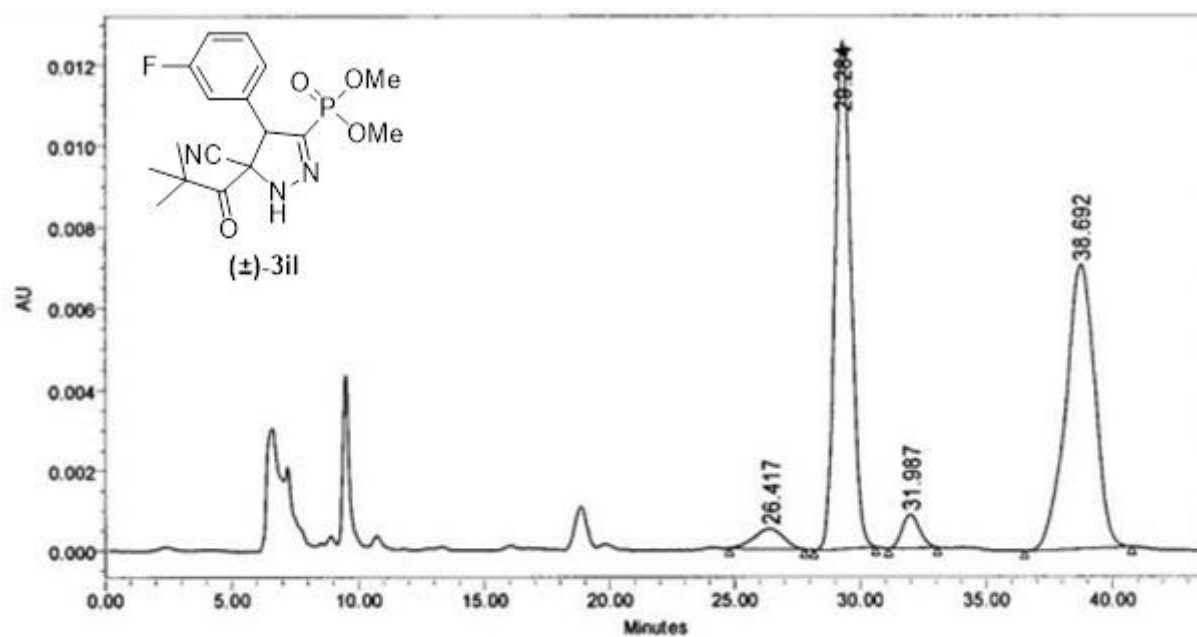
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	13.397	97372	3.05	3948	4.12
2	19.393	3064633	95.87	90728	94.79
3	20.711	34765	1.09	1037	1.08



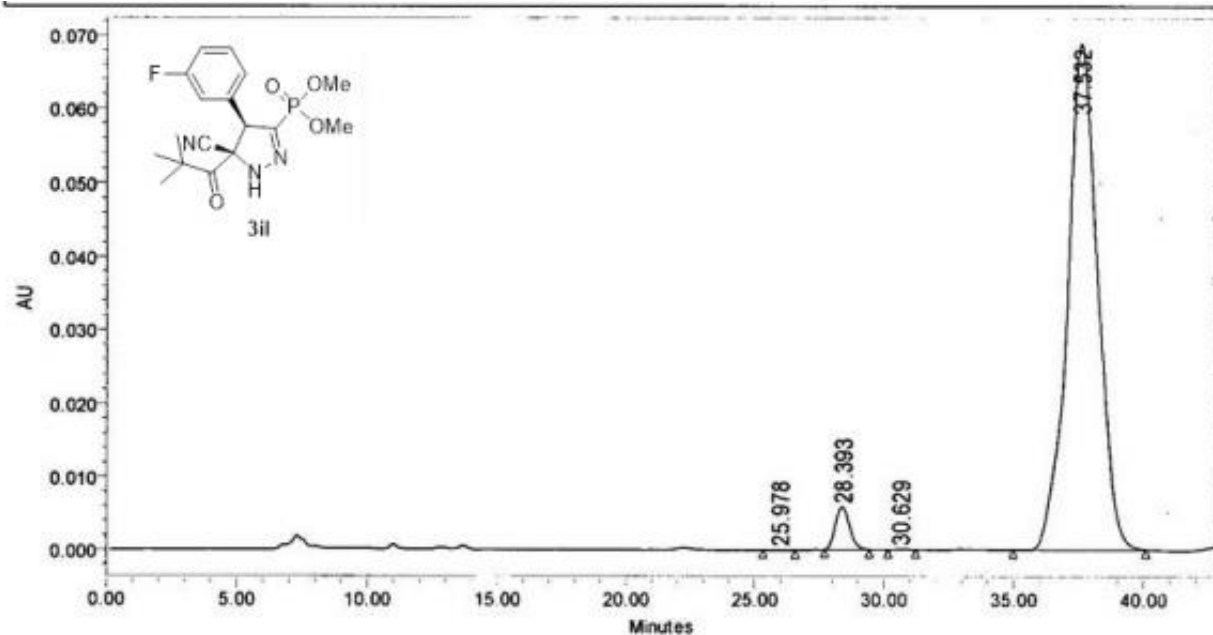
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	16.634	181563	5.72	6179	7.08
2	17.442	1517157	47.76	44368	50.87
3	21.992	1477691	46.52	36667	42.04



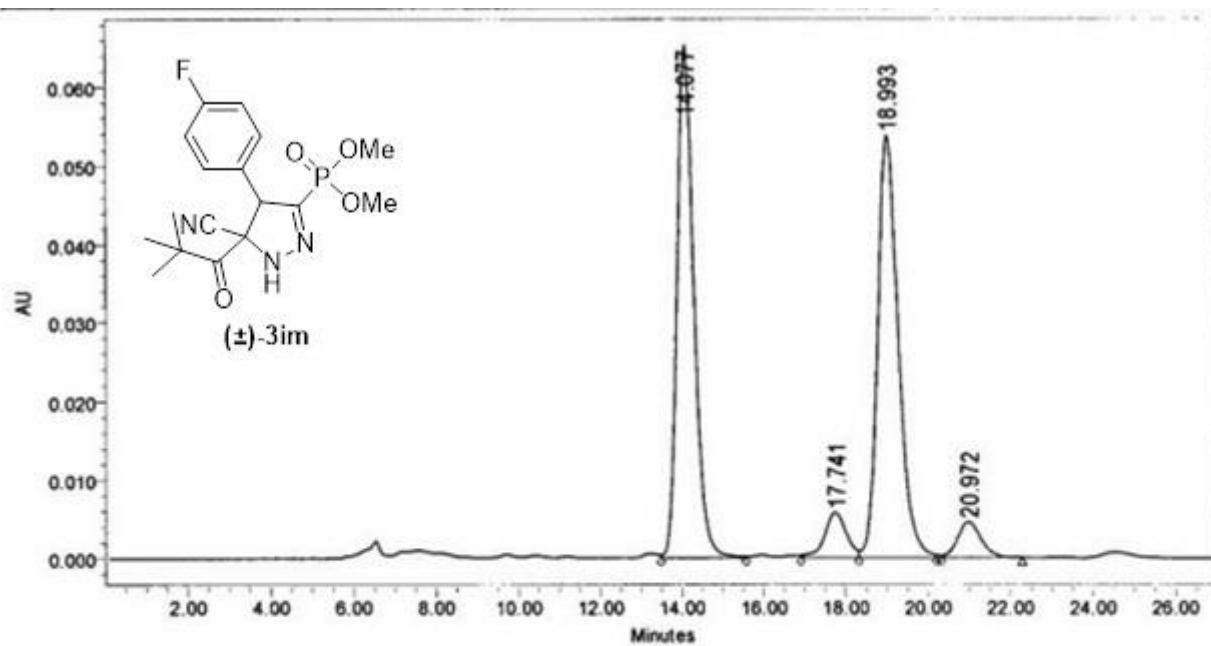
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.333	38993	0.84	1349	1.13
2	18.026	321911	6.95	10320	8.65
3	22.461	4269299	92.21	107609	90.22



