Asymmetric Cyclization/Nucleophilic Tandem Reaction of *o*-alkynylacetophenone with (Diazomethyl)phosphonate for the Synthesis of Functional Isochromenes

Liu Cai,[†,§] Yuan Chen,[†,§] Hao Cao,[†] Qi Wei,[†] Yi Yang,[†] Qin Ouyang*[,‡] and Yungui Peng*[,†]

[†]Key Laboratory of Applied Chemistry of Chongqing Municipality, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China

[‡]College of Pharmacy, Third Military Medical University, Chongqing 400038, China

ouyangq@tmmu.edu.cn; pengyungui@hotmail.com

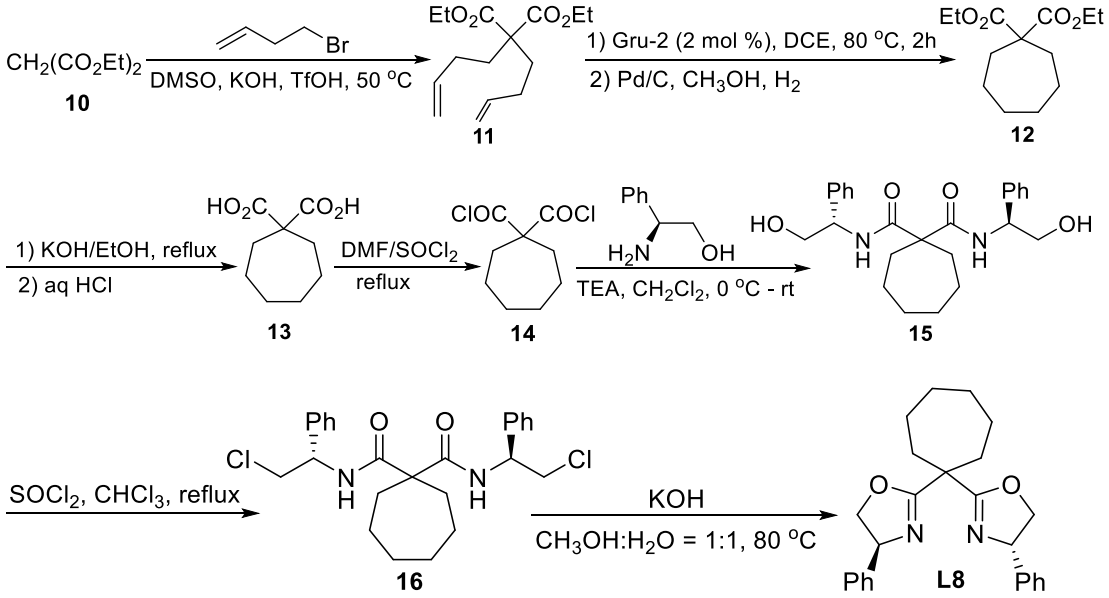
Contents

1. General information

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 was 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 Bruker Avance 600 MHz instruments. Chemical shifts (δ) are given in ppm relative to TMS, coupling constants (*J*) in Hz. ^{1}H NMR chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm, $(CD_3)_2CO$ at 2.05 ppm, CD_3OD at 3.31 ppm). ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.00 ppm, $(CD_3)_2CO$ at 29.84 ppm, CD_3OD at 49.00 ppm). Melting points were determined on an X–6 digital melting-point apparatus and were uncorrected. Optical rotations were measured on a Perkin Elmer 341 Polarimeter at λ = 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.

Bis(oxazolines) **L1**−**L13** were obtained following the reported procedure.[1] (Diazomethyl)phosphonate **2a** and **2b** were prepared according to the reference.[2]

2. General procedure for the synthesis of L8 and L12



Trifluoromethanesulfonic acid (6.7 mL, 75.7 mmol) was added to a stirred mixture of potassium hydroxide (9.81 g, 175 mmol) in DMSO (50 mL) at 0 ℃, and then the resulted

mixture was stirred at rt for 15 min. Diethyl malonate **10** (4.0 g, 25.0 mmol) and 4-bromo-1-butene (5.8 mL, 57.1 mmol) were added slowly at rt, and the reaction mixture was stirred at 50 ℃ for 6 h. Cooled to rt and a large amount of diethyl ether was added, and washed with 1N hydrochloric acid, saturated $NaHCO_3$ solution and brine. The organic layer was dried over with anhydrous sodium sulfate and concentrated. The residue was purified by column chromatography (PE/EA = 100/1 to 50/1) to afford **11** (4.81 g, 17.9 mmol, 72% yield).[3]

At the atmosphere of N_2, the second-generation Grubbs catalyst (25.5 mg, 0.03 mmol) was rapidly added to the solution of compound **11** (1.61 g, 6 mmol) in degassed dry 1,2-dichloroethane (15 mL), then stirred at 80 ℃ for 3h, cooled to room temperature, suction filtered, and concentrated under reduce pressure, the residue was purified by flash chromatography on silica gel. The obtained product was dissolved in methanol, 10% Pd/C was added, the reaction was carried out overnight in hydrogen atmosphere, the Pd/C is suction filtered, and concentrated under reduce pressure to obtain compound **12**.[4]

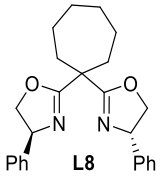
KOH (1.12 g, 20 mmol) was added to the solution of **12** (1.21 g, 5 mmol) in ethanol (15 mL) at rt, and reflux for 8 h, then cooled to 0 ℃, slowly add 1N hydrochloric acid until the pH = 2-3, extracted with dichloromethane and combined the organic phase, dried over with anhydrous sodium sulfate and concentrated under reduce pressure. The residue was purified by column chromatography (PE/EA = 1/1) to obtain **13** (0.912 g, 4.9 mmol, 98% yield).

Compound **13** (186.2 mg, 1 mmol) was dissolved in thionyl chloride under ice bath conditions. Then 2 drops of DMF were added and refluxed for 2 h, removed off the excess thionyl chloride under reduce pressure to obtain **14**. At the atmosphere of N_2, the solution of **14** in dichloromethane was added slowly to the stirring mixture of (*S*)-2-amino-2-phenylethan-1-ol (549.6 mg, 3 mmol) and triethylamine (0.55 mL, 4 mmol) in dichloromethane (10 mL) at 0 ℃, then the reaction mixture was warmed to rt and continued reaction for 4 h. Saturated ammonium chloride aqueous solution was added at 0 ℃ and extracted with dichloromethane. Combined the organic layers and washed with saturated brine, dried over with anhydrous sodium sulfate and concentrated under reduce pressure, the residue was purified by column chromatography (PE/EA = 5/1 to 3/1) to obtain **15** (0.335 g, 0.79 mmol, 79% yield).

Thionyl chloride (277.3 uL, 2 mmol) was added slowly to the solution of **15** (212.3 mg, 0.5 mmol) in dichloromethane at 0 ℃, then reflux at 45 ℃ for 3 h, removed off the excess thionyl chloride under reduce pressure. The residue was dissolved in dichloromethane and washed with saturated $NaHCO_3$ solution and brine, dried over with anhydrous sodium sulfate and concentrated. The residue was purified by column chromatography (PE/EA = 15/1) to give 1**6** (219.2 mg, 0.475 mmol, 95% yield).

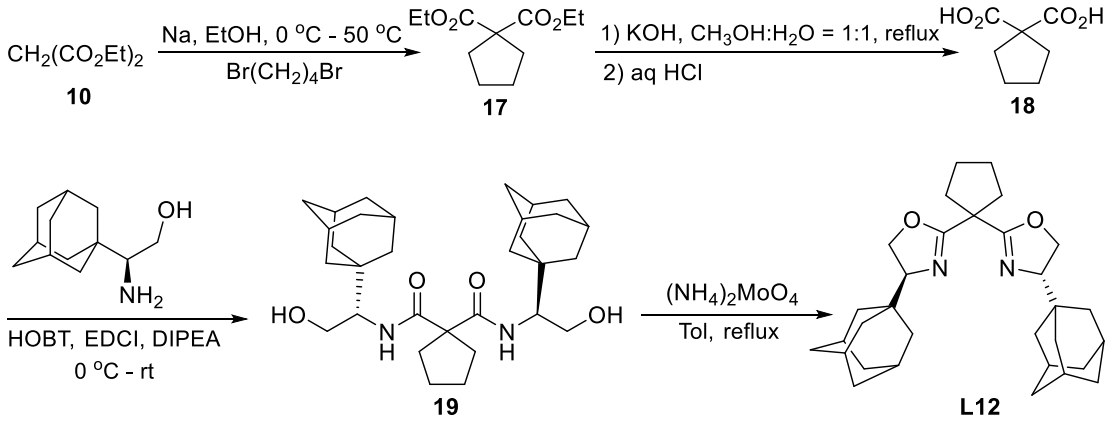
Potassium hydroxide (106.4 mg, 1.9 mmol) was added the solution of **16** (219.2 mg, 0.475 mmol) in a mixture of methanol and water (10 mL, 1:1) at low temperature, and then heated to 80 ℃ and reaction for 1 h. Cooled down to 0 ℃, quenched with saturated ammonium chloride, extracted with dichloromethane, dried over anhydrous sodium sulfate, and the residue was purified by column chromatography (PE/EA = 5/1 to 3/1) to obtain **L8** (120 mg, 0.308 mmol, 65% yield).[5]

(4*S*, 4'*S*)-2, 2'-(cycloheptane-1,1-diyl)bis(4-phenyl-4,5-dihydrooxazole) (L8)



L8

Colorless oil. $[\alpha]_D^{25}$ = -132.1 ° (*c* = 0.78, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45–7.16 (m, 10H), 5.22 (dd, *J* = 10.0, 7.8 Hz, 2H), 4.64 (dd, *J* = 10.0, 8.4 Hz, 2H), 4.11 (t, *J* = 8.0 Hz, 2H), 2.37 (dd, *J* = 11.0, 4.7 Hz, 4H), 1.69 (s, 4H), 1.61 (d, *J* = 2.2 Hz, 4H). ^{13}C NMR(151 MHz, $CDCl_3$) δ 170.4, 142.6, 128.7, 127.5, 126.7, 75.3, 69.5, 46.7, 34.9, 30.1, 23.5. HRMS (ESI) calcd. for $C_{25}H_{29}N_2O_2$ $[M+Na]^+$: 389.2224, found: 389.2224.



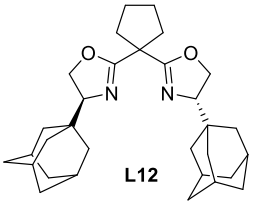
Diethyl malonate **10** (100 mmol, 15.2 mL) was added slowly to the solution of sodium (4.6 g, 200 mmol) in absolute ethyl alcohol (175 mL) at 0 ℃, then the reaction mixture was warmed to 50 ℃ and stirred for 1 h, 1,4-dibromobutane (90 mmol, 10.7 mL) was added and continuously reaction for 3-4 h at 50 ℃, quenched with saturated ammonium chloride, removed off the ethyl alcohol under reduce pressure. The residue was diluted with ethyl acetate, washed with saturated brine, dried over with anhydrous sodium sulfate and concentrated under reduce pressure. The residue was purified by column chromatography column (PE/EA = 100/1 to 50/1) to obtain **17** (4.3 g, 170 mmol, 85% yield).[6]

Potassium hydroxide (10 mmol, 560 mg) was added to the solution of **17** (1.1 g, 5 mmol) in the mixture of methanol and water (20 mL, 1:1) and refluxed for 4 h. Cooled to rt and adjust the pH to 2-3 with 1N hydrochloric acid, extracted the solution with dichloromethane three times (3 x 50 mL). Combined the organic layers and washed with saturated saline, dried over anhydrous sodium sulfate, concentrated under reduce pressure to obtain **18** (711 mg, 4.5 mmol, 90% yield).

EDCI (575.1 mg, 3.0 mmol) was added to the mixture of **18** (237.1 mg, 1.5 mmol) DIPEA (744.0 uL, 4.5 mmol), HOBT (473.0 mg, 3.5 mmol) and (*S*)-2-(adamantan-1-yl)-2-aminoethan-1-ol (586.0 mg, 3.0 mmol) (prepared according the reported procedure)[7] in anhydrous dichloromethane (10 mL) at 0 ℃, warmed to rt and reacted overnight. Saturated ammonium chloride aqueous solution was added and extracted with dichloromethane for three times (3 x 50 mL). Combined the organic layers and washed with 1N dilute hydrochloric acid, saturated saline, dried over with anhydrous sodium sulfate, concentrated under reduce pressure and purified by column chromatography (PE/EA = 2/1) to obtain **19** (422 .7 mg, 55% yield).

Ammonium molybdate solid (15.7 mg, 0.08 mmol) was added to the solution of **19** (422.7 mg, 0.825 mmol) in 15 mL of anhydrous toluene at rt, then the mixture was refluxed for 2-3 h, concentrated under reduce pressure and purified by low-temperature column chromatography (PE/EA = 15/1) to obtain **L12** (294 mg, 0.62 mmol, 75% yield).[8]

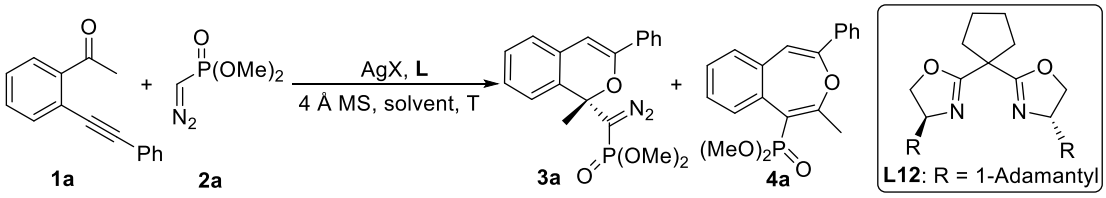
(4*S*, 4'*S*)-2, 2'-(cycloheptane-1,1-diyl)bis(4-adamantyl-4,5-dihydrooxazole) (L12)



White solid, mp: 291.0–294.0 ℃, $[\alpha]_D^{25}$ = -91.2 ° (*c* = 0.36, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 4.16 (t, *J* = 7.9 Hz, 2H), 4.09–4.04 (t, 2H), 3.67 (dd, *J* = 9.9, 7.3 Hz, 2H), 2.36 (dt, *J* = 12.9, 6.7 Hz, 2H), 2.16–2.06 (m, 2H), 1.96 (s, 6H), 1.64 (ddd, *J* = 27.0, 18.5, 11.7 Hz, 22H), 1.42–1.34 (m, 6H). ^{13}CNMR (151 MHz, $CDCl_3$) δ 167.9, 75.5, 67.6, 49.3, 38.4, 37.2, 35.7, 35.5, 25.1. HRMS (ESI) calcd. for $C_{31}H_{44}N_2O_2$ $[M+H]^+$: 477.3476, found: 477.3486.

3. Optimization of reaction conditions

Table 1. Partial results of reaction conditions optimization[a]

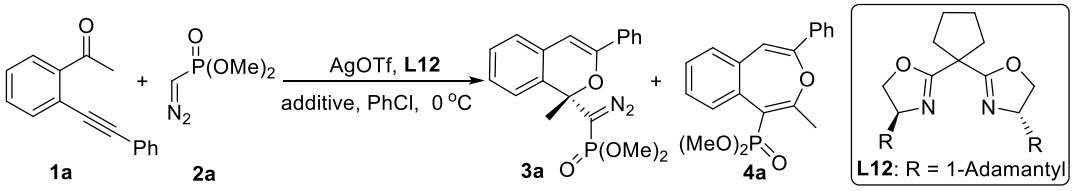


entry	solvent	temp/ ℃	con. (mol/L)	Ratio (**L12**:AgOTf)	yield of **3a** (%)[b]	*Ee* of **3a**[c]	yield of **4a** (%)[b]
1	PhCl	0	0.2	1.2:1	92	93	3
2	THF	0	0.2	1.2:1	15	90	-
3	Tol	0	0.2	1.2:1	50	89	-
4	hexane	0	0.2	1.2:1	63	67	7
5	CH_2Cl_2	0	0.2	1.2:1	88	93	7

6	CH_3CN	0	0.2	1.2:1	12	84	-
7	EA	0	0.2	1.2:1	38	89	-
8	PhF	0	0.2	1.2:1	93	92	5
9	acetone	0	0.2	1.2:1	27	88	-
10	dichloro benzene	0	0.2	1.2:1	90	90	4
11	PhCl	-10	0.2	1.2:1	84	93	3
12	PhCl	-20	0.2	1.2:1	40	95	-
13[d]	PhCl	0	0.2	1.2:1	86	90	6
14[e]	PhCl	0	0.2	1.2:1	80	93	trace
15[e,f]	PhCl	0	0.2	1.2:1	98	94	trace
16[e,f]	PhCl	0	0.1	1.2:1	97	94	trace
17[e,f]	PhCl	0	0.05	1.2:1	86	94	trace

[a]Conditions: Unless noted otherwise, all of the reactions were carried out with **1a** (0.2 mmol), **2a** (0.2 mmol), **L12** (12 mol%) and AgOTf (10 mol%) in 1.0 mL of PhCl at 0 ℃ for 1-2 days; [b]Isolated yield; [c]Determined by chiral HPLC; [d]15 mol% of AgOTf was used; [e]5 mol% of AgOTf was used; [f]**1a**/**2a** (0.2 mmol) = 1.2:1; [g]4Å MS was not added.

Table 2. The influence of additive (MS) on the reaction[a]

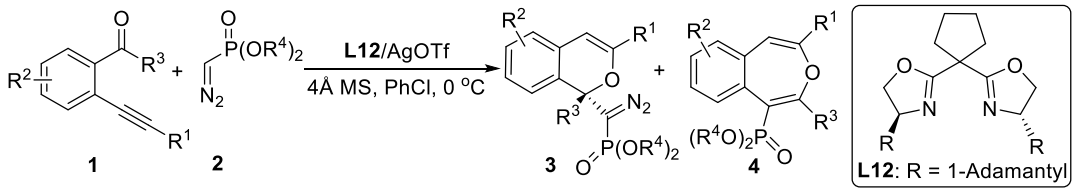


entry	additive	yield of **3a** (%)[b]	yield of **4a** (%)[b]	*ee* of **3a** (%)[c]
1	-	47	trace	89
2	3Å MS	62	trace	92
3	4Å MS	98	trace	94
4	5Å MS	93	trace	94

[a]Conditions: Unless noted otherwise, all of the reactions were carried out with **1a** (0.24 mmol), **2a** (0.2 mmol), **L12** (6 mol%) and AgOTf (5 mol%), MS (100 mg) in 1.0 mL of PhCl at 0 ℃ for 1-2 days; [b]Isolated yield; [c]Determined by chiral HPLC.

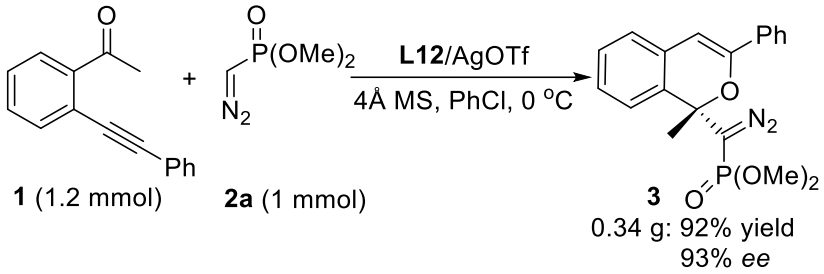
The molecular sieve was added to scavenge the trace amount of water present in the reaction system. 4Å MS has shown the best performance.

4. General procedure for the synthesis of functional isochromenes 3



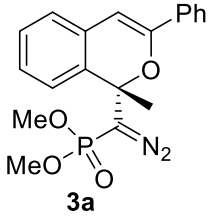
Chiral bis(oxazoline) **L12** (0.012 mmol), AgOTf (0.01 mmol) and anhydrous PhCl (1 mL) was added to a dried reaction tube at the nitrogen atmosphere, and stirred in dark about 2 h at rt, 4 Å MS and *o*-alkynylacetophenone **1** (0.24 mmol) was added and the mixture was cooled to 0 ℃. The (diazomethyl)phosphonate **2** (0.2 mmol) was added and stirred at 0 ℃ until the reaction completion monitored by TLC. The reaction mixture was directly purified on a silica gel chromatography column PE/EA (5/1 to 3/1) to give chiral functional isochromenes **3** and accompany by product **4**

1 mmol-scale experiment



Chiral bis(oxazoline) **L12** (28.6 mg, 0.06 mmol), AgOTf (12.8 mg, 0.05 mmol) and anhydrous PhCl (5 mL) was added to a dried reaction tube at the nitrogen atmosphere, and stirred in dark about 3 h at rt, 4 Å MS (500 mg) and *o*-alkynylacetophenone **1** (150.0 mg, 1.0 mmol) was added and the mixture was cooled to 0 ℃. The (diazomethyl)phosphonate **2** (264.5 mg, 1.2 mmol) was added and stirred at 0 ℃ until the reaction completion monitored by TLC. The reaction mixture was directly purified on a silica gel chromatography column PE/EA (5/1 to 3/1) to give **3** (0.34 g, 92% yield, 93% *ee*)

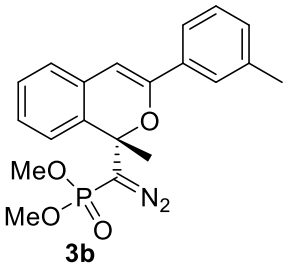
Dimethyl (*S*)-(diazo(1-methyl-3-phenyl-1H-isochromen-1-yl)methyl)phosphonate (3a)



Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-(phenylethynyl)phenyl)ethan-1-one **1a** (52.9 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3a** as a green oil, 72.6 mg (98% yield, 94% *ee*); $[\alpha]_D^{25}$ = +106.12 ° (*c* = 0.91, EA). ^{1}H NMR (600 MHz, Acetone) δ 7.82–7.63 (m, 2H), 7.29–7.23 (m, 3H), 7.23–7.08 (m, 4H), 6.55 (s, 1H), 3.48 (dd, *J* = 35.3, 11.8 Hz, 6H), 1.97 (s, 3H). ^{13}C NMR (151 MHz, Acetone) δ 151.1, 134.3, 131.2, 131.1 (d, *J* = 5.5 Hz), 129.0, 128.9, 128.3, 127.3, 125.2, 124.8, 124.1, 100.9, 80.8 (d, *J* = 9.5 Hz), 52.3 (dd, *J* = 7.0, 5.6 Hz), 49.9 (d, *J* = 219.8 Hz), 24.8. HRMS (ESI) calcd. for $C_{19}H_{19}N_2O_4P$ $[M+Na]^+$: 393.0975, found: 393.0978; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH =

70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 17.816 min, t_{minor} = 14.961 min).

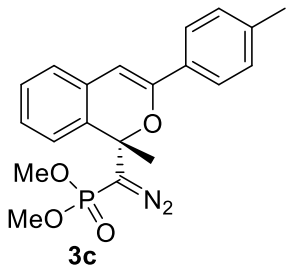
Dimethyl (*S*)-(diazo(1-methyl-3-(m-tolyl)-1H-isochromen-1-yl)methyl)phosphonate (3b)



3b

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-(*m*-tolylethynyl)phenyl)ethan-1-one **1b** (56.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3b** as a green oil, 74.6 mg (97% yield, 94% *ee*); $[\alpha]_D^{25}$ = +94.2 °(*c* = 0.93, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 9.3 Hz, 2H), 7.32-7.20 (m, 4H), 7.15 (t, *J* = 5.9 Hz, 2H), 6.44 (s, 1H), 3.66 (dd, *J* = 11.4, 8.9 Hz, 6H), 2.39 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.3, 137.9, 134.2, 131.2, 130.9 (d, *J* = 5.0 Hz), 129.8, 129.0, 128.3, 127.1, 125.7, 124.6, 124.0, 122.3, 100.7, 80.9 (d, *J* = 9.9 Hz), 52.9 (dd, *J* = 7.8, 5.7 Hz), 50.4 (d, *J* = 226.6 Hz), 25.4, 21.5, 25.5. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_4P$ $[M+Na]^+$: 407.1131, found: 407.1135; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.546 min, t_{minor} = 13.925 min).

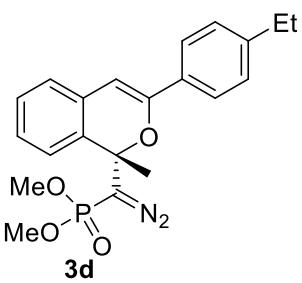
Dimethyl (*S*)-(diazo(1-methyl-3-(*p*-tolyl)-1H-isochromen-1-yl)methyl)-phosphonate (3c)



3c

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-(*p*-tolylethynyl)phenyl)ethan-1-one **1c** (56.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3c** as a green solid 75.3 mg (98% yield, 92% *ee*), mp: 82.8–84.1 ℃; $[\alpha]_D^{25}$ = +116.7 °(*c* = 0.94, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.31–7.17 (m, 5H), 7.14 (d, *J* = 7.4 Hz, 1H), 6.41 (s, 1H), 3.65 (dd, *J* = 11.7, 8.8 Hz, 6H), 2.37 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.3, 139.0, 131.4, 131.3, 130.8 (d, *J* = 5.0 Hz), 129.1, 129.0, 126.9, 125.1, 124.6, 124.0, 100.0, 80.8 (d, *J* = 10.0 Hz), 52.9 (t, *J* = 5.7 Hz), 50.3 (d, *J* = 226.4 Hz), 25.4, 21.3. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_4P$ $[M+Na]^+$: 407.1131, found: 407.1133; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.625 min, t_{minor} = 15.153 min).

Dimethyl (*S*)-(diazo(3-(4-ethylphenyl)-1-methyl-1H-isochromen-1-yl)methyl)phosphonate (3d)

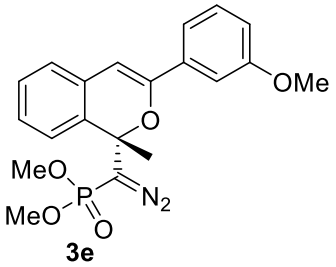


3d

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol)

with1-(2-((4-ethylphenyl)ethynyl)phenyl)ethan-1-one **1d** (59.6 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3d** as a green oil 66.1 mg (83% yield, 93% *ee*), $[\alpha]_D^{25}$ = +100 ° (*c* = 0.82, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.0 Hz, 2H), 7.32–7.19 (m, 5H), 7.14 (d, *J* = 7.3 Hz, 1H), 6.42 (s, 1H), 3.77–3.56 (m, 6H), 2.67 (q, *J* = 7.5 Hz, 2H), 2.07 (s, 3H), 1.25 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.3, 145.4, 131.7, 131.3, 130.8 (d, *J* = 5.0 Hz), 129.0, 127.9, 126.9, 125.2, 124.6, 124.0, 100.0, 80.8 (d, *J* = 10.0 Hz), 52.9 (t, *J* = 5.6 Hz), 50.4 (d, *J* = 226.4 Hz), 28.7, 25.4, 15.4. HRMS (ESI) calcd. for $C_{21}H_{23}N_2O_4P$ $[M+Na]^+$: 421.1288, found: 421.1291; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.716 min, t_{minor} = 14.608 min).

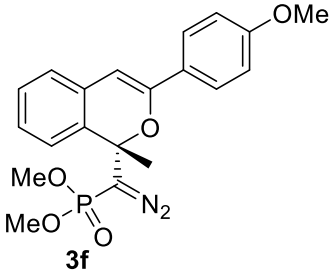
Dimethyl (*S*)-(diazo(3-(3-methoxyphenyl)-1-methyl-1H-isochromen-1-yl)methyl)phosphonate (3e)



3e

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((3-methoxyphenyl)ethynyl)phenyl)ethan-1-one **1e** (60.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3e** as a green oil, 76.9 mg (96% yield, 94% *ee*), $[\alpha]_D^{25}$ = +137.1 ℃ (*c* = 0.96, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 12.1 Hz, 2H), 7.33–7.22 (m, 4H), 7.16 (d, *J* = 6.2 Hz, 1H), 6.90 (d, *J* = 7.3 Hz, 1H), 6.58–6.22 (m, 1H), 3.86 (s, 3H), 3.67 (t, *J* = 12.1 Hz, 6H), 2.07 (d, *J* = 28.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.8, 151.0, 135.7, 131.0, 130.9 (d, *J* = 5.2 Hz), 129.3, 129.0, 127.2, 124.7, 124.0, 117.6, 114.7, 110.8, 101.1, 80.9 (d, *J* = 9.9 Hz), 55.3, 52.9 (t, *J* = 5.7 Hz), 50.3 (d, *J* = 226.6 Hz), 25.5. HRMS (ESI) calcd. for $C_{20}H_{21}N_2NaO_5P$ $[M+Na]^+$: 423.1080, found: 423.1082; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 19.940 min, t_{minor} = 17.550 min).

Dimethyl (*S*)-(diazo(3-(4-methoxyphenyl)-1-methyl-1H-isochromen-1-yl)methyl)phosphonate (3f)

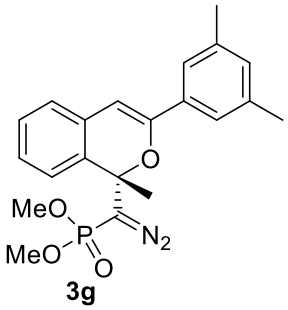


3f

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((4-methoxyphenyl)ethynyl)phenyl)ethan-1-one **1f** (60.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL)

at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3f** as a green solid 75.3 mg (94% yield, 92% *ee*), mp: 41.7–43.0 ℃; $[\alpha]_D^{25}$ = +84.6 °(*c* = 0.94, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.31–7.18 (m, 3H), 7.13 (d, *J* = 7.3 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 2H), 6.35 (s, 1H), 3.84 (s, 3H), 3.66 (dd, *J* = 15.1, 12.0 Hz, 6H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.4, 151.1, 131.4, 130.6 (d, *J* = 5.0 Hz), 129.0, 126.8, 126.7, 126.7, 124.4, 123.9, 113.8, 99.2, 80.7 (d, *J* = 9.9 Hz), 55.3, 52.9 (t, *J* = 4.7 Hz), 50.2 (d, *J* = 226.2 Hz), 25.4. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_5P$ $[M+Na]^+$: 423.1080,found: 423.1082; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 20.430 min, t_{minor} = 18.990 min).

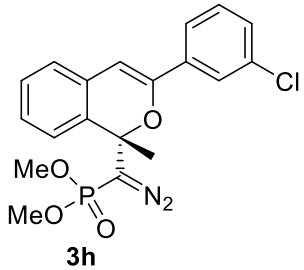
Dimethyl (*S*)-(diazo(3-(3,5-dimethylphenyl)-1-methyl-1H-isochro-men-1-yl)-methyl)phosphonate (3g)



3g

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((3,5-dimethylphenyl)ethynyl)phenyl)ethan-1-one **1g** (59.6 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3g** as a green oil, 78.9 mg (99% yield, 94% *ee*), mp: 92.9–95.9 ℃, $[\alpha]_D^{25}$ = +128.0 °(*c* = 0.75, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (s, 2H), 7.33–7.19 (m, 3H), 7.14 (d, *J* = 7.4 Hz, 1H), 6.99 (s, 1H), 6.42 (s, 1H), 3.67 (dd, *J* = 11.8, 6.3 Hz, 6H), 2.35 (s, 6H), 2.07 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.4, 137.8, 134.2, 131.3, 130.9 (d, *J* = 5.0 Hz), 130.7, 129.0, 127.0, 124.6, 124.0, 123.0, 100.6, 80.8 (d, *J* = 9.9 Hz), 52.9 (dd, *J* = 8.9, 5.6 Hz), 50.5 (d, *J* = 226.9 Hz), 25.4, 21.4. HRMS (ESI) calcd. for $C_{21}H_{23}N_2O_4P$ $[M+Na]^+$: 421.1288, found: 421.1292; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.204 min, t_{minor} = 12.844 min).

Dimethyl (*S*)-((3-(3-chlorophenyl)-1-methyl-1H-isochromen-1-yl)(diazo)methyl)phosphonate (3h)

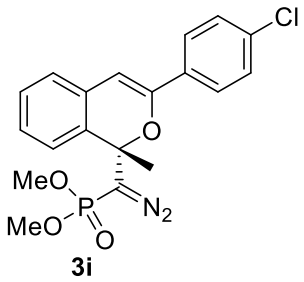


3h

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with1-(2-((3-chlorophenyl)ethynyl)phenyl)ethan-1-one **1h** (61.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3h** as a green solid, 76.1 mg (94% yield, 95% *ee*), mp: 83.0–83.7 ℃, $[\alpha]_D^{25}$ = +108.5 °(*c* = 0.95, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.65 (d, *J* = 4.0 Hz, 1H),

7.36–7.22 (m, 5H), 7.16 (d, *J* = 7.2 Hz, 1H), 6.46 (s, 1H), 3.68 (dd, *J* = 11.6, 8.6 Hz, 5H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 136.1, 134.5, 131.0 (d, *J* = 5.4 Hz), 130.6, 129.6, 129.1, 128.8, 127.6, 125.3, 125.0, 124.0, 123.1, 101.8, 81.1 (d, *J* = 9.7 Hz), 52.9 (dd, *J* = 12.4, 5.7 Hz), 50.4 (d, *J* = 227.1 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}ClN_2O_4P$ $[M+Na]^+$: 427.0585, found: 427.0586; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.648 min, t_{minor} = 14.237 min).

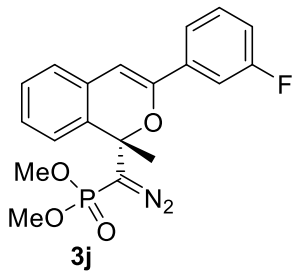
Dimethyl (*S*)-((3-(4-chlorophenyl)-1-methyl-1H-isochromen-1-yl)-(diazo)methyl) phosphonate (3i)



3i

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((4-chlorophenyl)ethynyl)phenyl)ethan-1-one **1i** (61.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3i** as a green solid 76.1 mg (94% yield, 89% *ee*), mp: 62.1–65.4 ℃, $[\alpha]_D^{25}$ = +91.9 °(*c* = 0.95, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.6 Hz, 2H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.33–7.23 (m, 3H), 7.16 (d, *J* = 7.2 Hz, 1H), 6.45 (s, 1H), 3.65 (dd, *J* = 16.2, 11.8 Hz, 6H), 2.10 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.1, 134.8, 132.7, 130.8, 130.8,129.1, 128.6, 127.4, 126.4, 124.8, 124.0, 101.2, 81.0 (d, *J* = 9.9 Hz), 52.9 (t, *J* = 6.1 Hz), 50.2 (d, *J* = 227.1 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}ClN_2O_4P$ $[M+Na]^+$: 427.0585, found: 427.0586; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.374 min, t_{minor} = 14.188 min).