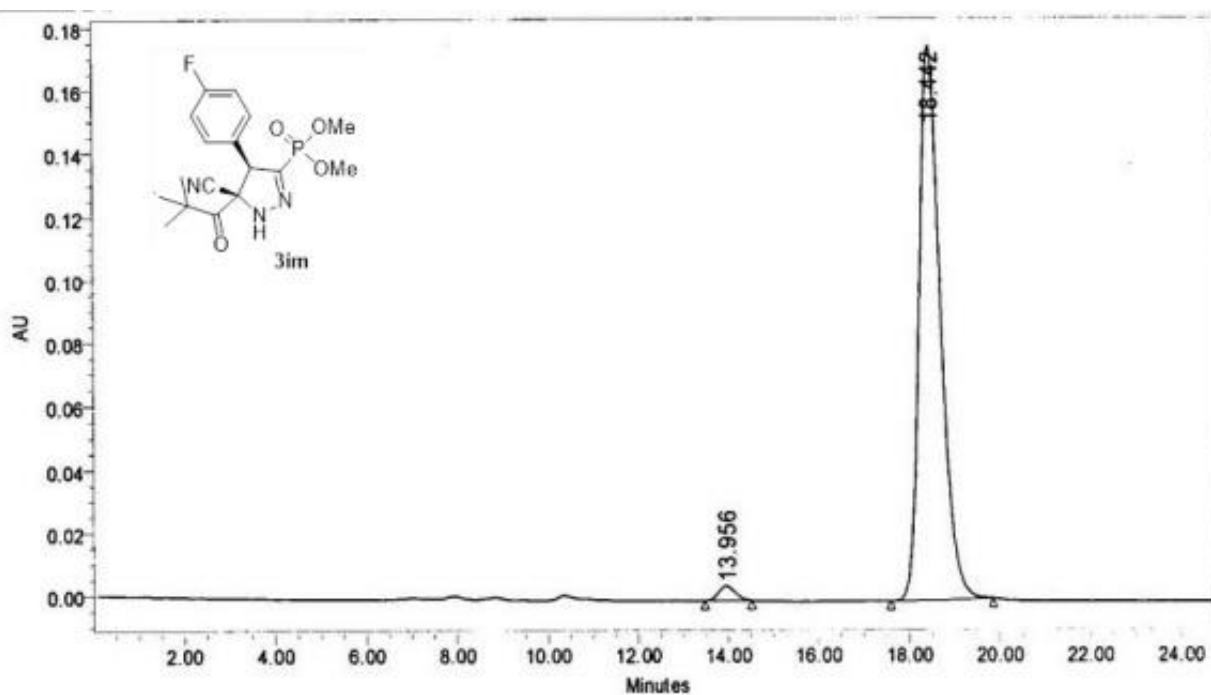
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	26.417	40560	3.36	506	2.42
2	29.284	565159	46.82	12548	60.00
3	31.987	40065	3.32	834	3.99
4	38.692	561412	46.51	7025	33.59



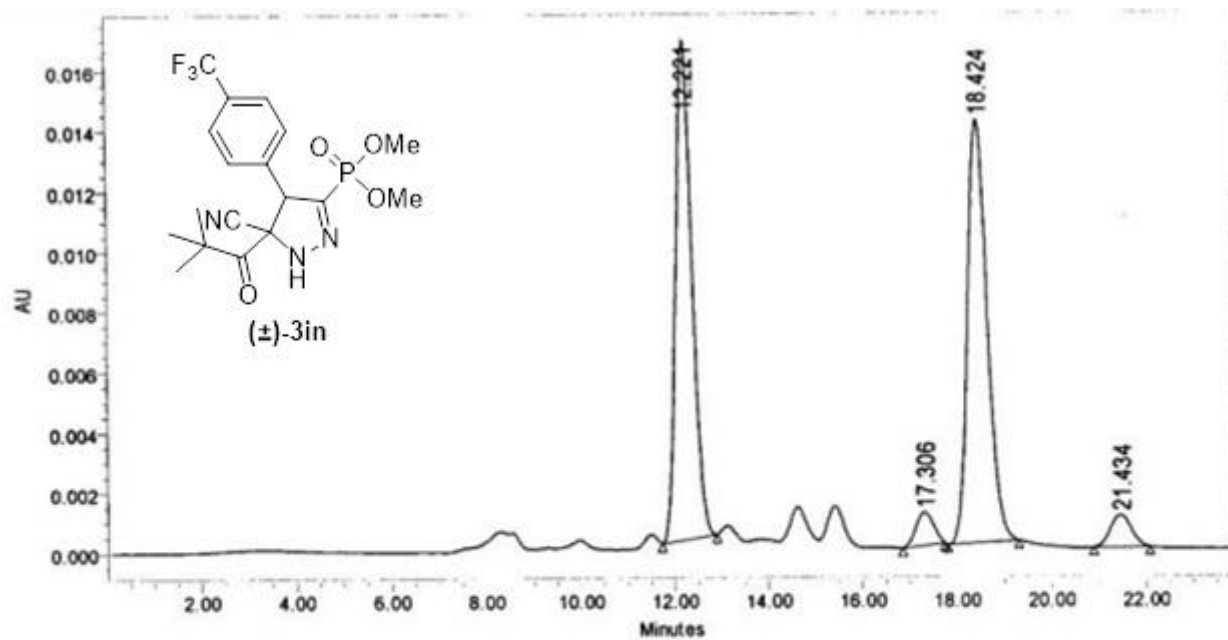
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	25.978	672	0.01	24	0.03
2	28.393	219345	3.81	5799	7.76
3	30.629	2070	0.04	72	0.10
4	37.532	5540453	96.15	68854	92.11



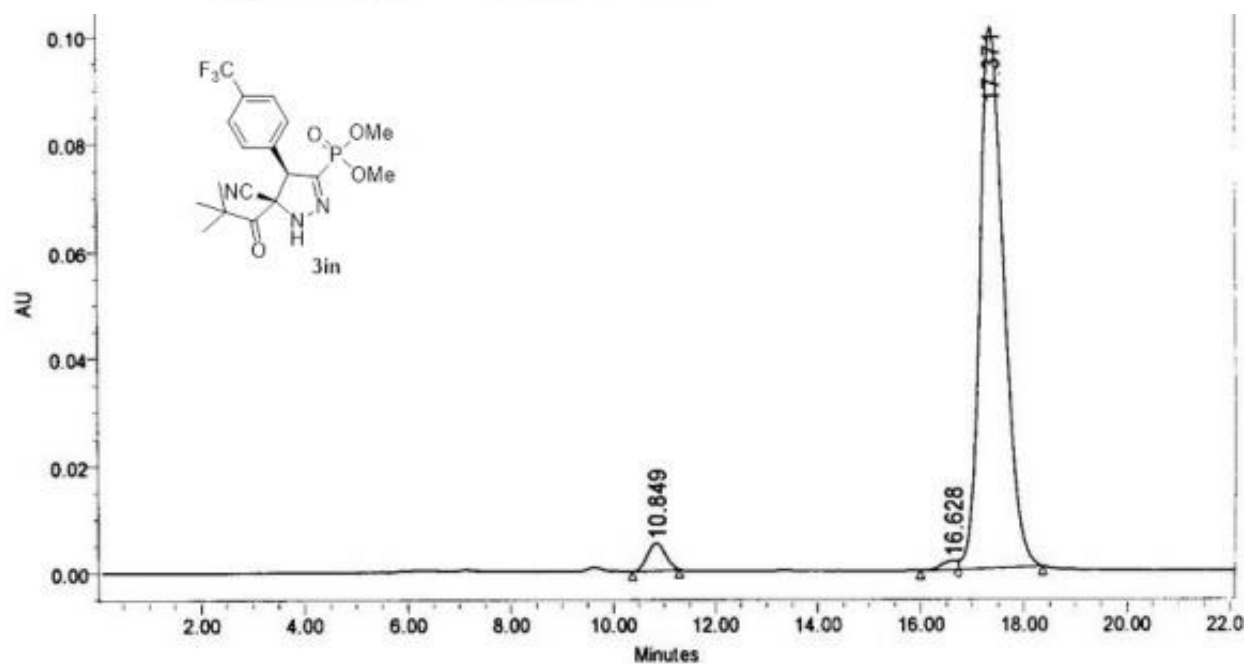
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	14.077	1857121	45.21	65357	50.51
2	17.741	209256	5.09	5743	4.44
3	18.993	1861815	45.33	53728	41.52
4	20.972	179127	4.36	4578	3.54