Dimethyl (*S*)-(diazo(3-(3-fluorophenyl)-1-methyl-1H-isochromen-1-yl)-methyl)phosphonate (3j)

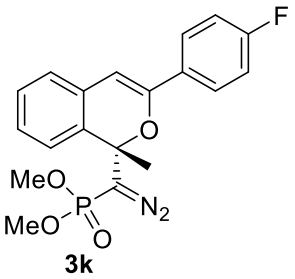


3j

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((3-fluorophenyl)ethynyl)phenyl)ethan-1-one **1j** (57.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3j** as a green oil, 37.2 mg (48% yield, 90% *ee*), mp: 63.4–64.7 ℃, $[\alpha]_D^{25}$ = +111.3 °(*c* = 0.74, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.0, 5.7 Hz, 2H), 7.26 (m, *J* = 14.8, 7.3 Hz, 3H), 7.13 (d, *J* = 7.3 Hz, 1H), 7.06 (t, *J* = 8.5 Hz, 2H), 6.38 (s, 1H), 3.64 (dd, *J* = 18.8, 11.7 Hz, 6H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.3 (d, *J* = 249.1 Hz), 150.3, 131.0, 130.7 (d, *J* = 5.3 Hz), 130.4 (d, *J* = 3.1 Hz), 129.1, 127.2, 127.1, 127.0, 124.7, 124.0, 115.4, 115.2, 100.6,

80.9 (d, J = 9.9 Hz), 52.9 (t, J = 5.8 Hz), 50.2 (d, J = 226.3 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}FN_2O_4P$ $[M+Na]^+$: 411.0880, found: 411.0880; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.596 min, t_{minor} = 14.047 min).

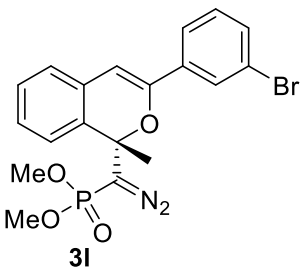
Dimethyl (*S*)-(diazo(3-(4-fluorophenyl)-1-methyl-1H-isochromen-1-yl)me-thyl)phosphonate (3k)



3k

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((4-fluorophenyl)ethynyl)phenyl)ethan-1-one **1k** (57.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3k** as a green solid 73.8 mg (95% yield, 90% *ee*), mp: 63.6–68.3 ℃, $[\alpha]_D^{25}$ = +96.1 °(*c* = 0.92, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, J = 7.8 Hz, 1H), 7.48 (d, J = 10.3 Hz, 1H), 7.38–7.23 (m, 4H), 7.17 (d, J = 7.3 Hz, 1H), 7.04 (td, J = 8.2, 2.1 Hz, 1H), 6.47 (s, 1H), 3.68 (dd, J = 11.7, 7.4 Hz, 6H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.0 (d, J = 245.2 Hz), 149.9 , 136.6 (d, J = 8.0 Hz), 131.0 (d, J = 5.2 Hz), 130.7, 129.8 (d, J = 8.2 Hz), 129.1, 127.6, 124.9, 124.0, 120.6 (d, J = 2.7 Hz), 115.7 (d, J = 21.4 Hz), 112.1 (d, J = 23.4 Hz), 101.8, 81.1 (d, J = 9.8 Hz), 52.9 (dd, J = 9.6, 5.7 Hz), 50.4 (d, J = 226.6 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}FN_2O_4P$ $[M+Na]^+$: 411.0880, found: 411.0882; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.233 min, t_{minor} = 14.083 min).

Dimethyl (*S*)-((3-(3-bromophenyl)-1-methyl-1H-isochromen-1-yl)(diazo)methyl) phosphonate (3l)

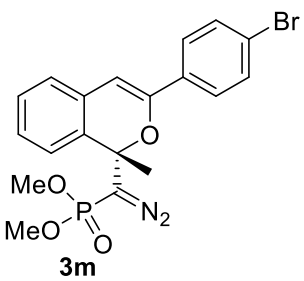


3l

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((3-bromophenyl)ethynyl)phenyl)ethan-1-one **1l** (71.8 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3l** as a white solid 55.7 mg (62% yield, 89% *ee*), mp: 80.3–83.0 ℃, $[\alpha]_D^{25}$ = +102.1 °(*c* = 0.70, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.70 (d, J = 6.5 Hz, 1H), 7.47 (d, J = 6.5 Hz, 1H), 7.29 (m, J = 15.7 Hz, 4H), 7.17 (d, J = 5.8 Hz, 1H), 6.46 (s, 1H), 3.69 (dd, J = 14.2, 5.0 Hz, 6H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.6, 136.3, 131.7, 131.0 (d, J = 5.4 Hz), 130.6, 129.8, 129.1, 128.2, 127.7, 125.0, 124.0, 123.6, 122.6, 101.8, 81.1 (d, J = 9.7 Hz), 53.0 (dd, J = 13.8, 5.6 Hz), 50.4 (d, J = 227.1 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}BrN_2O_4P$ $[M+Na]^+$:

471.0080, found: 471.0088; The *ee* was determined by a chiral phase Chiralpak ADH column (hexane/^{i}PrOH = 60/40, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 17.042 min, t_{minor} = 14.417 min).

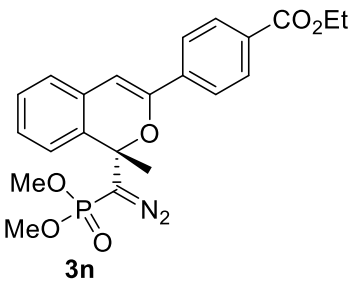
Dimethyl (*S*)-((3-(4-bromophenyl)-1-methyl-1H-isochromen-1-yl)(diazo)methyl) phosphonate (3m)



3m

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-((4-bromophenyl)ethynyl)phenyl)ethan-1-one **1m** (71.8 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3m** as a green solid 58.4 mg (65% yield, 90% *ee*), mp: 69.0–72.5 ℃, $[\alpha]_D^{25}$ = +78.8 °(*c* = 0.73, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.6 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.35–7.22 (m, 3H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.46 (s, 1H), 3.65 (dd, *J* = 15.2, 11.8 Hz, 6H), 2.10 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.2, 133.2, 131.5, 130.9 (d, *J* = 5.2 Hz), 130.8, 129.1, 127.5, 126.6, 124.8, 124.0, 123.0, 101.3, 81.0 (d, *J* = 9.9 Hz), 52.9 (t, *J* = 6.0 Hz), 50.2 (d, *J* = 226.1 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}BrN_2O_4P$ $[M+Na]^+$: 471.0080, found: 471.0083; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 14.756 min, t_{minor} = 16.015 min).

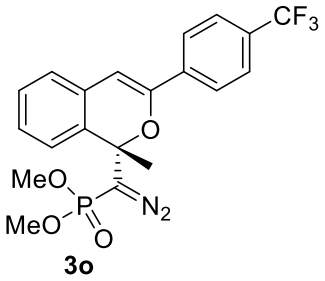
Ethyl (*S*)-3-(1-(diazo(dimethoxyphosphoryl)methyl)-1-methyl-1H-isochromen-3-yl)benzoate (3n)



3n

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with ethyl 4-((2-acetylphenyl)ethynyl)benzoate **1n** (70.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3n** as a green solid 29.2 mg (33% yield, 89% *ee*), mp: 77.3–80.3 ℃, $[\alpha]_D^{25}$ = +55.9 °(*c* = 0.58, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.34–7.27 (m, 3H), 7.19 (d, *J* = 7.2 Hz, 1H), 6.58 (s, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.65 (dd, *J* = 11.7, 8.8 Hz, 6H), 2.12 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.2, 150.1, 138.3, 131.1 (d, *J* = 5.3 Hz), 130.6 (d, *J* = 4.8 Hz), 129.6, 129.1, 127.8, 125.1, 124.8, 124.0, 102.8, 81.0 (d, *J* = 9.9 Hz), 61.0, 52.9 (dd, *J* = 9.2, 5.7 Hz), 50.3 (d, *J* = 226.5 Hz), 25.5, 14.3. HRMS (ESI) calcd. for $C_{22}H_{23}N_2O_6P$ $[M+Na]^+$: 465.1186, found: 465.1187; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 40.146 min, t_{minor} = 26.289 min).

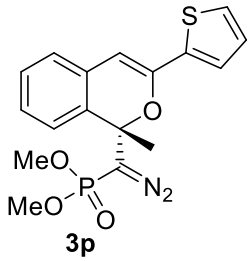
Dimethyl (*S*)-(diazo(1-methyl-3-(4-(trifluoromethyl)phenyl)-1H-isochromen-1-yl)methyl)phosphonate (3o)



3o

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with1-(2-((4-(trifluoromethyl)phenyl)ethynyl)phenyl)ethan-1-one **1o** (54.8 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3o** as a green oil, 42.1 mg (48% yield, 89% *ee*), $[\alpha]_D^{25}$ = +57.8 °(*c* = 0.69, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.35–7.27 (m, 3H), 7.19 (d, *J* = 7.2 Hz, 1H), 6.55 (s, 1H), 3.66 (dd, *J* = 16.7, 11.7 Hz, 6H), 2.12 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.7, 137.6, 131.1 (d, *J* = 5.2 Hz), 130.6 (q, *J* = 32.4 Hz), 130.5, 129.2, 127.9, 125.3 (dd, *J* = 7.6, 3.8 Hz), 125.2, 125.1, 124.1 (q, *J* = 272.0 Hz), 102.6, 81.1 (d, *J* = 9.9 Hz), 52.9 (dd, *J* = 7.9, 5.8 Hz), 50.4 (d, *J* = 226.9 Hz), 25.5. HRMS (ESI) calcd. for $C_{20}H_{18}F_3N_2O_4P$ $[M+Na]^+$: 461.0848, found: 461.0849; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 12.408 min, t_{minor} = 11.663 min).

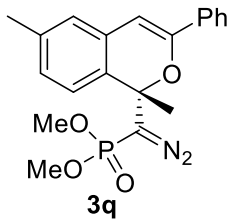
Dimethyl (*S*)-(diazo(1-methyl-3-(thiophen-2-yl)-1H-isochromen-1-yl)methyl) phosphonate (3p)



3p

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-(thiophen-2-ylethynyl)phenyl)ethan-1-one **1p** (54.3 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3p** as a green oil, 73.8 mg (98% yield, 84% *ee*), $[\alpha]_D^{25}$ = +98.3 °(*c* = 0.68, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.35–7.18 (m, 4H), 7.12 (d, *J* = 6.4 Hz, 1H), 7.05 (s, 1H), 6.32 (s, 1H), 3.70 (t, *J* = 12.8 Hz, 6H), 2.03 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 146.9, 138.5, 130.9 (d, *J* = 4.6 Hz), 130.8, 129.0, 127.6, 127.1, 126.0, 124.9, 124.5, 124.1, 100.1, 81.3 (d, *J* = 10.2 Hz), 53.0 (dd, *J* = 10.3, 5.5 Hz), 50.4 (d, *J* = 226.2 Hz), 25.4. HRMS (ESI) calcd. for $C_{17}H_{17}N_2O_4PS$ $[M+Na]^+$: 399.0539, found: 399.0538; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 21.099 min, t_{minor} = 16.699 min).

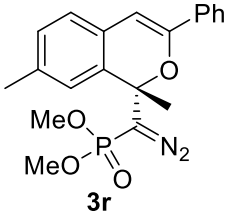
Dimethyl (*S*)-(diazo(1,6-dimethyl-3-phenyl-1H-isochromen-1-yl)methyl)phosphonate (3q)



3q

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(4-methyl-2-(phenylethynyl)phenyl)ethan-1-one **1q** (56.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3q** as a green solid, 70.0 mg (91% yield, 94% *ee*), mp: 80.0–80.5 ℃, $[\alpha]_D^{25}$ = +159.4 °(*c* = 0.88, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.41–7.30 (m, 3H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.97 (s, 1H), 6.41 (s, 1H), 3.66 (t, *J* = 11.5 Hz, 6H), 2.34 (s, 3H), 2.07 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.1, 138.8, 134.3, 131.0, 128.9, 128.3, 128.2 (d, *J* = 5.3 Hz), 127.9, 125.3, 125.1, 123.9, 100.82, 80.9 (d, *J* = 9.9 Hz), 52.9 (dd, *J* = 8.7, 5.6 Hz), 50.4 (d, *J* = 226.0 Hz), 25.6, 21.2. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_4P$ $[M+Na]^+$: 407.1131, found: 407.1136; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 18.883 min, t_{minor} = 15.028 min)

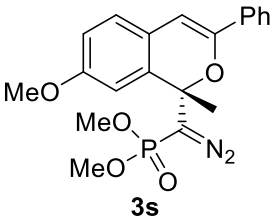
Dimethyl (*S*)-(diazo(1,7-dimethyl-3-phenyl-1H-isochromen-1-yl)methyl)phosphonate(3r)



3r

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(4-methyl-2-(phenylethynyl)phenyl)ethan-1-one **1r** 56.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3r** as a green solid, 74.6 mg (97% yield, 92% *ee*), mp: 104.7–105.8 ℃, $[\alpha]_D^{25}$ = +159.4 °(*c* = 0.93, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.13–7.03 (m, 3H), 6.44 (s, 1H), 3.66 (dd, *J* = 11.7, 8.9 Hz, 6H), 2.37 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.3, 137.1, 134.4, 131.0 (d, *J* = 5.2 Hz), 129.6, 128.7, 128.3, 128.3, 125.0, 124.7, 124.6, 100.8, 80.9 (d, *J* = 9.8 Hz), 52.9 (t, *J* = 5.7 Hz), 50.3 (d, *J* = 226.4 Hz), 25.5, 21.5. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_4P$ $[M+Na]^+$: 407.1131, found: 407.1136; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.760 min, t_{minor} = 14.809 min).

Dimethyl (*S*)-(diazo(7-methoxy-1-methyl-3-phenyl-1H-isochrom-en-1-yl)-methyl)phosphonate (3s)

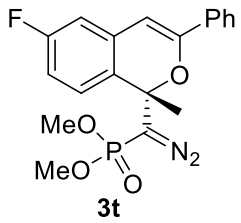


3s

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(5-methoxy-2-(phenylethynyl)phenyl)ethan-1-one **1s** (60.0 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5

mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3t** as a green solid, 74.6 mg (97% yield, 91% *ee*), mp: 112.3–113.7 ℃, $[\alpha]_D^{25}$ = +184.9 °(*c* = 0.93, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.4 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.92–6.81 (m, 2H), 6.43 (s, 1H), 3.83 (s, 3H), 3.66 (dd, *J* = 14.5, 11.8 Hz, 6H), 2.06 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.2, 149.1, 134.4, 132.6 (d, *J* = 5.2 Hz), 128.5, 128.3, 126.0, 124.8, 124.1, 113.9, 110.6, 100.6, 80.7 (d, *J* = 10.1 Hz), 55.5, 52.9 (dd, *J* = 7.5, 5.7 Hz), 50.1 (d, *J* = 226.6 Hz), 25.4. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_5P$ $[M+Na]^+$: 423.1080, found: 423.1803; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 21.955 min, t_{minor} = 17.748 min).

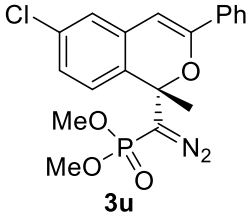
Dimethyl (*S*)-(diazo(6-fluoro-1-methyl-3-phenyl-1H-isochromen-1-yl)-methyl) phosphonate (3t)



3t

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(4-fluoro-2-(phenylethynyl)phenyl)ethan-1-one **1t** (57.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3t** as a green oil, 75.3 mg (97% yield, 93% *ee*), $[\alpha]_D^{25}$ = +137.6 °(*c* = 0.72, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.2 Hz, 2H), 7.45–7.30 (m, 3H), 7.25 (dd, *J* = 8.5, 5.4 Hz, 1H), 6.92 (td, *J* = 8.5, 2.4 Hz, 1H), 6.85 (dd, *J* = 9.1, 2.3 Hz, 1H), 6.41 (s, 1H), 3.65 (t, *J* = 12.2 Hz, 6H), 2.08 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.1 (d, *J* = 246.9 Hz), 152.3, 133.8, 133.5 (d, *J* = 9.1 Hz), 129.4, 128.4, 126.6 (dd, *J* = 4.7, 2.9 Hz), 126.0 (d, *J* = 8.9 Hz), 125.3, 113.6 (d, *J* = 22.2 Hz), 111.0 (d, *J* = 22.6 Hz), 100.1 (d, *J* = 2.1 Hz), 80.8 (d, *J* = 10.1 Hz), 53.7-52.3 (m), 50.5 (d, *J* = 227.1 Hz), 25.6. HRMS (ESI) calcd. for $C_{19}H_{18}FN_2O_4P$ $[M+Na]^+$: 411.0880, found: 411.0880; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.804 min, t_{minor} = 13.922 min).

Dimethyl (*S*)-((6-chloro-1-methyl-3-phenyl-1H-isochromen-1-yl)(diazo)-methyl) phosphornate (3u)

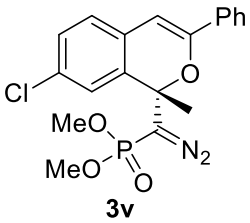


3u

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(4-chloro-2-(phenylethynyl)phenyl)ethan-1-one **1u** (61.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3u** as a green oil, 74.5 mg (92% yield, 85% *ee*), $[\alpha]_D^{25}$ = +126.8 °(*c* = 0.93, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.2 Hz,

2H), 7.45–7.34 (m, 3H), 7.24–7.17 (m, 2H), 7.14 (d, *J* = 0.5 Hz, 1H), 6.39 (s, 1H), 3.66 (dd, *J* = 12.9, 12.0 Hz, 6H), 2.06 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.4, 134.9, 133.7, 133.0, 129.4, 129.2 (d, *J* = 4.9 Hz), 128.4, 126.8, 125.6, 125.2, 124.3, 99.7, 80.8 (d, *J* = 10.1 Hz), 53.0 (t, *J* = 5.2 Hz), 50.4 (d, *J* = 227.2 Hz), 25.5. HRMS (ESI) calcd. for $C_{19}H_{18}ClN_2O_4P$ $[M+Na]^+$: 427.0585, found: 427.0585; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 16.596 min, t_{minor} = 14.047 min).

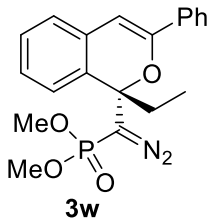
Dimethyl (*S*)-((7-chloro-1-methyl-3-phenyl-1H-isochromen-1-yl)(diazo)methyl)phosphonate (3v)



3v

Following the general procedure, treatment of dimethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(5-chloro-2-(phenylethynyl)phenyl)ethan-1-one **1v** (61.1 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3v** as a green solid, 17 mg (21% yield, 84% *ee*), mp: 113.1–114.3 ℃, $[\alpha]_D^{25}$ = +65.8 °(*c* = 0.93, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.2 Hz, 2H), 7.43–7.33 (m, 3H), 7.31–7.20 (m, 2H), 7.09 (d, *J* = 8.6 Hz, 1H), 6.43 (s, 1H), 3.67 (dd, *J* = 25.3, 11.7 Hz, 6H), 2.06 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.5, 133.9, 132.4 (d, *J* = 4.9 Hz), 132.3, 129.8, 129.3, 129.1, 128.4, 125.8, 125.2, 124.5, 99.9, 80.6 (d, *J* = 10.1 Hz), 53.0 (dd, *J* = 5.3, 4.4 Hz), 50.3 (d, *J* = 227.5 Hz), 25.4. HRMS (ESI) calcd. for $C_{19}H_{18}ClN_2O_4P$ $[M+Na]^+$: 427.0585, found: 427.0580; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 15.681 min, t_{minor} = 14.07 5 min).

Dimethyl (*S*)-(diazo(1-ethyl-3-phenyl-1H-isochromen-1-yl)methyl)phosphonate (3w)

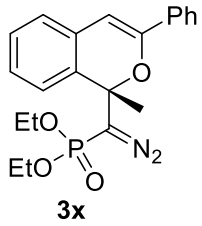


3w

Following the general procedure, treatment of diethyl (diazomethyl)phosphonate **2a** (30.0 mg, 0.2 mmol) with 1-(2-(phenylethynyl)phenyl)propan-1-one **1w** (56.2 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3w** as a green oil, 36.1 mg (47% yield, 93% *ee*); $[\alpha]_D^{25}$ = +89.3 °(*c* = 0.72, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.31–7.27 (m, 1H), 7.25–7.20 (m, 2H), 7.15 (d, *J* = 7.5 Hz, 1H), 6.43 (s, 1H), 3.58 (dd, *J* = 11.8, 6.0 Hz, 6H), 2.68 (dd, *J* = 14.6, 7.3 Hz, 1H), 2.44 (dd, *J* = 14.5, 7.3 Hz, 1H), 1.06 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.1, 134.1, 131.9, 128.9, 128.9, 128.3, 128.2 (d, *J* = 4.2 Hz), 126.8, 125.0, 124.8, 124.8, 100.0 (d, *J* = 10.9 Hz), 83.4 (d, *J* = 10.1 Hz), 52.9 (t, *J* = 5.6 Hz), 50.5 (d, *J* = 224.5 Hz),

31.25, 9.05. HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_4P$ $[M+Na]^+$: 407.1131, found: 407.1132; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 17.262 min, t_{minor} = 13.830 min).

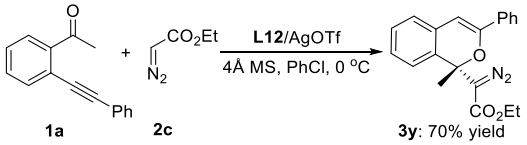
Diethyl (*S*)-(diazo(1-methyl-3-phenyl-1H-isochromen-1-yl)methyl)phosphonate (3x)



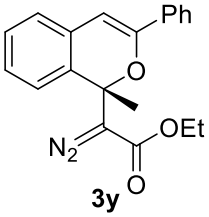
3x

Following the general procedure, treatment of diethyl (diazomethyl)phosphonate **2b** (35.6 mg, 0.2 mmol) with 1-(2-(phenylethynyl)phenyl)ethan-1-one **1a** (52.9 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3x** as a green solid, 62.9 mg (79% yield, 90% *ee*), mp: 80.9–82.0 ℃, $[\alpha]_D^{25}$ = +121.7 ° (*c* = 0.79, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90–7.68 (m, 2H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.36–7.32 (m, 1H), 7.32–7.27 (m, 2H), 7.27–7.22 (m, 1H), 7.17–7.13 (m, 1H), 6.45 (s, 1H), 4.13–3.96 (m, 4H), 2.10 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H), 1.22 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.2, 134.3, 131.1, 129.0 (s), 128.9, 128.5 (d, *J* = 12.1 Hz), 128.3, 127.2, 125.2, 124.7, 124.1, 100.8, 81.1 (d, *J* = 10.0 Hz), 62.6 (dd, *J* = 5.6, 3.0 Hz), 51.1 (d, *J* = 225.2 Hz), 25.5, 16.1 (dd, *J* = 14.0, 7.1 Hz). HRMS (ESI) calcd. for $C_{21}H_{23}N_2O_4P$ $[M+Na]^+$: 421.1288, found: 421.1288; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 13.715 min, t_{minor} = 11.930 min).

Employing diazoacetate as nucleophile



Ethyl (*S*)-2-diazo-2-(1-methyl-3-phenyl-1H-isochromen-1-yl) acetate (3y)

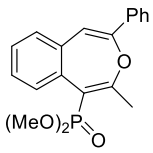


3y

Following the general procedure, treatment of ethyl 2-diazoacetate **2c** (22.8 mg, 0.2 mmol) with 1-(2-(phenylethynyl)phenyl)ethan-1-one **1a** (52.9 mg, 0.24 mmol) in the presence of catalyst **L12** (6 mol %)/AgOTf (5 mol %) and 4 Å MS (100 mg) in PhCl (1 mL) at 0 ℃ for 48 h, followed by column chromatography (PE/EA = 6/1 to 4/1) to afford **3y** as a green oil, 46.8 mg (70% yield, 93% *ee*), $[\alpha]_D^{25}$ = +230.5 ° (*c* = 0.94, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.29 (dd, *J* = 14.0, 6.5 Hz, 2H), 7.25–7.21 (m, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 6.45 (s, 1H), 4.44–3.93 (m, 2H), 2.27 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.7, 151.7, 134.4, 131.2, 131.1, 129.0, 129.0, 128.4, 127.2, 125.6, 124.8, 123.9, 101.0, 79.3, 63.7, 60.6, 24.7, 14.4. HRMS (ESI) calcd. for $C_{20}H_{18}N_2O_3$ $[M+Na]^+$: 357.1210, found: 357.1211; The *ee* was

determined by a chiral phase Chiralpak ASH column (hexane/^{i}PrOH = 90/10, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 9.413 min, t_{minor} = 8.914 min).

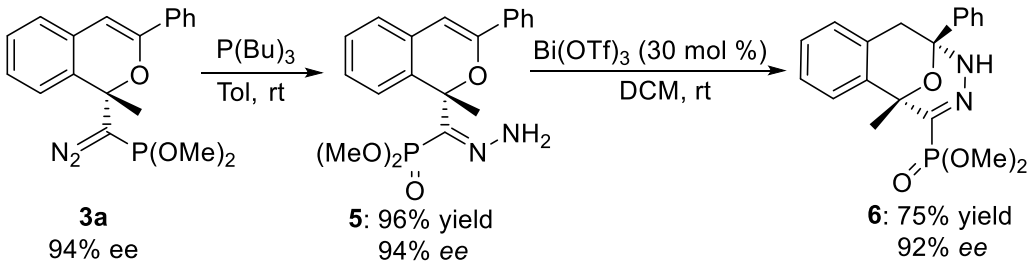
Dimethyl (2-methyl-4-phenylbenzo[*d*]oxepin-1-yl)phosphonate (4a)



4a

White oil, ^{1}H NMR (600 MHz, Acetone) δ 7.70 (m, 2H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.31 (m, 2H), 7.24 (m, 2H), 7.16–7.08 (m, 2H), 6.98 (s, 1H), 3.46 (d, *J* = 11.3 Hz, 6H), 2.34 (d, *J* = 2.6 Hz, 3H). ^{13}C NMR (151 MHz, Acetone) δ 172.5 (d, *J* = 27.9 Hz), 157.5, 135.8 (d, *J* = 9.8 Hz), 134.7, 134.7 (d, *J* = 7.4 Hz), 129.5 (d, *J* = 3.0 Hz), 128.9, 128.8, 128.6, 126.7, 125.9, 124.9, 115.0 (d, *J* = 179.7 Hz), 114.1 (d, *J* = 0.8 Hz), 51.5 (d, *J* = 5.6 Hz), 21.3. HRMS (ESI) calcd. for $C_{19}H_{20}O_4P$ $[M+H]^+$: 343.1094, found: 343.1089.

5. General procedure for the synthesis of the phosphine-containing tricycle compound 6 and isochromatic compound 9



3a
94% ee

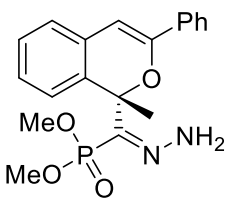
5: 96% yield
94% *ee*

6: 75% yield
92% *ee*

Tributylphosphine (0.3 mmol, 60.7 mg) were added to the solution of **3a** (0.2 mmol, 74.1 mg) in Tol at rt under nitrogen atmosphere. The reaction mixture was stirred for 3 h, diluted with ethyl acetate and washed with saturated $NaHCO_3$ solution and brine. The organic phase was dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by flash chromatography using (PE / EA = 3 / 1) to give **5** as white solid (71.5 mg, 96% yield, 93% *ee*).[9]

$Bi(OTf)_3$ (3.9 mg, 0.3 equiv.) was added to a solution of **5** (74.4 mg, 0.2 mmol) in dry CH_2Cl_2 and stirred at rt. After the reaction was completion monitored by TLC, quenched with saturated $NaHCO_3$ and extracted with dichloromethane (3 × 30 mL). Combined the organic layer and dried over Na_2SO_4, concentrated under reduce pressure and purified by column chromatography (PE/EA = 3/1 to 1/1) to give **6** (55.8 mg, 75% yield, 92% *ee*).[10]

Dimethyl (*S*, *E*)-(hydrazono(1-methyl-3-phenyl-1H-isochromen-1-yl)methyl) phosphonate (5)

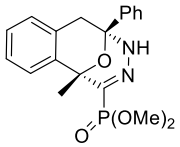


5

The compound **5** was a colorless solid, $[\alpha]_D^{25}$ = 61.7 °(*c* = 0.34, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.3 Hz, 2H), 7.71 (s, 2H), 7.38

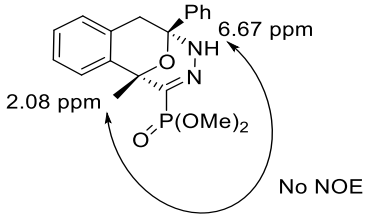
(t, J = 7.4 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.19 (td, J = 7.4, 1.0 Hz, 1H), 7.13 (td, J = 7.5, 1.0 Hz, 1H), 7.07 (d, J = 7.4 Hz, 1H), 6.99 (d, J = 7.5 Hz, 1H), 6.34 (s, 1H), 3.68 (d, J = 11.8 Hz, 3H), 3.14 (d, J = 11.2 Hz, 3H), 1.73 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.0, 135.2 (d, J = 151.3 Hz), 134.9, 133.8, 129.9, 128.6, 128.3, 127.9, 126.5, 124.8, 124.3, 124.0, 98.9, 84.2 (d, J = 20.5 Hz), 52.6 (dd, J = 22.3, 5.8 Hz), 25.8 (d, J = 3.6 Hz). HRMS (ESI) calcd. for $C_{19}H_{21}N_2NaO_4P$ $[M+Na]^+$: 395.1131, found: 395.1125; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 19.949 min, t_{minor} = 18.462 min).

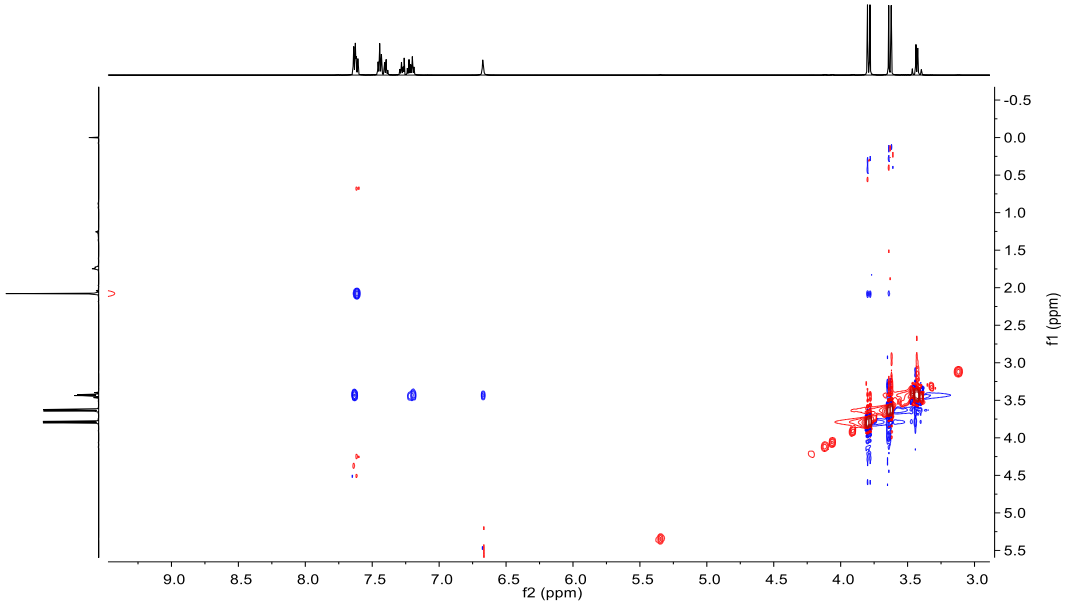
(1-methyl-5-phenyl-1,4,5,6-tetrahydro-1,5-epoxybenzo[e][1,2]diazocin-2-yl)phosphonate (6)

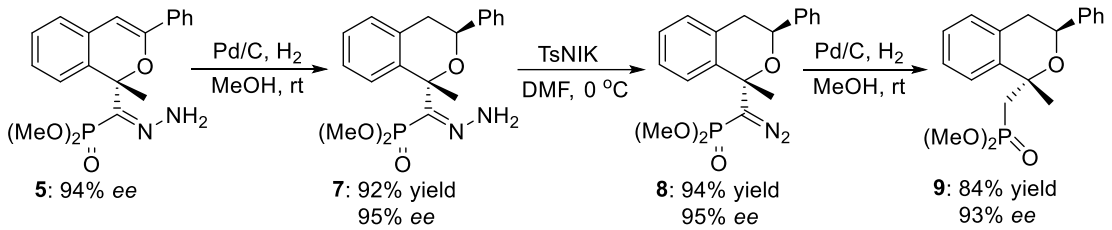


6

The compound **6** was a colorless oil, $[\alpha]_D^{25}$ = 68.6 °(*c* = 1.5, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67–7.58 (m, 3H), 7.44 (t, J = 7.5 Hz, 2H), 7.42–7.37 (m, 1H), 7.28 (t, J = 7.4 Hz, 1H), 7.22 (ddd, J = 21.4, 10.8, 4.1 Hz, 2H), 6.67 (s, 1H), 3.79 (d, J = 11.2 Hz, 3H), 3.63 (d, J = 11.1 Hz, 3H), 3.51–3.31 (m, 2H), 2.08 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.0, 137.0 (d, J = 228.4 Hz), 135.6, 131.1, 129.0, 129.0, 128.8, 127.1, 127.0, 125.7, 124.0, 85.1, 73.1 (d, J = 29.5 Hz), 53.1 (dd, J = 12.0, 6.1 Hz), 41.2, 23.3. HRMS (ESI) calcd. for $C_{19}H_{21}N_2O_4P$ $[M+Na]^+$: 395.1131, found: 395.1138; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 70/30, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 23.237 min, t_{minor} = 18.874 min).