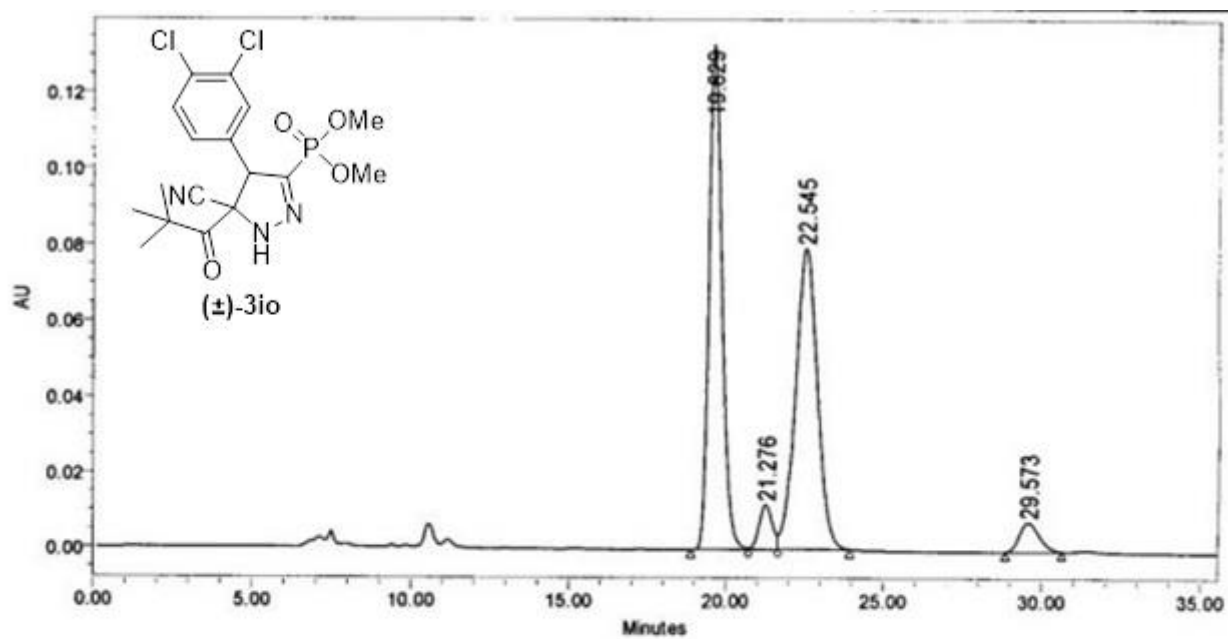
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	13.956	116765	2.01	4600	2.55
2	18.442	5681174	97.99	175616	97.45



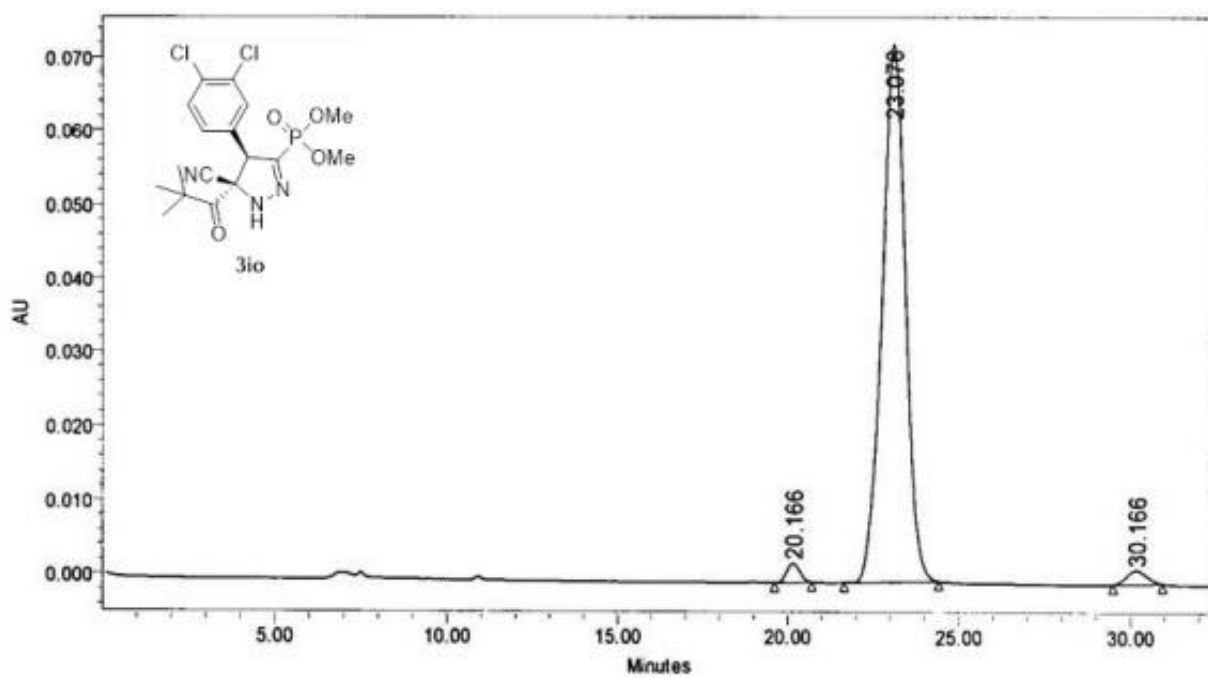
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	12.221	396825	46.26	16594	50.63
2	17.306	27708	3.23	1091	3.33
3	18.424	400818	46.72	14034	42.82
4	21.434	32483	3.79	1059	3.23