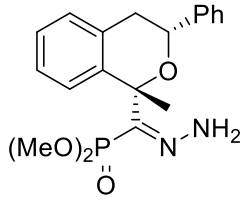


To a solution of **5** (0.2 mmol, 74.5 mg) in MeOH (5.0 mL) was added 10% Pd/C. Hydrogenation under 1 atm of H_2 (balloon) until the reaction completed, filtrated and the solution was concentrated under reduce pressure and the residue was purified by flash chromatography using (PE / EA = 3 / 1) to give **7** as white solid (68.9 mg, 92% yield, 95% *ee*, >20:1 *dr*)

Potassium *N*-iodo *p*-toluenesulfonamide (40.3 mg, 0.12 mmol) was added to the solution of **7** (37.4 mg, 0.1 mmol) in THF (1 mL), then aqueous potassium hydroxide was added slowly (the final volume ratio KOH (1 M)/THF was 1:4). The reaction was complete after stirring for 1 h at room temperature and the mixture was poured into aqueous potassium hydroxide (1M, 5 mL) and extracted with ether (30 mL). The organic layer was washed with aqueous potassium hydroxide (1M, 5 mL), saturated brine (5 mL) and dried over Na_2SO_4. Concentrated under reduce pressure and the residue was purified by flash chromatography (PE / EA = 3 / 1) to give **8** as green oil (35.0 mg, 94% yield, 95% *ee*, >20:1 *dr*).[11]

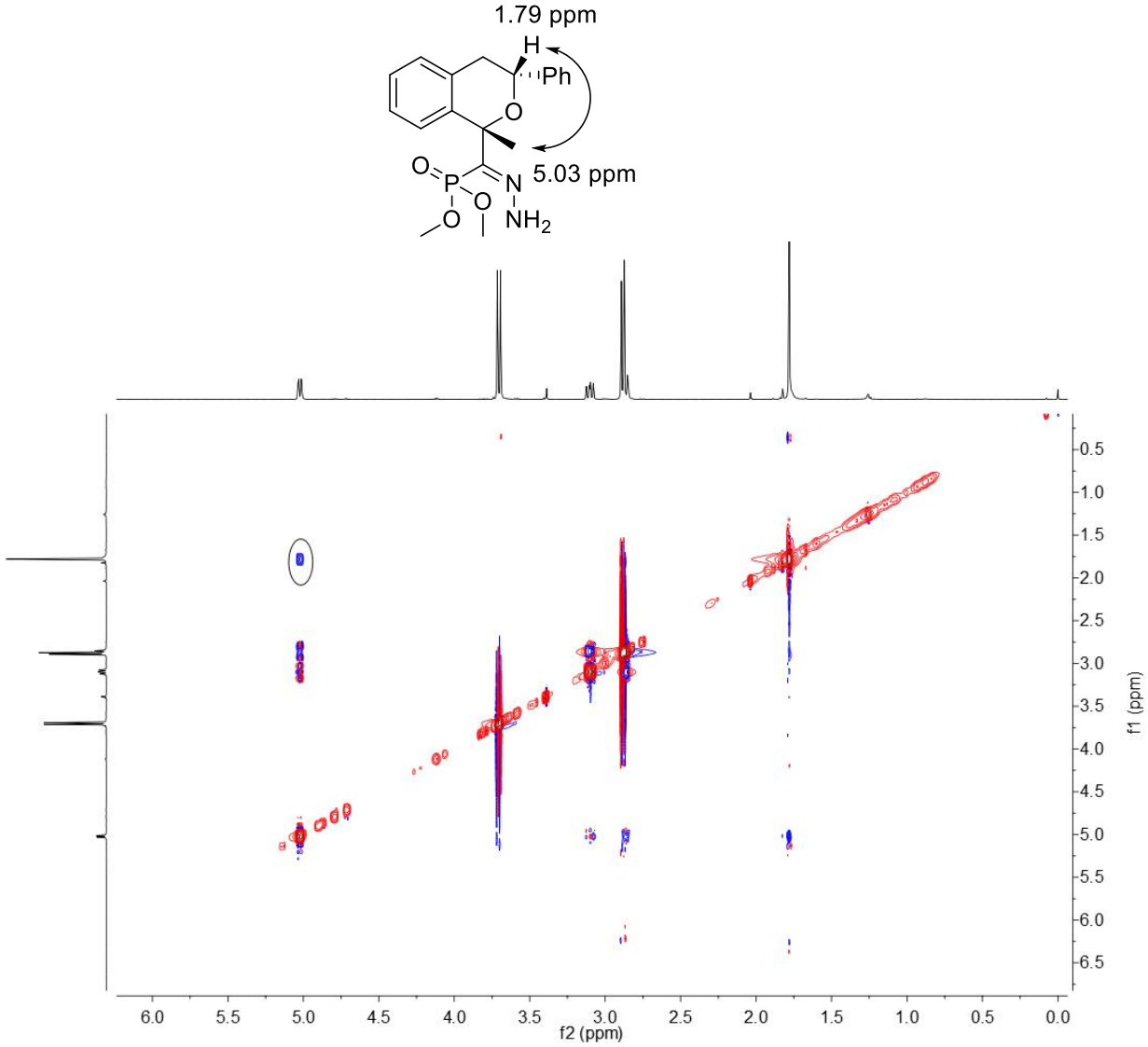
10% Pd/C was added to the solution of **8** (37.2 mg, 0.1 mmol) in MeOH (2.0 mL), hydrogenation under 1 atm of H_2 (balloon) with ice baths. After the reaction completed, filtrated through a plug of celite, then the filtrate was concentrated under vacuum, the residue was purified by flash chromatography using (PE / EA = 3 / 1 to 2 / 1) to give **9** as white oil (29.1mg, 84% yield, 93% *ee*, >20:1 *dr*). [12]

Dimethyl (I-hydrazono((1*S*, 3*S*)-1-methyl-3-phenylisochroman-1-yl)methyl)phosphonate (7)

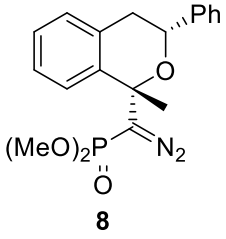


7

The compound **7** was a colorless solid, mp: 131–134 ℃, $[\alpha]_D^{25}$ = 54.1 ° (*c* = 0.48, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 2H), 7.52 (d, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 7.21–7.09 (m, 4H), 5.03 (dd, *J* = 11.4, 2.5 Hz, 1H), 3.71 (d, *J* = 12.2 Hz, 3H), 3.11 (dd, *J* = 15.7, 11.5 Hz, 1H), 2.93–2.84 (m, 4H), 1.79 (s, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.7, 139.6, 135.8 (d, *J* = 146.4 Hz), 134.0, 128.5, 128.4, 127.5, 126.6, 126.4, 126.3, 126.3, 81.8 (d, *J* = 20.4 Hz), 71.6, 51.8 (dd, *J* = 24.4, 4.5 Hz), 36.8, 26.8 (d, *J* = 4.0 Hz). HRMS (ESI) calcd. for $C_{19}H_{23}O_4P$ $[M+Na]^+$: 397.1288, found: 397.1283; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 90/10, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 45.053 min, t_{minor} = 52.327 min).



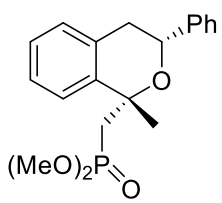
Dimethyl (diazo (1*S*, 3*S*)-1-methyl-3-phenylisochroman-1-yl)methyl)phosphonate (8)



8

The compound **8** was green oil; $[\alpha]_D^{25}$ = 58.2 ° (*c* = 1.7, EA); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.4 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.36–7.30 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 4.91 (dd, *J* = 11.2, 1.8 Hz, 1H), 3.70 (dd, *J* = 120.2, 11.9 Hz, 6H), 3.05 (dd, *J* = 15.8, 11.5 Hz, 1H), 2.89 (dd, *J* = 15.9, 2.0 Hz, 1H), 1.85 (s, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.9, 139.2 (d, *J* = 3.5 Hz), 134.2, 128.7, 128.4, 127.7, 127.4, 127.0, 126.5, 126.0, 79.1 (d, *J* = 8.9 Hz), 72.3, 53.2 (d, *J* = 229.7 Hz), 52.9 (dd, *J* = 14.3, 5.1 Hz), 36.7, 26.3 (d, *J* = 2.6 Hz). HRMS (ESI) calcd. for $C_{19}H_{22}N_2O_4P$ $[M+H]^+$: 373.1312, found: 373.1307; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 90/10, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 55.136 min, t_{minor} = 45.397 min).

Dimethyl (((1*S*)-1-methyl-3-phenylisochroman-1-yl)methyl)phosphonate (9)

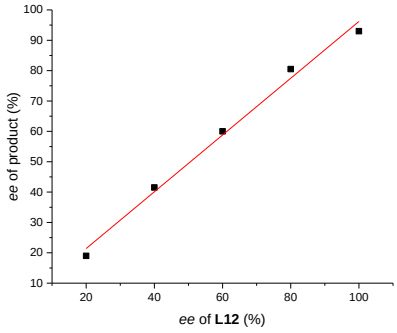


9

The compound **9** was a colorless oil, $[\alpha]_D^{25}$ = 42.3 ° (*c* = 0.52, EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.13 (dd, *J* = 17.1, 7.6 Hz, 2H), 4.86 (dd, *J* = 11.3, 2.0 Hz, 1H), 3.53 (d, *J* = 11.0 Hz, 2H), 3.46 (d, *J* = 10.9 Hz, 2H), 3.13 (dd, *J* = 15.6, 11.4 Hz, 1H), 2.88 (dd, *J* = 15.8, 2.2 Hz, 1H), 2.57 (ddd, *J* = 50.4, 17.9, 15.6 Hz, 2H), 1.75 (d, *J* = 1.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.4, 140.8 (d, *J* = 7.7 Hz), 133.8, 128.8, 128.3, 127.5, 126.6, 126.5, 126.3, 125.4, 76.3 (d, *J* = 6.3 Hz), 71.4, 52.0 (dd, *J* = 50.0, 6.4 Hz), 40.4 (d, *J* = 140.5 Hz), 37.2, 29.0 (d, *J* = 11.9 Hz). HRMS (ESI) calcd. for $C_{19}H_{23}O_4P$ $[M+Na]^+$: 369.1226, found: 369.1235; The *ee* was determined by a chiral phase Chiralpak IC column (hexane/^{i}PrOH = 80/20, flow rate 0.5 mL/min, λ = 254 nm, t_{major} = 37.082 min, t_{minor} = 28.250 min).

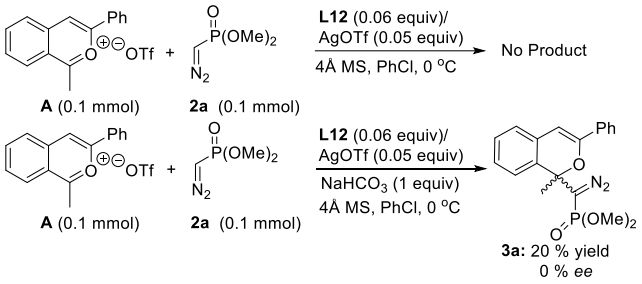
6. Nonlinear effects were investigated

To gain insight into the mechanism and the origin of enantioselectivity of this asymmetric cyclization/nucleophile tandem reaction, nonlinear effects were studied.[13] The enantiomeric excess of the product was not in a linear correlation with the *ee* value of the chiral bis(oxazoline) **L12**, which suggests that **L12** coordinated with the AgOTf to form the active monoligated complex (Figure 1). A HRMS spectrum of a mixture of **L12** and Ag^+ (1/1) confirmed the coordination of the chiral bis(oxazoline) to the Ag^+, peaks were observed at m/z 803.3336.



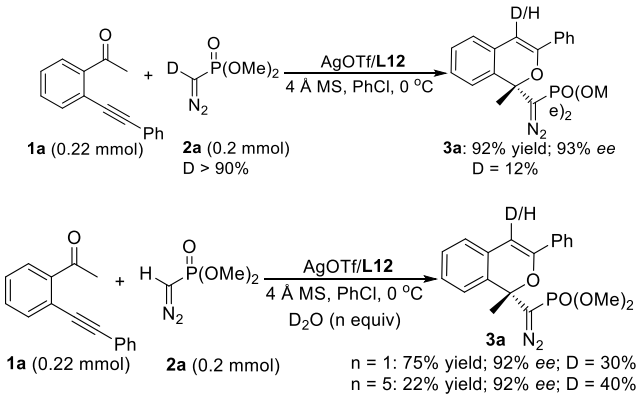
Plot of ee (%) of 3a vs. ee (%) of L12

7. Isochromenylium triflate as start material



Control experiments were conducted in conditions otherwise identical to the established optimal conditions. The starting *o*-(alkynyl) aryl ketone (**1a**) was replaced with a preformed isochromenylium triflate (**A**) in which the 4-position was protonated. In this case, no product was observed (Scheme 5). If 1 equiv. of $NaHCO_3$ was added, the reaction took place and afforded a racemic product in low yield (20%). Comparison of this result with that of the model reaction demonstrated that the coordinated central metal Ag (I) attachment to the 4-position of the isochromenylium ion is vital to achieving efficient stereocontrol.

8. Deuterium labeling study

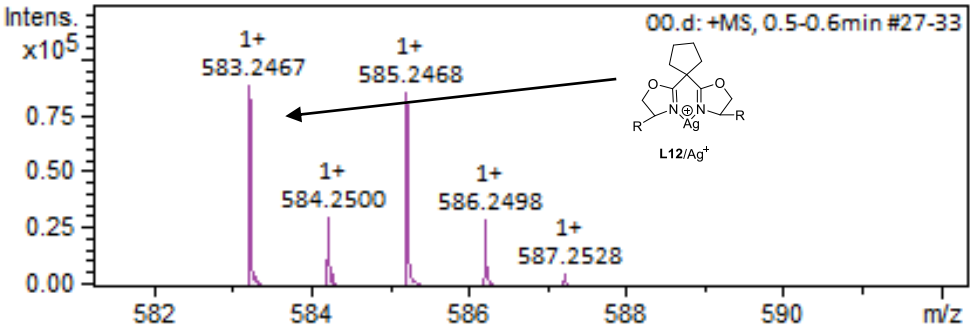


A deuterium labeling experiment was performed by employing α-deuterium substituted diazomethylphosphonate as the nucleophile resulting in 12% deuterium incorporation at the C4 position of the product. This result demonstrated that the proton at the C4 position could come from the α-proton of diazomethylphosphonate (Scheme 6). Furthermore, the model reaction was conducted in the presence of 1 equiv. of deuterium oxide and the reaction proceeded well and gave the product (75% yield, 92% *ee*) with 30% deuterium at the C4 position. When the deuterium oxide was increased to 5 equiv., the yield decreased dramatically with the same enantioselectivity, and the deuterium incorporation up to 40% at the C4 position. These results suggest that the proton at the C4 position of the product could either be derived from residual water present in the reaction system or the

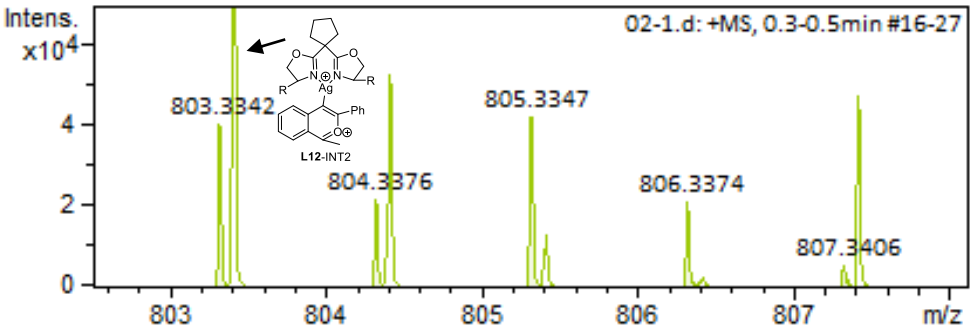
diazomethylphosphonate.

9. ESI-MS determination of L12/Ag^+, L12-INT2 and L12-INT3

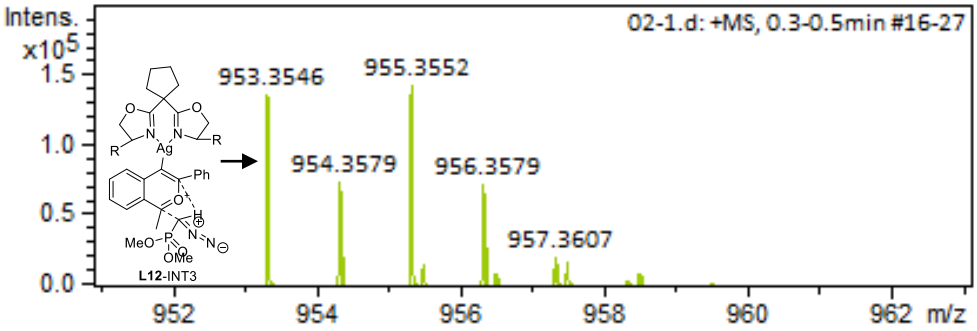
The mixture of **L12** (0.5 mmol) and AgOTf (0.5 mmol) in anhydrous PhCl (10 mL) was stirred at rt for 3h in a dried Schlenk tube, then **1a** (0.5 mmol) and 500 mg 4 Å MS were added. Cooled the resulted mixture to 0 ℃, **2a** (0.5 mmol) was added and the reaction was subjected to analysis by ESI-MS every hour.



$C_{31}H_{44}AgN_2O_2$ calculated as 584.2521, was found to be 584.2500.



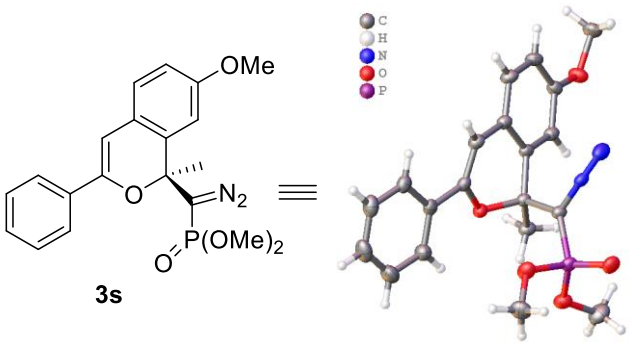
$C_{47}H_{56}AgN_2O_3$ calculated as 803.3342, was found to be 803.3342.



$C_{50}H_{63}AgN_4O_6P$ calculated as 953.3531, was found to be 953.3546.

10. X-ray crystal structure of 3s

Recrystallization of the product **3s** from EA/PE afforded crystals suitable for diffraction analysis. The absolute configuration **3s** was determined to be *S* by X–ray diffraction analysis and thus, the absolute configuration of others were deduced.