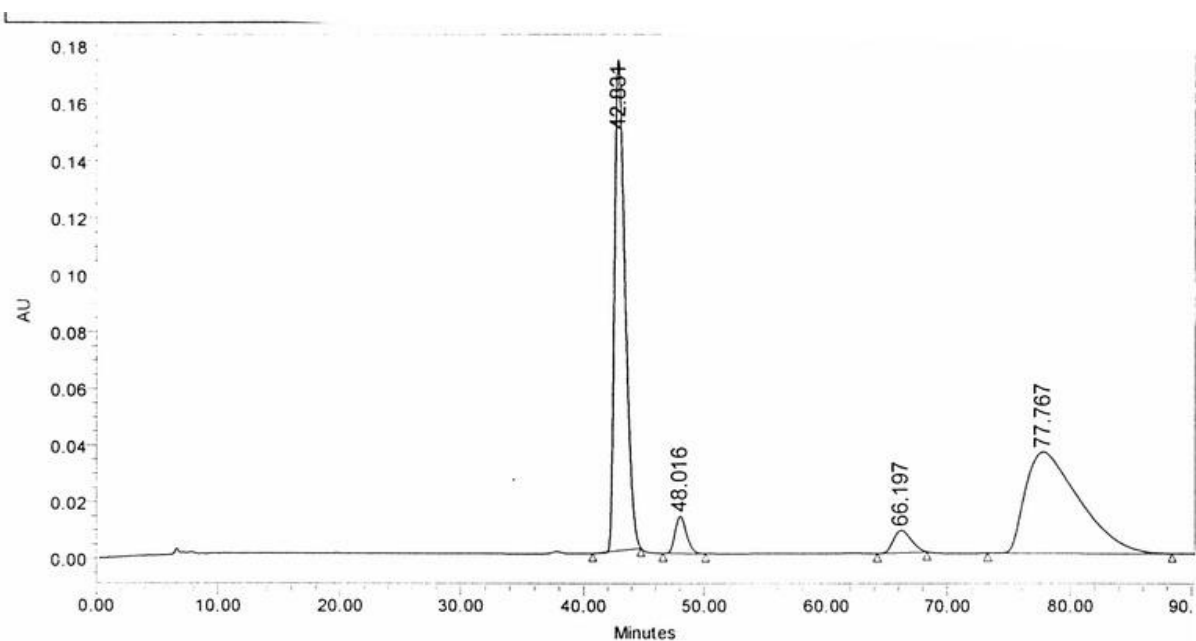
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	10.849	122358	3.61	5071	4.72
2	16.628	33782	1.00	1592	1.48
3	17.371	3232851	95.39	100828	93.80



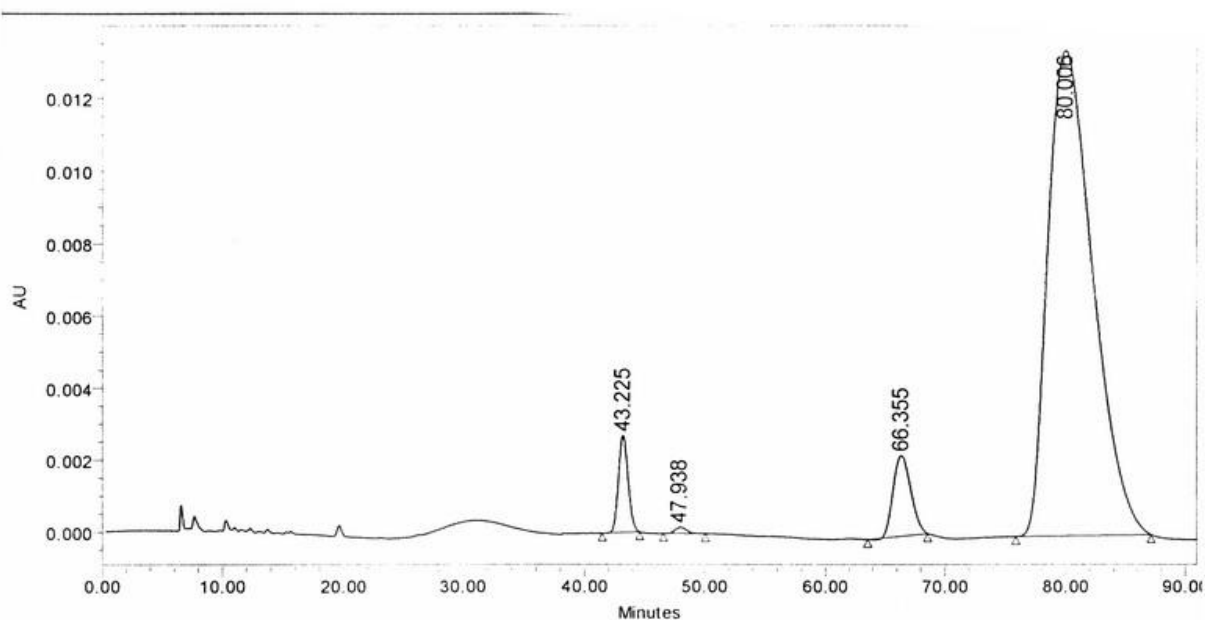
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	19.629	3836816	45.97	133176	57.27
2	21.276	345337	4.14	11923	5.13
3	22.545	3829650	45.88	79678	34.26
4	29.573	334842	4.01	7773	3.34



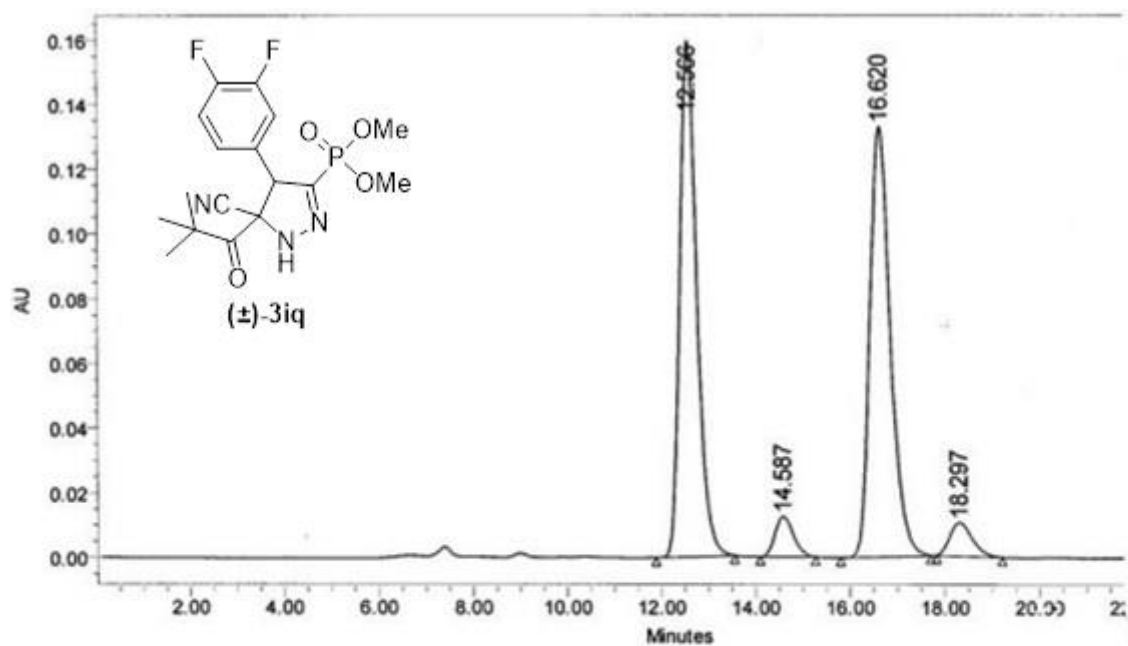
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	20.166	67242	1.89	2529	3.28
2	23.076	3422332	96.03	72767	94.36
3	30.166	74106	2.08	1824	2.37



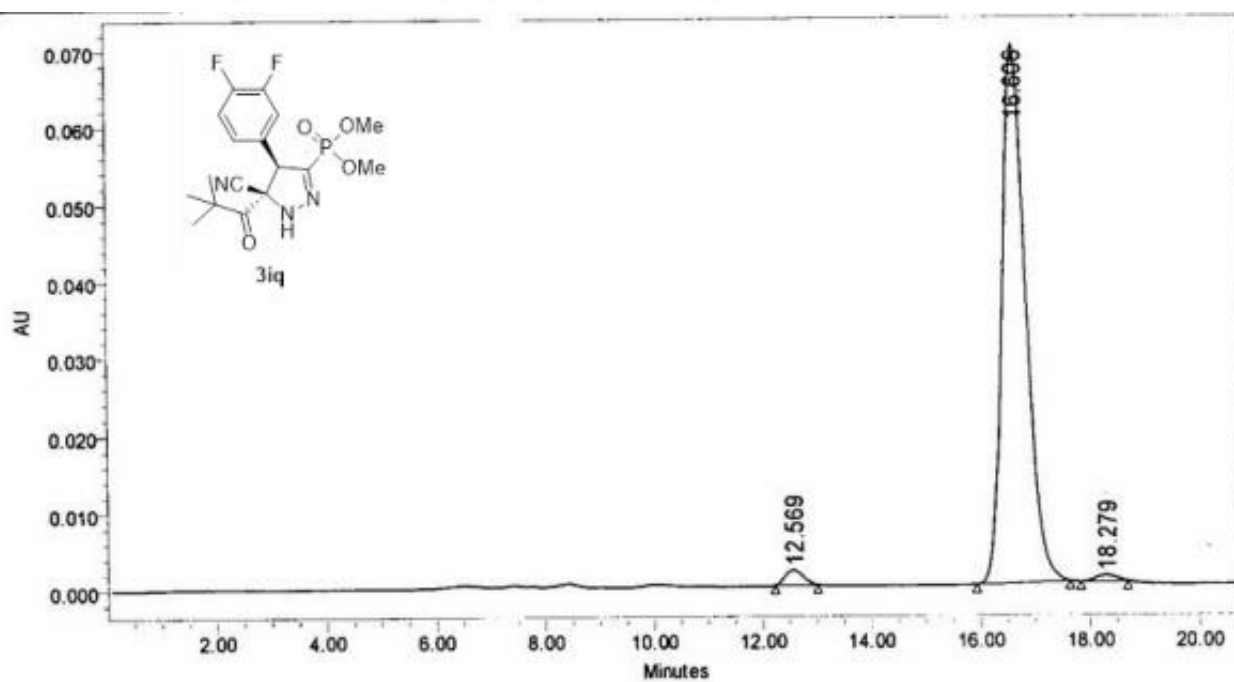
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	42.831	10622240	45.94	172407	75.22
2	48.016	860132	3.72	13157	5.74
3	66.197	797863	3.45	7869	3.43
4	77.767	10843338	46.89	35762	15.60



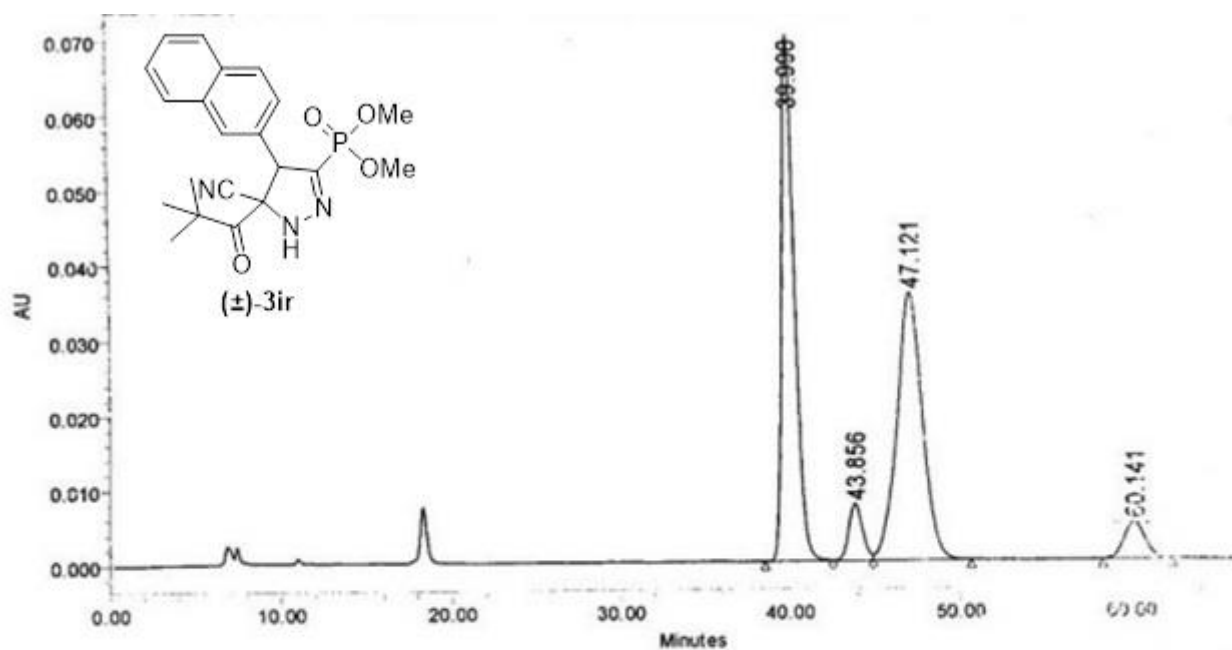
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	43.225	153323	3.95	2701	14.57
2	47.938	10484	0.27	173	0.93
3	66.355	231061	5.95	2237	12.07
4	80.006	3486146	89.83	13428	72.43



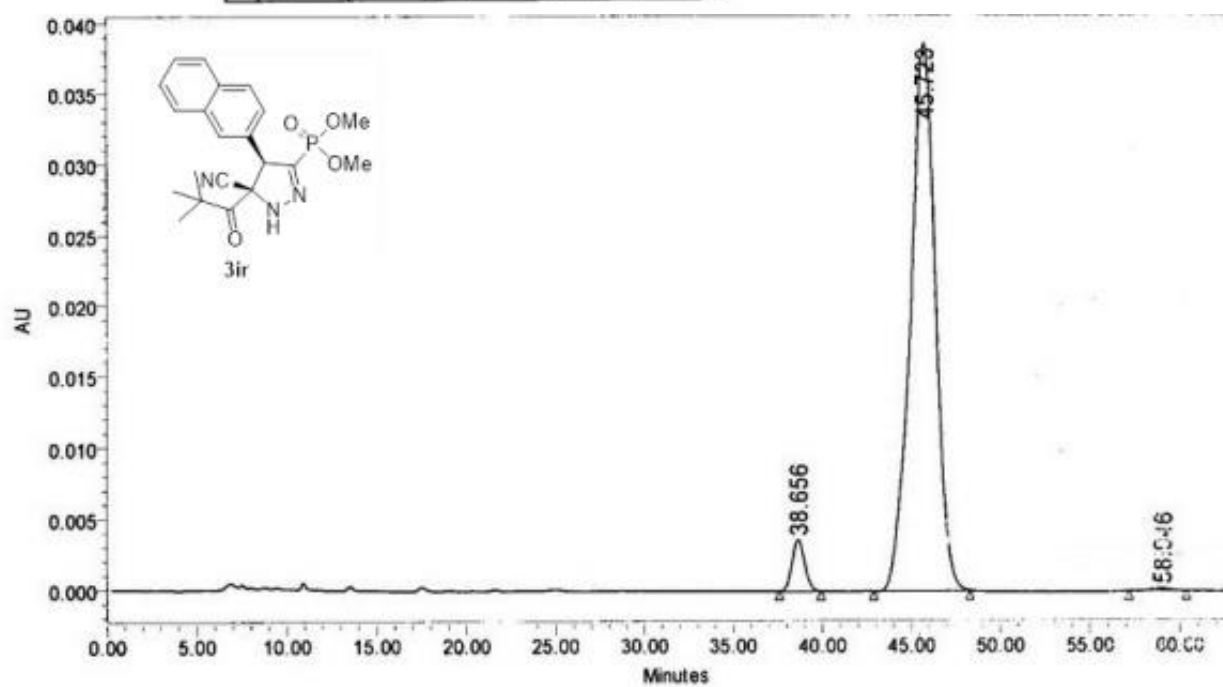
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	12.566	3992072	46.30	159396	50.58
2	14.587	336594	3.90	12534	3.98
3	16.620	3959476	45.92	132837	42.16
4	18.297	334102	3.87	10343	3.28