3s

Crystal data and structure refinement for **pyg0329**	
Identification code	pyg0329
Empirical formula	$C_{20}H_{21}N_2O_5P$
Formula weight	400.36
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.84956(6)
b/Å	10.90982(6)
c/Å	18.14926(11)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1950.26(2)
Z	4
ρ_{calc}g/cm^3	1.364
μ/mm^{-1}	1.550
F(000)	840.0
Crystal size/mm^3	0.2 ×0.2 ×0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.458 to 145.826
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -21 ≤ l ≤ 22
Reflections collected	28560
Independent reflections	3868 [R_{int}= 0.0282, R_{sigma}= 0.0160]
Data/restraints/parameters	3868/0/257
Goodness-of-fit on F^2	0.914
Final R indexes [I>=2σ (I)]	R_1 = 0.0274, wR_2 = 0.0783

Final R indexes [all data]	R_1 = 0.0276, wR_2 = 0.0786
Largest diff. peak/hole / e Å^{-3}	0.27/-0.29
Flack parameter	-0.001(5)

11. DFT computational calculation studies

1. The possible pathway

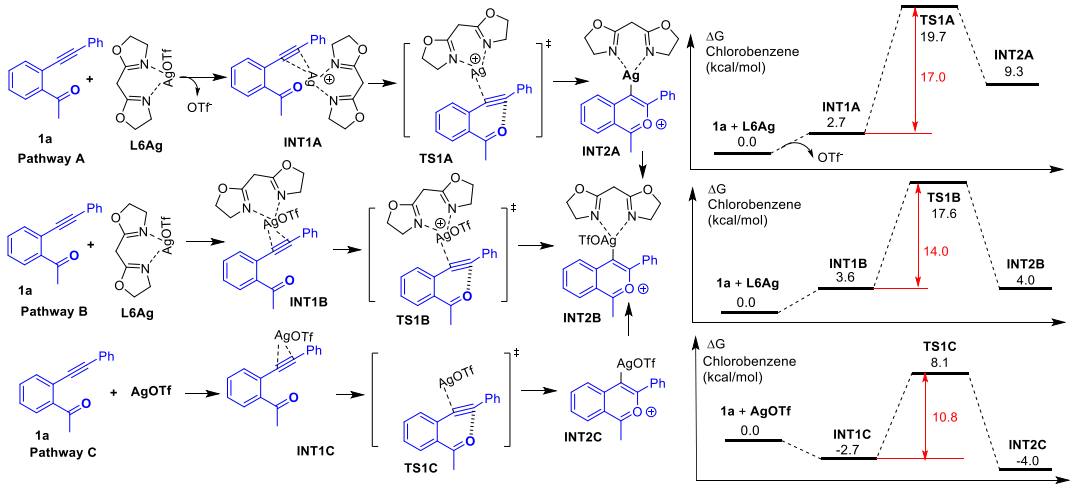


Figure 1. Computed potential energy surface of possible cyclization reactions.

According to the experimental results, a potential pathway involving the formation of complexes of Ag and ligand (**L6**) was proposed and rationalized by DFT calculated. These geometries of intermediates were optimized using M06-2x functional together with the standard 6-31G(d) basis set, and the energy was calculated at 6-31++G(d,p) level (chlorobenzene as solvent).

The reaction process could be divided into three steps, as cyclization, proton exchange, and **2a** addition. As the pre-reaction of **AgOTf** and **L6** at 25 ℃ is important for the stereoselectivity, it was necessary for the formation of **L6Ag**, which would attack the alkyne to promote the cyclization reaction via **TS1** to form **INT2**. There possible cyclization reactions pathways (**pathway A**, **B**, and **C**) were proposed and the energies were calculated as figure 1. The energy barrier of **TS1C** in **pathway C** is lowest among **TS1A**, **TS1B**, and **TS1C** with value of 10.8 kcal/mol. **INT2C** and also could transfer to **INT2A** or **INTB** by ligand exchange, suggesting the cyclization directly catalyzed by **AgOTf** should be theoretically favorable. However, due to a necessary re-reaction of **AgOTf** and **L6** in actual operation, the Ag salt should present as coordination compound **L6Ag** rather than **AgOTf** and the former should have much higher concentration in chlorobenzene due to its better solubility. Therefore, the actual reaction has less possibility to conduct as **pathway A** and **pathway B**. Although the energy barrier of **TS1A** with value of 17.0 kcal/mol is reasonable for this reaction, the OTf anion may promote the cyclization as **pathway C**, in which the energy barrier of **TS1C** was

3.0 kcal/mol lower than **TS1**. The results suggested that the different Ag salts may affect the reaction rate, which was consistent with experimental results of Ag salts (Table 1, entries 13, 19-22) of the main manuscript.

After the cyclization, the **INT2A** as cation or **INT2B** as salt may conduct the following reactions as **Pathway A** and **Pathway B** in figure 2. In the pathway A, after producing the complex of **INT2A** and **2a**, the hydrogen of **2a**, as an acid, would react with Lewis base **INT2A** to form **INT3A** with energy barrier of **TS2A** with value of 18.1 kcal/mol. The **INT4** as complex of **L6Ag** and final product **3a** would be easily produced through a low energy barrier (**TS3A**) with value of 1.3 kcal/mol.

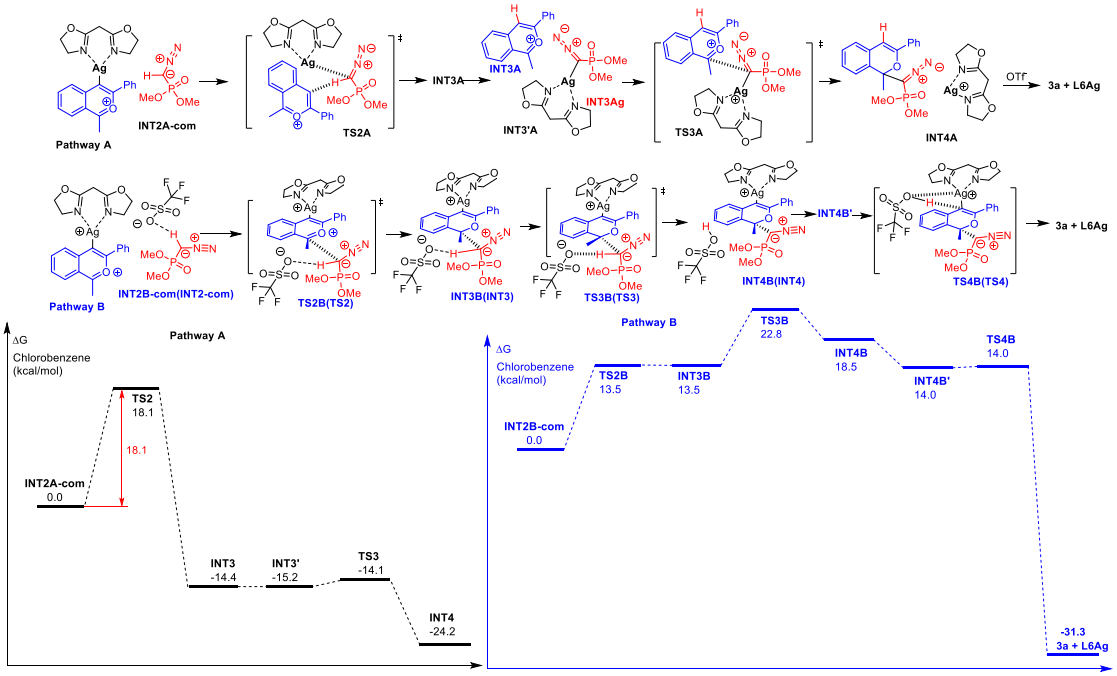


Figure 2. Computed potential energy surface of the reaction.

As a Lewis base, **INT2A** may react with **2a** to form **INT3A** as figure 2. However, the possibility for **INT2A** attacking to **2a** can't be simply excluded. The calculation results showed that the energy barriers, with value of 31.7 kcal/mol for **TS2C** and 21.1 kcal/mol for **TS3C**, were too high to conduct, suggesting this pathway by directly **2a** attacking was unfavorable.

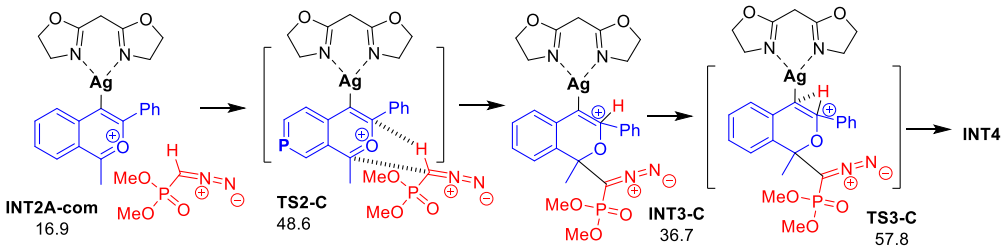


Figure 3. The possibility for **INT2** attacking to **2a** directly.

For the third step, the energy barrier of **TS3A** is very low with value of 1.4 kcal/mol. The

formation of the **INT3Ag** would be important to promote this reaction. Besides the reaction with **INT2A**, other condition also may produce the **INT3Ag** as shown in figure 4. In the **pathway D**, **L6Ag** reacted with **2a** and the energy barrier of **TS2D** was 23.5 kcal/mol, which was higher than that of T**S2**. On the other hand, the proposed **INT2A** also was able to react with **2a** via a higher energy barrier than **TS2** with value of 20.8 kcal/mol, meaning that the reaction pathway proposed in figure 1 should be more favorable and also reasonable for the stereoselectivity.

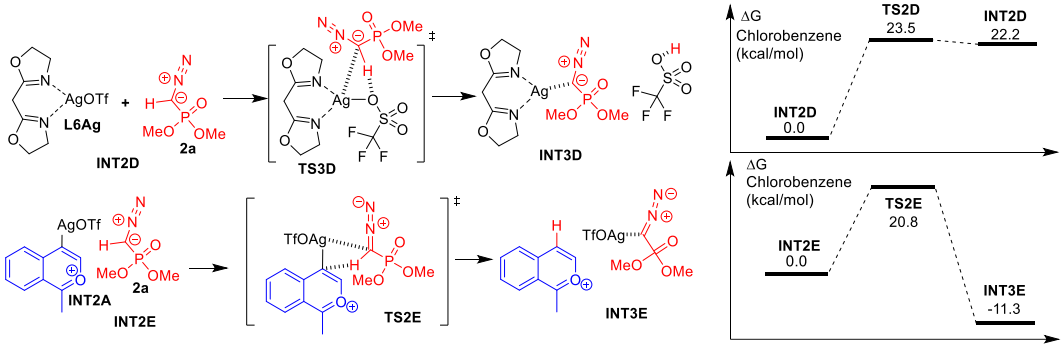


Figure 4. The possibility for the formation of **INT3Ag**.

In the pathway B, the OTf anion participated in the reaction as a hydrogen acceptor. **2a** attacked **INT2B-com** to form a C-C bond, then was dehydrogenized by OTf anion. The formed HOTf was reaction with the Ag complex to produce the final product. The energy barriers of **TS2B** and **TS3B** with respective value of 13.5 kcal/mol and 9.3 kcal/mol are lower than that of **TS2A** (18.1 kcal/mol). Moreover, the related energy of the **INT2A** was much higher than **INT2B**. These results suggested that **pathway B** may be the favorable processes for this reaction.

The stereoselectivity

As shown in Figure 2, in **Pathway A**, the stereoselectivity was determined by the step3, while the **TS2B** in **Pathway B** involved the C-C bond formation should be the key transition state for the stereoselectivity. As the step3 of **Pathway A** is not the rate limited step and the energy barrier of step3 is too low, the reaction through the processes as **Pathway A** should not employ good stereoselectivity. On the other hand, the pathway should be more reaction to produce products with good *ee* value. So the energies of different poses of ***R*-TS2B** and ***S*-TS3B** were the most important factor of the stereoselectivity. As showed in figure 5, the energy barrier of ***R*-TS2B** is 1.5 kcal/mol higher than that of ***S*-TS2B**, suggesting the S-TS2B corresponding product ***S*-3a** should be the main isomer, which is consistent with our experiments.

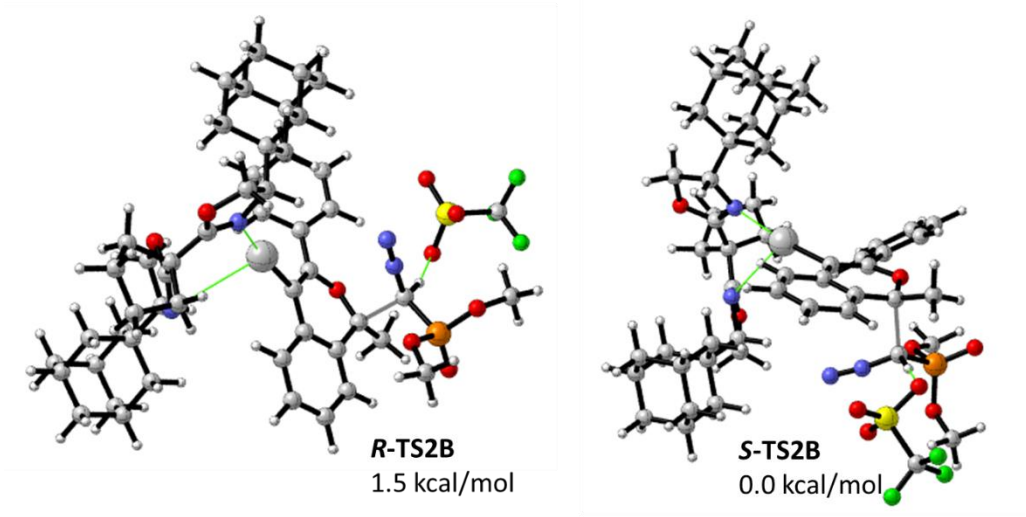


Figure 5. The structure and energy of **R-TS2B** and **S-TS2B**.

Computational method

All calculations were carried out with the GAUSSIAN 09 packages.[14] The recently developed B3LYP functional, together with LANL2DZ for Ag atom and 6-31G(d) basis set for the rest, were used for optimizing the geometry of all the minima and transition states. All the optimized structures were confirmed by frequency calculations to be either minima or transition states using the same level of theory. For transition states, intrinsic reaction coordinate analysis (IRC) was done to verify that they connect the right reactants.[15] To take solvent effects into account, solution-phase single-point calculations were performed on the gas-phase geometries.[16] The solution-phase single point energy calculations were done using M06L method using LANL2DZ for Ag and 6-311++G(d,p) for the rest. Solvent effect was accounted for using self-consistent reaction field (SCRF) method, using SMD model and UAKS radii.[17] Dichloromethane was used as the solvent. Solution-phase single-point energies corrected by the gas-phase Gibbs free energy corrections were used to describe all the reaction energetics. All of these energies correspond to the reference state of 1 mol/L, 298 K. All energetics reported throughout the text are in kcal/mol, and the bond lengths are in angstroms (Å). Structures were generated using GaussView 5.0.8 and CYL view.

Computational data:

1a

Zero-point correction= 0.229244 (Hartree/Particle)
Thermal correction to Energy= 0.243854
Thermal correction to Enthalpy= 0.244798
Thermal correction to Gibbs Free Energy= 0.184943
E(sov) = -692.210195370 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.848843	-0.042719	0.000116
2	6	0	2.487322	0.300292	-0.000049
3	6	0	1.520536	-0.746620	-0.000156
4	6	0	1.970342	-2.084088	-0.000180
5	6	0	3.325043	-2.392787	-0.000078
6	6	0	4.273939	-1.367850	0.000091
7	1	0	4.595315	0.744091	0.000250
8	1	0	1.227461	-2.875366	-0.000275
9	1	0	3.640684	-3.432564	-0.000127
10	1	0	5.335215	-1.598867	0.000216
11	6	0	2.072596	1.740440	-0.000132
12	6	0	3.155487	2.814312	0.000655
13	1	0	2.663551	3.788285	0.000559
14	1	0	3.798365	2.736458	0.885305
15	1	0	3.799421	2.736779	-0.883250
16	8	0	0.897551	2.072100	-0.000680
17	6	0	0.115366	-0.532873	-0.000147
18	6	0	-1.100741	-0.493637	-0.000115
19	6	0	-2.508654	-0.284619	-0.000021
20	6	0	-3.411365	-1.365949	0.000281
21	6	0	-3.015683	1.031751	-0.000236
22	6	0	-4.784344	-1.134448	0.000360
23	1	0	-3.023006	-2.379989	0.000449
24	6	0	-4.389596	1.252628	-0.000151
25	1	0	-2.314222	1.860184	-0.000487
26	6	0	-5.277517	0.172844	0.000150
27	1	0	-5.472236	-1.975765	0.000587
28	1	0	-4.770625	2.270370	-0.000324
29	1	0	-6.349765	0.349514	0.000218

L6Ag

Zero-point correction= 0.203560 (Hartree/Particle)
Thermal correction to Energy= 0.224713
Thermal correction to Enthalpy= 0.225658
Thermal correction to Gibbs Free Energy= 0.145956
E(sov) = -1640.25485031 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.340898	0.726354	-0.870318
2	1	0	3.271966	0.723378	-1.967061
3	1	0	4.357133	1.074581	-0.651375
4	6	0	2.367815	1.744033	-0.347069
5	8	0	2.542320	2.960694	-0.913089

6	6	0	3.232406	-0.694160	-0.396277
7	8	0	4.383412	-1.380844	-0.564149
8	7	0	2.226174	-1.332673	0.071072
9	7	0	1.453672	1.604528	0.529751
10	6	0	1.491959	3.815806	-0.367143
11	1	0	1.972564	4.704061	0.048512
12	1	0	0.840335	4.105129	-1.195497
13	6	0	0.792112	2.917745	0.681149
14	1	0	-0.278046	2.796381	0.497887
15	1	0	0.935858	3.272806	1.707379
16	6	0	4.124446	-2.754841	-0.162591
17	1	0	4.290866	-3.392525	-1.034204
18	1	0	4.841658	-3.012772	0.619476
19	6	0	2.653575	-2.724107	0.316750
20	1	0	2.547383	-2.956215	1.381114
21	1	0	2.009166	-3.409137	-0.242052
22	47	0	0.177676	-0.483112	0.652504
23	8	0	-1.950452	-0.602525	1.279153
24	16	0	-2.760310	0.366512	0.436495
25	8	0	-3.945919	0.900427	1.105285
26	8	0	-1.882908	1.316564	-0.294549
27	6	0	-3.392256	-0.757364	-0.903376
28	9	0	-4.159450	-1.726090	-0.392822
29	9	0	-2.352879	-1.334173	-1.543214
30	9	0	-4.106668	-0.068838	-1.800575