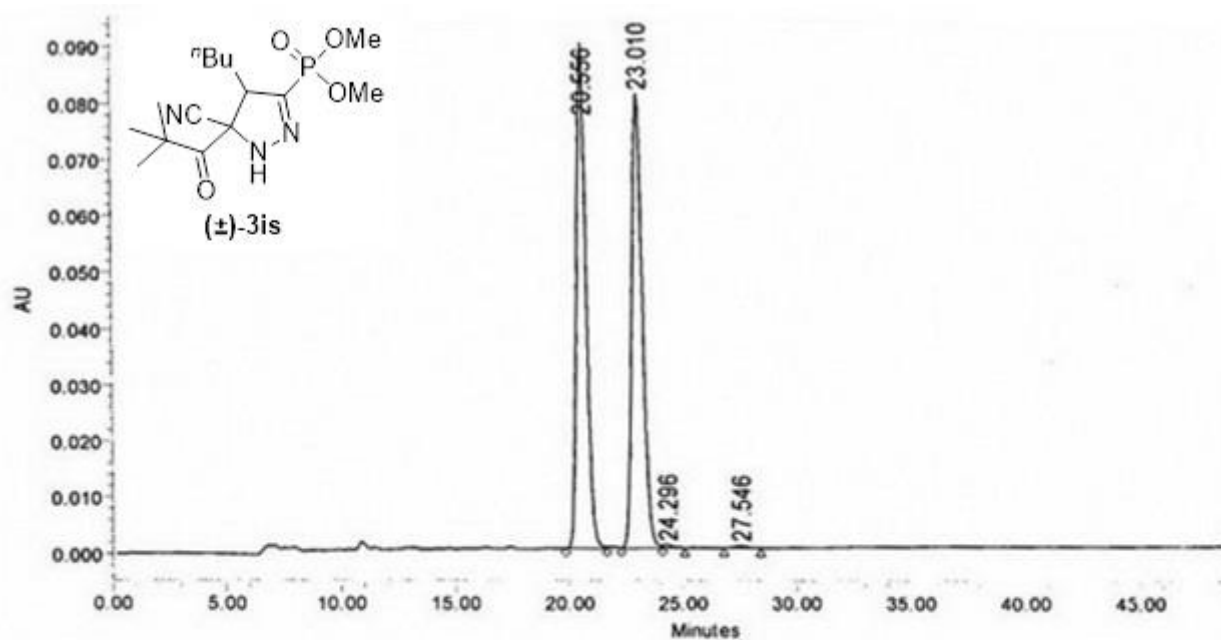
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	12.569	43930	2.07	1954	2.70
2	16.606	2062107	96.96	69738	96.22
3	18.279	20814	0.98	783	1.08



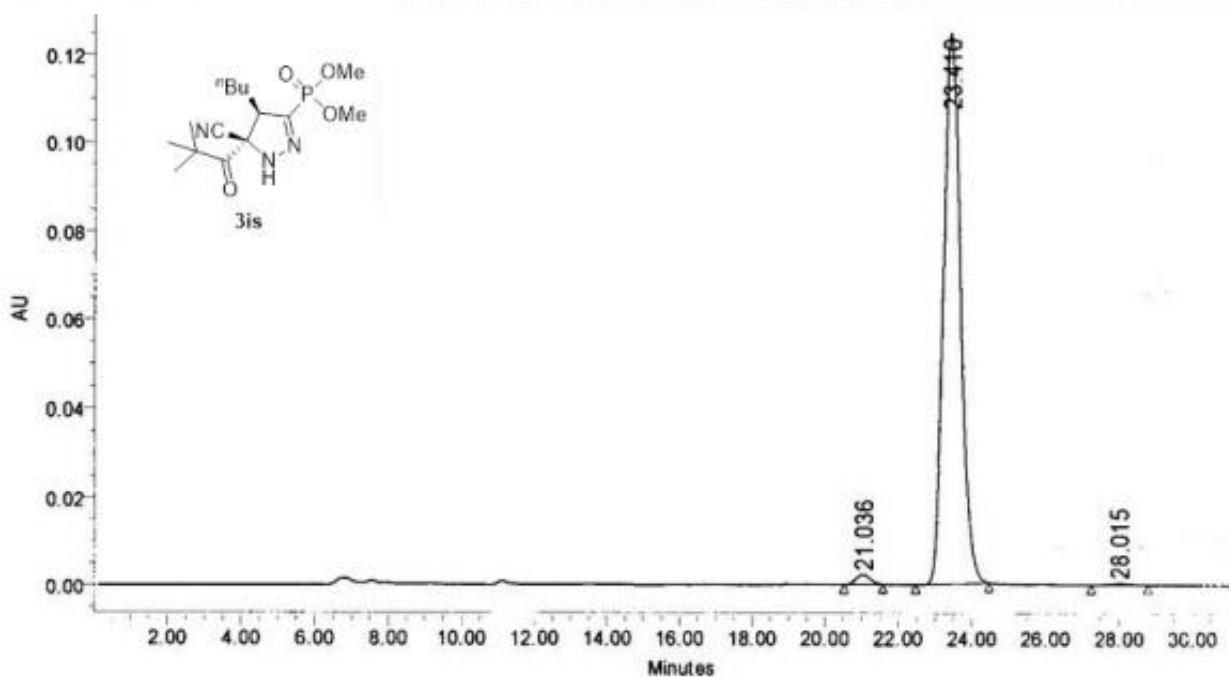
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	39.990	3691998	44.94	70174	59.44
2	43.856	423865	5.16	7514	6.36
3	47.121	3688833	44.91	35532	30.10
4	60.141	410024	4.99	4838	4.10



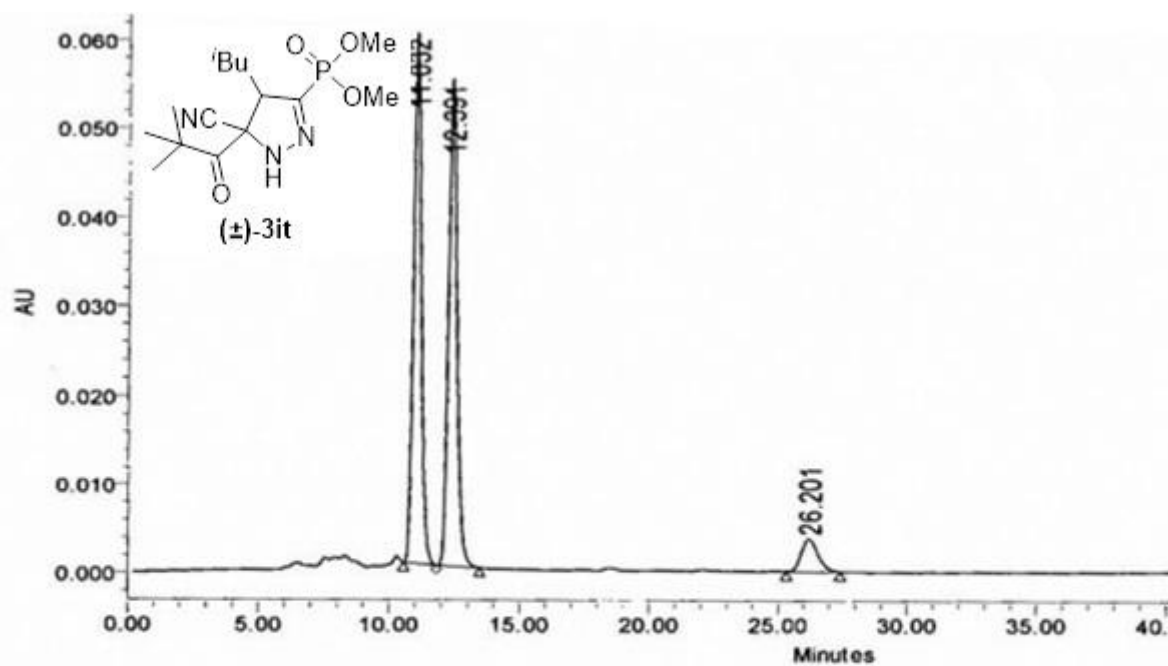
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	38.656	177226	4.51	3628	8.52
2	45.723	3737763	95.09	38731	90.98
3	58.946	15617	0.40	214	0.50



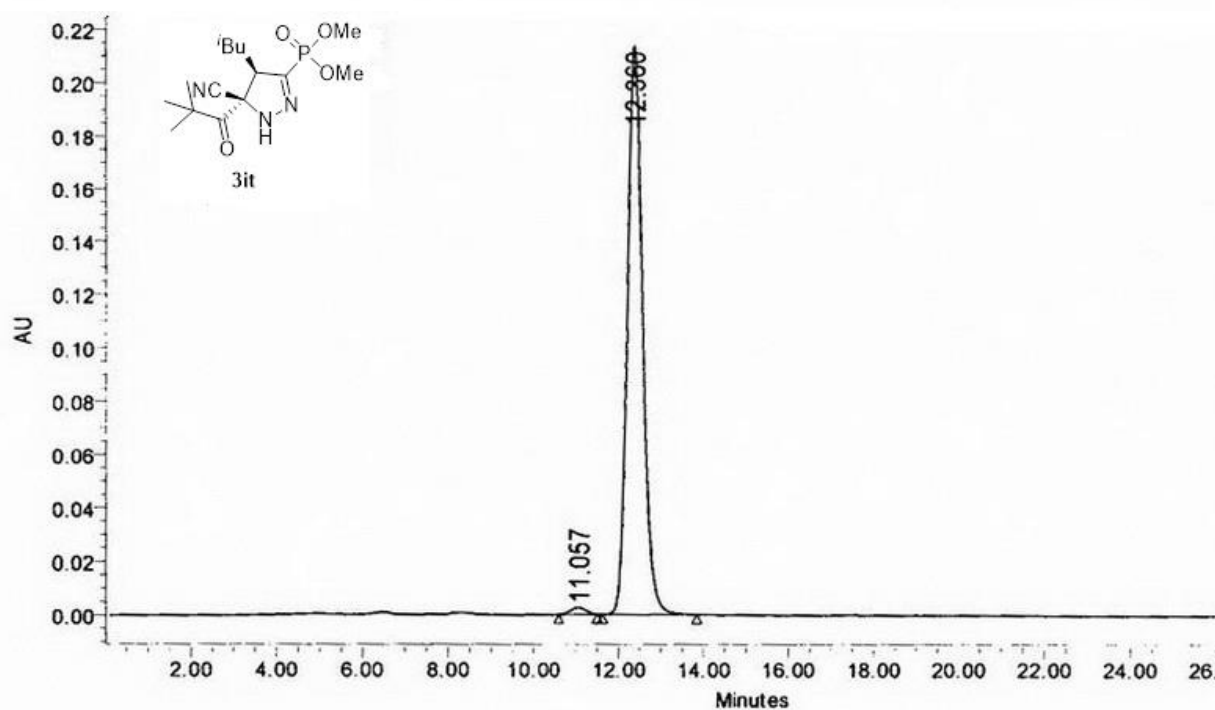
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	20.556	2617039	49.83	89921	52.33
2	23.010	2598126	49.47	80877	47.06
3	24.296	18734	0.36	620	0.36
4	27.546	17700	0.34	432	0.25



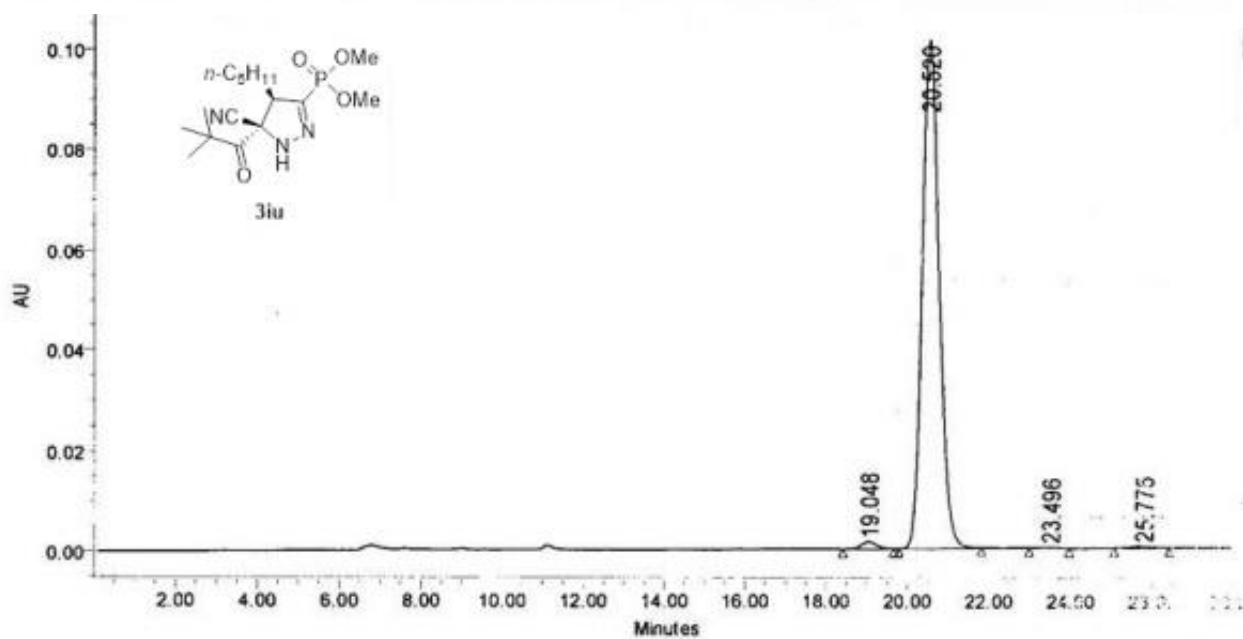
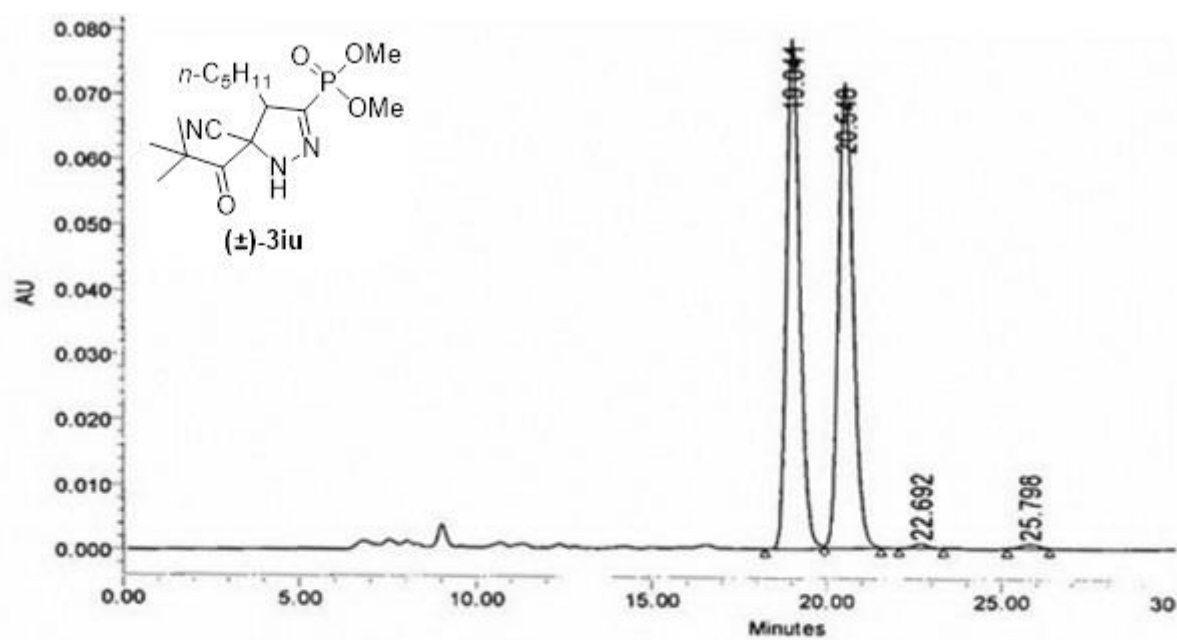
	RT (min)	Area ($\mu\text{V}\cdot\text{sec}$)	% Area	Height (μV)	% Height
1	21.036	59846	1.46	2208	1.73
2	23.410	4022357	98.20	124869	97.99
3	28.015	13976	0.34	355	0.28