INT1A

Zero-point correction= 0.405391 (Hartree/Particle)
Thermal correction to Energy= 0.434257
Thermal correction to Enthalpy= 0.435201
Thermal correction to Gibbs Free Energy= 0.335139
E(sov) = -1370.74104324 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.981852	-2.488554	-0.663574
2	1	0	3.353512	-2.124771	-1.632945
3	1	0	3.631408	-3.328898	-0.402516
4	6	0	3.201770	-1.403314	0.353143
5	8	0	4.461342	-1.389891	0.825473
6	6	0	1.594567	-3.029135	-0.874334
7	8	0	1.605743	-4.283273	-1.361891
8	7	0	0.458628	-2.462324	-0.704769
9	7	0	2.395400	-0.501797	0.771886
10	6	0	4.569019	-0.242565	1.718785

11	1	0	4.915138	-0.610029	2.686366
12	1	0	5.314789	0.434920	1.296653
13	6	0	3.134468	0.338026	1.737659
14	1	0	3.093465	1.383681	1.419325
15	1	0	2.659324	0.264323	2.721228
16	6	0	0.220033	-4.657154	-1.611819
17	1	0	0.115313	-4.839629	-2.683742
18	1	0	0.022999	-5.579803	-1.063192
19	6	0	-0.581074	-3.434112	-1.103784
20	1	0	-1.211830	-3.669283	-0.240358
21	1	0	-1.218288	-2.995215	-1.877168
22	47	0	0.141285	-0.308149	0.189547
23	6	0	-0.667261	2.091674	-0.567467
24	6	0	-1.655900	1.375743	-0.444418
25	6	0	-2.957854	0.775314	-0.428970
26	6	0	-3.721322	0.864231	-1.608113
27	6	0	-3.534268	0.173647	0.725367
28	6	0	-5.023202	0.372886	-1.658474
29	1	0	-3.282291	1.339626	-2.479256
30	6	0	-4.857058	-0.290489	0.653032
31	6	0	-5.596470	-0.205580	-0.524536
32	1	0	-5.592297	0.453685	-2.579747
33	1	0	-5.313507	-0.741098	1.527604
34	1	0	-6.613455	-0.583758	-0.554581
35	6	0	0.434736	2.993667	-0.696848
36	6	0	1.016143	3.575316	0.449420
37	6	0	0.929139	3.333624	-1.972092
38	6	0	2.069487	4.475947	0.315355
39	1	0	0.622536	3.326865	1.430570
40	6	0	1.985354	4.233031	-2.093379
41	1	0	0.476320	2.893550	-2.855212
42	6	0	2.557431	4.804770	-0.953521
43	1	0	2.503932	4.931644	1.200434
44	1	0	2.358765	4.493684	-3.079191
45	1	0	3.376465	5.510899	-1.053592
46	6	0	-2.761998	-0.000550	1.991140
47	6	0	-3.511053	-0.171436	3.297185
48	1	0	-4.308009	0.570776	3.407757
49	1	0	-3.975232	-1.164493	3.347120
50	1	0	-2.801514	-0.083926	4.121543
51	8	0	-1.530260	-0.021942	2.002150

TS1A

Zero-point correction= 0.405318 (Hartree/Particle)
Thermal correction to Energy= 0.433049
Thermal correction to Enthalpy= 0.433993

Thermal correction to Gibbs Free Energy= 0.338669

E(sov) = -1370.71752114 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.482431	-0.419905	0.204676
2	1	0	5.233908	0.120927	-0.384494
3	1	0	5.071987	-1.052754	0.881951
4	6	0	3.746926	0.584500	1.041604
5	8	0	4.590499	1.338627	1.770576
6	6	0	3.731464	-1.322269	-0.729370
7	8	0	4.565800	-2.076474	-1.470060
8	7	0	2.471983	-1.474410	-0.901337
9	7	0	2.491620	0.808225	1.156025
10	6	0	3.776343	2.266015	2.544965
11	1	0	3.989859	2.090551	3.601299
12	1	0	4.081508	3.278784	2.274125
13	6	0	2.328939	1.911189	2.127991
14	1	0	1.807168	2.745514	1.649636
15	1	0	1.717821	1.569470	2.968903
16	6	0	3.738087	-2.925751	-2.315498
17	1	0	4.008117	-2.722695	-3.353664
18	1	0	3.974147	-3.964170	-2.073554
19	6	0	2.295060	-2.506321	-1.945608
20	1	0	1.702780	-3.335352	-1.546315
21	1	0	1.746861	-2.080383	-2.791659
22	47	0	0.692637	-0.282353	0.126882
23	6	0	-1.859066	0.845659	-0.238267
24	6	0	-1.524782	-0.343717	0.073495
25	6	0	-2.325360	-1.525915	0.363177
26	6	0	-1.688947	-2.744980	0.648943
27	6	0	-3.749743	-1.483369	0.379986
28	6	0	-2.414385	-3.896875	0.934609
29	1	0	-0.602620	-2.771577	0.646717
30	6	0	-4.464069	-2.660529	0.674943
31	6	0	-3.811552	-3.856784	0.947219
32	1	0	-1.893292	-4.824899	1.151239
33	1	0	-5.547668	-2.642416	0.690993
34	1	0	-4.385793	-4.750376	1.170666
35	6	0	-1.683681	2.207710	-0.647617
36	6	0	-2.157228	3.265502	0.153663
37	6	0	-1.037384	2.495354	-1.867581
38	6	0	-1.973160	4.582883	-0.254248
39	1	0	-2.675213	3.039999	1.079711
40	6	0	-0.847782	3.817278	-2.261069
41	1	0	-0.693287	1.677568	-2.493489

42	6	0	-1.315819	4.860842	-1.457249
43	1	0	-2.343843	5.395287	0.363546
44	1	0	-0.347533	4.034272	-3.200142
45	1	0	-1.174920	5.890965	-1.771460
46	6	0	-4.498110	-0.237482	0.104296
47	6	0	-6.011660	-0.219844	0.172964
48	1	0	-6.446610	-0.915470	-0.553423
49	1	0	-6.366896	-0.511686	1.167440
50	1	0	-6.357327	0.790257	-0.050425
51	8	0	-3.933478	0.826962	-0.189266

INT2A

Zero-point correction= 0.407981 (Hartree/Particle)
Thermal correction to Energy= 0.435298
Thermal correction to Enthalpy= 0.436242
Thermal correction to Gibbs Free Energy= 0.343113
E(sov) = -1370.73859393 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.447005	-0.404892	-0.238105
2	1	0	-5.159784	0.375902	0.058116
3	1	0	-5.078119	-1.221665	-0.612636
4	6	0	-3.640581	0.119619	-1.388135
5	8	0	-4.425557	0.520371	-2.408062
6	6	0	-3.751979	-0.888967	0.999074
7	8	0	-4.628229	-1.321995	1.928320
8	7	0	-2.504335	-0.943596	1.275590
9	7	0	-2.373582	0.230983	-1.524710
10	6	0	-3.542724	1.006937	-3.458989
11	1	0	-3.733477	0.411114	-4.354041
12	1	0	-3.802491	2.049708	-3.653124
13	6	0	-2.128057	0.811769	-2.862227
14	1	0	-1.578295	1.751849	-2.756676
15	1	0	-1.510469	0.125965	-3.450259
16	6	0	-3.847616	-1.764997	3.074400
17	1	0	-4.162240	-1.175411	3.938133
18	1	0	-4.081341	-2.817580	3.247840
19	6	0	-2.385156	-1.509209	2.636028
20	1	0	-1.787101	-2.425076	2.601013
21	1	0	-1.866276	-0.796762	3.284874
22	47	0	-0.603905	-0.308073	-0.047791
23	6	0	2.270847	0.853622	0.250504
24	6	0	1.554930	-0.303096	0.046835
25	6	0	2.332270	-1.485084	-0.189029

26	6	0	1.720868	-2.750792	-0.399712
27	6	0	3.772430	-1.442438	-0.236220
28	6	0	2.472215	-3.881513	-0.632593
29	1	0	0.636380	-2.802148	-0.370601
30	6	0	4.532112	-2.625084	-0.483040
31	6	0	3.890232	-3.822233	-0.676313
32	1	0	1.977117	-4.835980	-0.787153
33	1	0	5.615425	-2.573731	-0.516206
34	1	0	4.461789	-4.725742	-0.863624
35	6	0	1.775790	2.215146	0.519782
36	6	0	2.454067	3.338463	0.011856
37	6	0	0.625983	2.417117	1.303782
38	6	0	1.978352	4.623928	0.260008
39	1	0	3.346364	3.202559	-0.590610
40	6	0	0.157429	3.705259	1.555242
41	1	0	0.123214	1.561363	1.743936
42	6	0	0.827985	4.812379	1.030067
43	1	0	2.506417	5.480124	-0.149329
44	1	0	-0.723434	3.845467	2.175264
45	1	0	0.462021	5.815851	1.226639
46	6	0	4.394393	-0.204658	-0.035661
47	6	0	5.865400	0.067707	-0.049678
48	1	0	6.380505	-0.529604	0.711155
49	1	0	6.301251	-0.189146	-1.022003
50	1	0	6.048933	1.124553	0.151289
51	8	0	3.661218	0.861904	0.198585

INT1B

Zero-point correction= 0.434154 (Hartree/Particle)
Thermal correction to Energy= 0.471735
Thermal correction to Enthalpy= 0.472679
Thermal correction to Gibbs Free Energy= 0.355359
E(sov) = -2332.48375187 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.531121	-2.356080	0.581916
2	6	0	3.488412	-1.948410	2.563455
3	1	0	3.795541	-2.657880	3.334463
4	1	0	4.136728	-1.069994	2.569084
5	6	0	1.357018	-3.033913	-1.573981
6	6	0	0.088907	-4.344720	-2.895741
7	1	0	-0.354958	-5.293622	-2.586123
8	1	0	0.271758	-4.364980	-3.973686
9	7	0	1.541545	-1.825606	1.195753

10	7	0	0.285784	-2.338456	-1.628063
11	8	0	1.375467	-4.218220	-2.231186
12	8	0	3.661447	-2.596730	1.270043
13	47	0	0.000262	-0.426636	-0.173924
14	8	0	1.762812	0.945407	-0.976540
15	16	0	2.756391	1.265621	0.105226
16	8	0	2.120804	1.551498	1.415000
17	8	0	3.929514	0.370238	0.134531
18	6	0	3.421816	2.911952	-0.444101
19	9	0	4.340948	3.353627	0.423704
20	9	0	3.983880	2.817123	-1.654517
21	9	0	2.430100	3.819546	-0.506700
22	6	0	-2.886290	4.523725	-0.193433
23	6	0	-3.115531	3.141611	-0.113253
24	6	0	-2.055045	2.302737	0.344589
25	6	0	-0.825634	2.887781	0.705093
26	6	0	-0.632111	4.262968	0.612301
27	6	0	-1.663704	5.087467	0.163170
28	1	0	-3.681262	5.175086	-0.539040
29	1	0	-0.008457	2.262390	1.051244
30	1	0	0.335802	4.675581	0.877636
31	1	0	-1.518536	6.161080	0.086181
32	6	0	-4.449403	2.583797	-0.495373
33	6	0	-5.484149	3.511693	-1.119781
34	1	0	-6.356044	2.913606	-1.389764
35	1	0	-5.793899	4.291743	-0.414092
36	1	0	-5.092880	4.011137	-2.013151
37	8	0	-4.730806	1.406826	-0.317136
38	6	0	-2.191740	0.882682	0.452940
39	6	0	-2.321282	-0.330424	0.620247
40	6	0	-2.915700	-1.620018	0.845939
41	6	0	-4.309304	-1.748801	0.665106
42	6	0	-2.164368	-2.740214	1.249629
43	6	0	-4.927825	-2.976202	0.886998
44	1	0	-4.877348	-0.879598	0.352050
45	6	0	-2.797512	-3.962447	1.469886
46	1	0	-1.091049	-2.643702	1.384419
47	6	0	-4.177625	-4.085277	1.289574
48	1	0	-6.001481	-3.067344	0.746183
49	1	0	-2.210664	-4.820710	1.786250
50	1	0	-4.666619	-5.040114	1.463029
51	6	0	2.641457	-2.680677	-0.882706
52	1	0	3.354949	-3.496673	-1.013034
53	1	0	3.071068	-1.784514	-1.352109
54	6	0	-0.695858	-3.095912	-2.421950
55	1	0	-1.556097	-3.348175	-1.792920
56	1	0	-1.055477	-2.481499	-3.253189

57	6	0	1.986955	-1.580808	2.584393
58	1	0	1.827575	-0.529031	2.830984
59	1	0	1.401603	-2.202249	3.272974

TS1B

Zero-point correction= 0.433664 (Hartree/Particle)
Thermal correction to Energy= 0.470155
Thermal correction to Enthalpy= 0.471100
Thermal correction to Gibbs Free Energy= 0.356690
E(sov) = -2332.46282891 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.498172	-2.303895	-1.147825
2	6	0	-3.459175	-1.559784	-3.030121
3	1	0	-3.714780	-2.104666	-3.941237
4	1	0	-4.161834	-0.739300	-2.866557
5	6	0	-1.370971	-3.253183	0.958306
6	6	0	-0.253657	-4.438892	2.516116
7	1	0	0.137629	-5.446635	2.354769
8	1	0	-0.473926	-4.303132	3.578603
9	7	0	-1.547297	-1.589244	-1.617696
10	7	0	-0.253245	-2.635699	0.956717
11	8	0	-1.501296	-4.323726	1.784674
12	8	0	-3.598632	-2.476752	-1.909435
13	47	0	0.100593	-0.531444	-0.234185
14	8	0	-1.775849	0.578668	1.058504
15	16	0	-2.958074	0.972068	0.232899
16	8	0	-2.602076	1.526599	-1.097531
17	8	0	-4.067588	-0.005040	0.244371
18	6	0	-3.618242	2.448873	1.149708
19	9	0	-4.719257	2.926318	0.552902
20	9	0	-3.923156	2.132373	2.415185
21	9	0	-2.695615	3.431865	1.173236
22	6	0	2.548095	4.601476	-0.106725
23	6	0	2.773209	3.207178	-0.127375
24	6	0	1.665195	2.323836	-0.302919
25	6	0	0.382310	2.876553	-0.463081
26	6	0	0.186824	4.251974	-0.436129
27	6	0	1.271524	5.121324	-0.255602
28	1	0	3.381941	5.281861	0.027614
29	1	0	-0.468065	2.219589	-0.608421
30	1	0	-0.821270	4.640778	-0.543011
31	1	0	1.116673	6.196028	-0.230889
32	6	0	4.132421	2.696175	0.026236

33	6	0	5.302214	3.638312	0.234936
34	1	0	6.215069	3.047677	0.325472
35	1	0	5.405135	4.330309	-0.608032
36	1	0	5.168175	4.237389	1.142350
37	8	0	4.412407	1.477554	-0.009936
38	6	0	1.845247	0.882529	-0.297004
39	6	0	2.941834	0.224215	-0.202275
40	6	0	3.664122	-1.025733	-0.210186
41	6	0	4.750324	-1.263631	0.652692
42	6	0	3.254160	-2.049321	-1.089293
43	6	0	5.401781	-2.494553	0.639440
44	1	0	5.077059	-0.477195	1.322476
45	6	0	3.905412	-3.280485	-1.088180
46	1	0	2.420548	-1.867384	-1.759798
47	6	0	4.981653	-3.507818	-0.226028
48	1	0	6.238587	-2.664600	1.311281
49	1	0	3.576790	-4.060126	-1.769869
50	1	0	5.491380	-4.467381	-0.230896
51	6	0	-2.627114	-2.932874	0.207177
52	1	0	-3.224819	-3.843805	0.118490
53	1	0	-3.222086	-2.219520	0.799399
54	6	0	0.629869	-3.316161	1.917133
55	1	0	1.514678	-3.699125	1.397112
56	1	0	0.970576	-2.600855	2.672363
57	6	0	-1.986767	-1.102751	-2.940902
58	1	0	-1.896593	-0.015226	-2.967790
59	1	0	-1.351793	-1.538903	-3.721918

INT2B

Zero-point correction= 0.436155 (Hartree/Particle)
Thermal correction to Energy= 0.472375
Thermal correction to Enthalpy= 0.473320
Thermal correction to Gibbs Free Energy= 0.360137
E(sov) = -2332.48215314 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.416802	-2.356306	-1.135667
2	6	0	-3.395204	-1.664313	-3.029339
3	1	0	-3.630162	-2.224276	-3.936964
4	1	0	-4.125078	-0.866545	-2.872823
5	6	0	-1.294017	-3.202786	1.018995
6	6	0	-0.197405	-4.222372	2.703990
7	1	0	0.189178	-5.242175	2.622448
8	1	0	-0.410018	-4.000801	3.753226