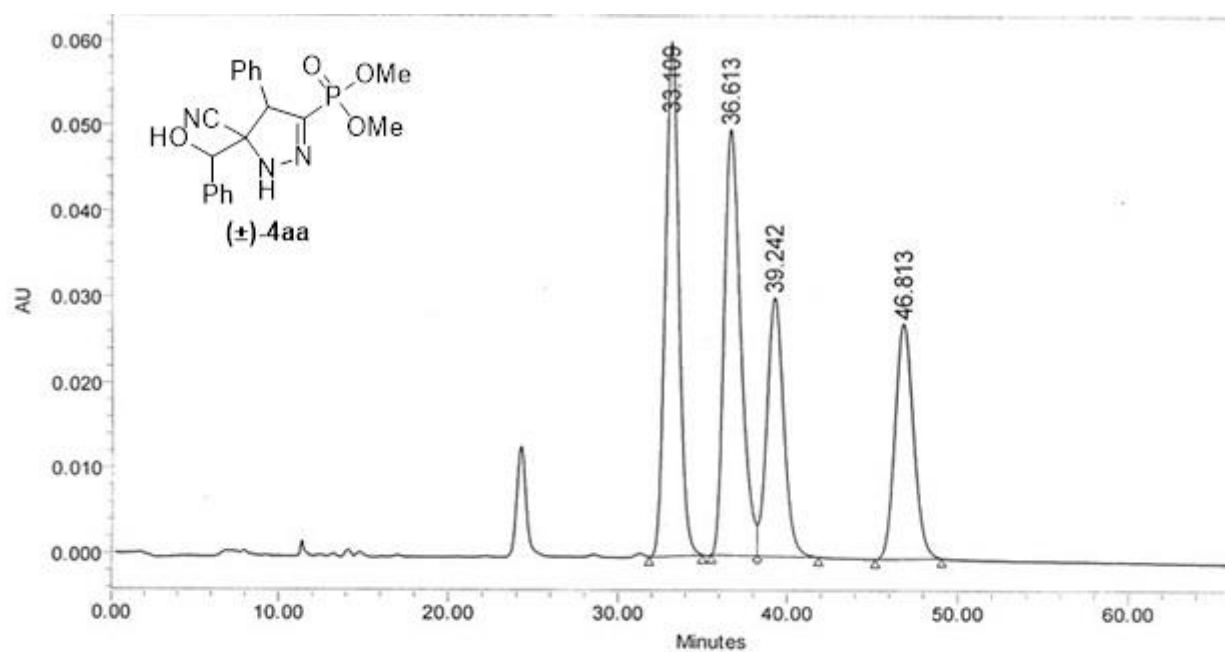


	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.032	1247340	46.65	59816	50.50
2	12.391	1261829	47.19	54932	46.38
3	26.201	164675	6.16	3688	3.11

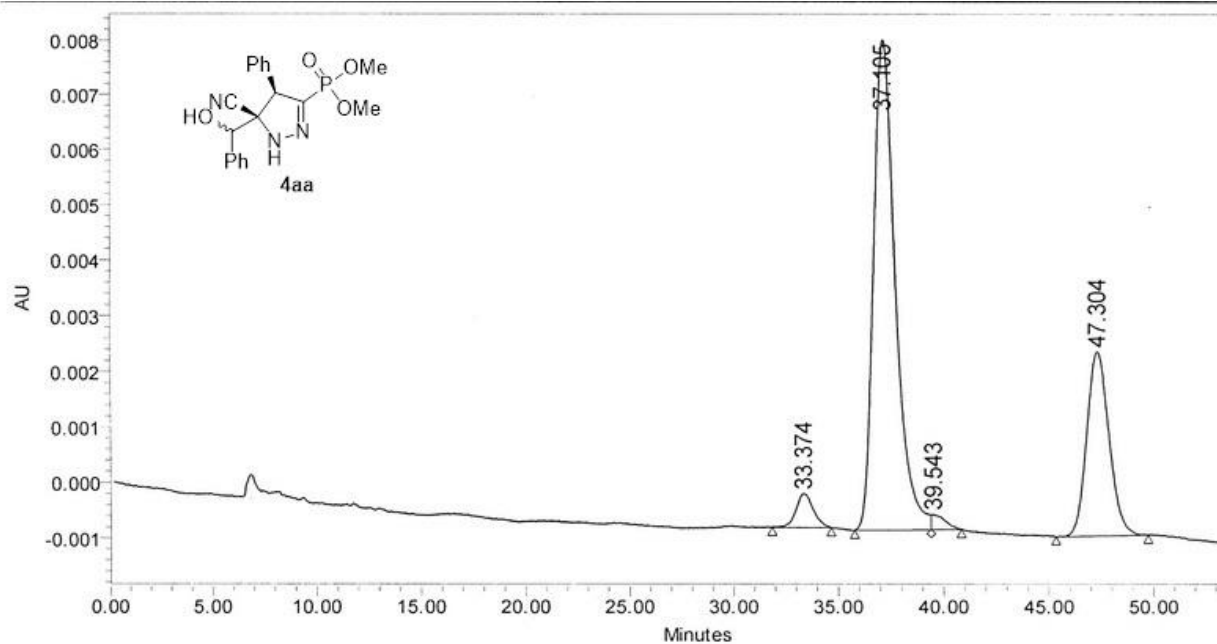


	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.057	62206	1.16	2514	1.16
2	12.360	5317348	98.84	213755	98.84





	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	33.109	3370058	30.77	60260	35.90
2	36.613	3418220	31.21	49734	29.63
3	39.242	2087504	19.06	30277	18.04
4	46.813	2077377	18.97	27589	16.44



	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	33.374	34701	3.74	606	4.64
2	37.105	635044	68.47	8866	67.81
3	39.543	11955	1.29	271	2.07
4	47.304	245814	26.50	3331	25.48