9	7	0	-1.488333	-1.616231	-1.611748
10	7	0	-0.168216	-2.606619	0.949204
11	8	0	-1.447726	-4.160782	1.972311
12	8	0	-3.505591	-2.576059	-1.902458
13	47	0	0.241683	-0.573624	-0.392879
14	8	0	-1.814709	0.514134	1.020890
15	16	0	-3.008524	0.882742	0.209608
16	8	0	-2.684873	1.498605	-1.103740
17	8	0	-4.080109	-0.137954	0.184303
18	6	0	-3.744758	2.298165	1.165360
19	9	0	-4.870308	2.736185	0.583125
20	9	0	-4.031933	1.934997	2.423393
21	9	0	-2.875313	3.330015	1.218191
22	6	0	2.290668	4.646416	-0.011325
23	6	0	2.613819	3.257901	-0.089405
24	6	0	1.585619	2.272020	-0.322230
25	6	0	0.257844	2.747238	-0.489535
26	6	0	-0.032072	4.091844	-0.403883
27	6	0	0.987314	5.049748	-0.160754
28	1	0	3.074695	5.375185	0.169328
29	1	0	-0.540958	2.038834	-0.678113
30	1	0	-1.063903	4.411812	-0.510659
31	1	0	0.732343	6.103539	-0.094406
32	6	0	3.927054	2.804016	0.051443
33	6	0	5.141753	3.650336	0.282069
34	1	0	6.029787	3.017291	0.331172
35	1	0	5.272578	4.378534	-0.526323
36	1	0	5.055318	4.211328	1.219867
37	8	0	4.190153	1.516973	-0.022982
38	6	0	1.883367	0.866261	-0.360481
39	6	0	3.210835	0.539749	-0.212623
40	6	0	3.842505	-0.793424	-0.195493
41	6	0	5.017359	-1.027917	0.543633
42	6	0	3.285704	-1.858433	-0.925290
43	6	0	5.602125	-2.292224	0.568635
44	1	0	5.464460	-0.219372	1.112447
45	6	0	3.875937	-3.120806	-0.900929
46	1	0	2.394007	-1.684161	-1.517846
47	6	0	5.033536	-3.345331	-0.151708
48	1	0	6.502144	-2.455549	1.155273
49	1	0	3.433697	-3.928186	-1.478292
50	1	0	5.491807	-4.330413	-0.133450
51	6	0	-2.540864	-2.968752	0.225366
52	1	0	-3.087449	-3.912380	0.141170
53	1	0	-3.189795	-2.278571	0.787797
54	6	0	0.689632	-3.158916	2.008884
55	1	0	1.599463	-3.580371	1.568462

56	1	0	0.990567	-2.353971	2.687472
57	6	0	-1.939686	-1.156982	-2.940767
58	1	0	-1.886890	-0.067145	-2.976752
59	1	0	-1.287396	-1.577087	-3.716270

INT1C

Zero-point correction= 0.258368 (Hartree/Particle)
Thermal correction to Energy= 0.284338
Thermal correction to Enthalpy= 0.285282
Thermal correction to Gibbs Free Energy= 0.194445
E(sov) = -1799.64650393 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.431535	0.889920	0.051831
2	8	0	2.474709	1.605632	0.431842
3	16	0	3.366557	0.742610	-0.453194
4	8	0	2.528845	-0.202697	-1.242746
5	8	0	4.431015	1.465206	-1.142813
6	6	0	4.203323	-0.339878	0.805653
7	9	0	5.003607	-1.220413	0.195843
8	9	0	4.928084	0.394189	1.652694
9	9	0	3.277203	-1.018284	1.506751
10	6	0	-1.976480	-4.220855	-0.244365
11	6	0	-2.311742	-2.871512	-0.064658
12	6	0	-1.360444	-1.876753	-0.440478
13	6	0	-0.123242	-2.281416	-0.980822
14	6	0	0.175820	-3.630739	-1.148136
15	6	0	-0.750467	-4.606840	-0.781169
16	1	0	-2.690534	-4.986850	0.036902
17	1	0	0.617892	-1.538283	-1.260024
18	1	0	1.139028	-3.910856	-1.563588
19	1	0	-0.521116	-5.660423	-0.908935
20	6	0	-3.644236	-2.493203	0.500025
21	6	0	-4.565813	-3.585746	1.018979
22	1	0	-5.451463	-3.111149	1.444247
23	1	0	-4.876649	-4.257381	0.209828
24	1	0	-4.075230	-4.196179	1.785458
25	8	0	-4.000437	-1.324335	0.547116
26	6	0	-1.626785	-0.477221	-0.286984
27	6	0	-1.869401	0.735001	-0.235867
28	6	0	-2.586649	1.979539	-0.155556
29	6	0	-3.911955	1.958745	0.326441
30	6	0	-2.009634	3.201077	-0.551015
31	6	0	-4.633501	3.146144	0.408836

32	1	0	-4.348945	1.011866	0.622468
33	6	0	-2.743220	4.381210	-0.464383
34	1	0	-0.991979	3.219561	-0.932682
35	6	0	-4.054456	4.356978	0.017124
36	1	0	-5.653911	3.126327	0.780990
37	1	0	-2.290054	5.318761	-0.772480
38	1	0	-4.623915	5.279521	0.086348

TS1C

Zero-point correction= 0.258622 (Hartree/Particle)
Thermal correction to Energy= 0.283348
Thermal correction to Enthalpy= 0.284293
Thermal correction to Gibbs Free Energy= 0.197308
E(sov) = -1799.63210183 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.593686	-0.604298	-0.242890
2	8	0	-2.614898	-1.420050	-0.397829
3	16	0	-3.556996	-0.251876	-0.660099
4	8	0	-2.794408	1.013824	-0.812056
5	8	0	-4.619429	-0.538319	-1.621374
6	6	0	-4.393578	-0.082755	0.991588
7	9	0	-5.267546	0.929996	0.967923
8	9	0	-5.042175	-1.206768	1.310883
9	9	0	-3.477411	0.167679	1.944662
10	6	0	2.684744	3.934784	-0.019577
11	6	0	2.655238	2.526060	0.023859
12	6	0	1.412032	1.853827	-0.163828
13	6	0	0.253643	2.619643	-0.387239
14	6	0	0.312763	4.008730	-0.432487
15	6	0	1.530908	4.672073	-0.247593
16	1	0	3.622896	4.459230	0.123159
17	1	0	-0.699750	2.116766	-0.527331
18	1	0	-0.596925	4.574738	-0.610347
19	1	0	1.577109	5.756431	-0.280069
20	6	0	3.904479	1.786700	0.262896
21	6	0	5.202745	2.528853	0.516768
22	1	0	5.992686	1.796849	0.690533
23	1	0	5.473804	3.150203	-0.344064
24	1	0	5.118934	3.186347	1.388927
25	8	0	3.964458	0.544275	0.266505
26	6	0	1.325852	0.401233	-0.119193
27	6	0	2.232234	-0.489070	0.008430
28	6	0	2.761841	-1.822929	0.025205

29	6	0	3.577591	-2.267446	1.083181
30	6	0	2.449431	-2.706175	-1.028415
31	6	0	4.061360	-3.571943	1.087878
32	1	0	3.826976	-1.581501	1.884945
33	6	0	2.927309	-4.013365	-1.006895
34	1	0	1.827099	-2.359126	-1.847398
35	6	0	3.734561	-4.447449	0.047964
36	1	0	4.689265	-3.909867	1.907088
37	1	0	2.673854	-4.691426	-1.816386
38	1	0	4.108731	-5.467242	0.059930

INT2C

Zero-point correction= 0.261398 (Hartree/Particle)
Thermal correction to Energy= 0.285693
Thermal correction to Enthalpy= 0.286637
Thermal correction to Gibbs Free Energy= 0.201669
E(sov) = -1799.65588734 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.523365	0.599333	-0.308665
2	8	0	2.556968	1.334564	-0.473546
3	16	0	3.541212	0.187047	-0.660536
4	8	0	2.846291	-1.115044	-0.795434
5	8	0	4.629456	0.486908	-1.589743
6	6	0	4.322063	0.109730	1.024792
7	9	0	5.229857	-0.873385	1.071247
8	9	0	4.923564	1.265569	1.325161
9	9	0	3.383210	-0.136654	1.957338
10	6	0	-2.648965	-3.944190	0.063197
11	6	0	-2.630887	-2.516829	0.041353
12	6	0	-1.396386	-1.796737	-0.156459
13	6	0	-0.212599	-2.567881	-0.332712
14	6	0	-0.258886	-3.944819	-0.312980
15	6	0	-1.480707	-4.641095	-0.111994
16	1	0	-3.585406	-4.470602	0.217598
17	1	0	0.735103	-2.056643	-0.484504
18	1	0	0.658704	-4.508988	-0.452625
19	1	0	-1.485441	-5.726860	-0.097412
20	6	0	-3.799367	-1.769350	0.208789
21	6	0	-5.178747	-2.309800	0.427154
22	1	0	-5.891398	-1.486093	0.497959
23	1	0	-5.477848	-2.964649	-0.398925
24	1	0	-5.226660	-2.899149	1.350136
25	8	0	-3.750719	-0.454306	0.174543

26	6	0	-1.368226	-0.362332	-0.162016
27	6	0	-2.577206	0.272206	-0.004668
28	6	0	-2.871675	1.715197	0.027881
29	6	0	-3.934577	2.213673	0.804197
30	6	0	-2.102031	2.620929	-0.723365
31	6	0	-4.201296	3.579880	0.845097
32	1	0	-4.539592	1.530391	1.391115
33	6	0	-2.374431	3.986411	-0.681788
34	1	0	-1.302696	2.247788	-1.355115
35	6	0	-3.421273	4.471678	0.104930
36	1	0	-5.016177	3.949422	1.461251
37	1	0	-1.770699	4.669960	-1.271581
38	1	0	-3.629915	5.537218	0.139192

INT2A-com

Zero-point correction= 0.525197 (Hartree/Particle)
Thermal correction to Energy= 0.565788
Thermal correction to Enthalpy= 0.566733
Thermal correction to Gibbs Free Energy= 0.439261
E(sov) = -2165.88794215 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.836971	4.087649	0.233644
2	1	0	1.607991	4.228788	-0.832604
3	1	0	2.194767	5.057025	0.590708
4	6	0	0.559349	3.768712	0.956566
5	8	0	-0.099965	4.867603	1.369155
6	6	0	2.958382	3.094719	0.355326
7	8	0	4.179684	3.660182	0.235330
8	7	0	2.884801	1.830648	0.516133
9	7	0	0.024204	2.629321	1.191914
10	6	0	-1.377410	4.411757	1.906086
11	1	0	-1.516564	4.887721	2.877715
12	1	0	-2.159326	4.746756	1.218423
13	6	0	-1.220540	2.877752	1.957000
14	1	0	-2.052383	2.336435	1.501004
15	1	0	-1.082621	2.505649	2.979139
16	6	0	5.145945	2.572644	0.299143
17	1	0	5.684964	2.551394	-0.651389
18	1	0	5.844615	2.797465	1.107531
19	6	0	4.269383	1.319624	0.548219
20	1	0	4.463260	0.855303	1.521084
21	1	0	4.397916	0.554434	-0.222046
22	47	0	0.713950	0.521673	0.642711

23	6	0	1.493921	-2.383672	-0.194178
24	6	0	0.555452	-1.630690	0.470178
25	6	0	-0.387414	-2.367602	1.265349
26	6	0	-1.469555	-1.724173	1.924825
27	6	0	-0.274150	-3.796086	1.431005
28	6	0	-2.348806	-2.437893	2.710862
29	1	0	-1.611758	-0.660014	1.767506
30	6	0	-1.187290	-4.510675	2.263035
31	6	0	-2.202600	-3.837941	2.895528
32	1	0	-3.171171	-1.920768	3.196965
33	1	0	-1.078183	-5.582793	2.389738
34	1	0	-2.900915	-4.374507	3.530301
35	6	0	2.539922	-1.941707	-1.133226
36	6	0	3.778774	-2.605943	-1.199877
37	6	0	2.302737	-0.862395	-2.002548
38	6	0	4.758954	-2.185931	-2.096560
39	1	0	3.977071	-3.444350	-0.540158
40	6	0	3.282410	-0.450894	-2.904445
41	1	0	1.338183	-0.365752	-1.983428
42	6	0	4.514824	-1.107983	-2.952160
43	1	0	5.713424	-2.703109	-2.130170
44	1	0	3.077297	0.373413	-3.581560
45	1	0	5.276138	-0.789986	-3.658649
46	6	0	1.053199	-5.918110	0.776123
47	1	0	1.323582	-6.237128	1.789536
48	1	0	0.180541	-6.504257	0.467550
49	1	0	1.882783	-6.142427	0.103445
50	8	0	1.558056	-3.766423	-0.038613
51	6	0	0.752217	-4.452938	0.742648
52	7	0	-2.687070	-0.566669	-3.131973
53	7	0	-2.836525	-0.765401	-4.241662
54	6	0	-2.539020	-0.331282	-1.854993
55	1	0	-1.629931	-0.693079	-1.388635
56	15	0	-3.721282	0.632815	-0.949466
57	8	0	-3.290657	0.811738	0.468159
58	8	0	-3.894227	1.939520	-1.865647
59	8	0	-5.184868	-0.030339	-1.134193
60	6	0	-4.986583	2.860321	-1.648382
61	1	0	-4.979008	3.228803	-0.618163
62	1	0	-4.822842	3.688626	-2.338356
63	1	0	-5.939283	2.372178	-1.865164
64	6	0	-5.569279	-1.152609	-0.320503
65	1	0	-6.607762	-1.371574	-0.571724
66	1	0	-4.944923	-2.022963	-0.550903
67	1	0	-5.483052	-0.903601	0.740514

TS2A

Zero-point correction= 0.523798 (Hartree/Particle)
Thermal correction to Energy= 0.563438
Thermal correction to Enthalpy= 0.564382
Thermal correction to Gibbs Free Energy= 0.441587
E(sov) = -2165.86138159 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.083040	-3.532123	-0.517343
2	1	0	-3.619325	-3.922281	0.360272
3	1	0	-3.338810	-4.211294	-1.335895
4	6	0	-3.648368	-2.177842	-0.841472
5	8	0	-4.818756	-2.252500	-1.505037
6	6	0	-1.609029	-3.665543	-0.255737
7	8	0	-1.159334	-4.911075	-0.500724
8	7	0	-0.769919	-2.804997	0.187585
9	7	0	-3.203612	-1.019240	-0.536906
10	6	0	-5.253232	-0.880257	-1.744155
11	1	0	-5.281004	-0.730028	-2.826100
12	1	0	-6.260582	-0.776871	-1.336467
13	6	0	-4.183926	-0.026238	-1.022166
14	1	0	-4.586299	0.520979	-0.163531
15	1	0	-3.684588	0.700147	-1.666778
16	6	0	0.242241	-4.943198	-0.104954
17	1	0	0.332393	-5.636613	0.734928
18	1	0	0.816402	-5.320757	-0.952699
19	6	0	0.546251	-3.473602	0.266590
20	1	0	1.236328	-2.987699	-0.430690
21	1	0	0.960563	-3.365588	1.272391
22	47	0	-1.138831	-0.521297	0.505911
23	6	0	3.073296	0.010843	0.013518
24	6	0	1.883365	0.471677	-0.491149
25	6	0	1.919992	0.834044	-1.878457
26	6	0	0.760687	1.339596	-2.534650
27	6	0	3.120379	0.720935	-2.674186
28	6	0	0.791431	1.690412	-3.867377
29	1	0	-0.152424	1.461216	-1.959696
30	6	0	3.127003	1.090011	-4.052917
31	6	0	1.978758	1.563921	-4.636324
32	1	0	-0.107083	2.076062	-4.341534
33	1	0	4.038021	0.996810	-4.635582
34	1	0	1.975428	1.847560	-5.684392
35	6	0	3.371883	-0.423680	1.389873
36	6	0	4.689284	-0.498296	1.880514

37	6	0	2.318445	-0.773032	2.254879
38	6	0	4.937818	-0.899204	3.191760
39	1	0	5.520306	-0.230313	1.237875
40	6	0	2.569582	-1.174575	3.564389
41	1	0	1.301497	-0.738255	1.878525
42	6	0	3.881995	-1.237908	4.040518
43	1	0	5.961269	-0.941611	3.553137
44	1	0	1.741242	-1.441003	4.215507
45	1	0	4.079252	-1.548180	5.062414
46	6	0	5.618755	0.050187	-2.674056
47	1	0	5.561046	-0.643089	-3.520798
48	1	0	6.010745	1.000816	-3.053601
49	1	0	6.320486	-0.350476	-1.940339
50	8	0	4.234408	-0.094311	-0.772239
51	6	0	4.274000	0.240160	-2.042212
52	7	0	-0.224373	1.646890	2.661590
53	7	0	-0.037161	1.674068	3.776295
54	6	0	-0.445001	1.568304	1.352726
55	1	0	0.474986	1.303570	0.744038
56	15	0	-1.614002	2.739810	0.650706
57	8	0	-1.904913	2.404330	-0.772701
58	8	0	-2.804171	2.663153	1.724526
59	8	0	-1.086283	4.247043	0.890273
60	6	0	-3.851709	3.661554	1.750590
61	1	0	-4.368506	3.697841	0.787304
62	1	0	-4.544202	3.347360	2.531623
63	1	0	-3.431106	4.640394	1.990079
64	6	0	-0.231331	4.888186	-0.079654
65	1	0	-0.187741	5.940154	0.204191
66	1	0	0.773893	4.455769	-0.041994
67	1	0	-0.646429	4.783015	-1.084651

INT3A

Zero-point correction= 0.527087 (Hartree/Particle)
Thermal correction to Energy= 0.567333
Thermal correction to Enthalpy= 0.568277
Thermal correction to Gibbs Free Energy= 0.442289
E(sov) = -2165.91186305 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.817666	0.483616	0.043813
2	1	0	-7.270722	0.874557	0.965770
3	1	0	-7.638070	0.473233	-0.683693
4	6	0	-5.789308	1.467934	-0.427975

5	8	0	-6.336206	2.656832	-0.771951
6	6	0	-6.413696	-0.939785	0.296818
7	8	0	-7.485593	-1.736908	0.486536
8	7	0	-5.252583	-1.472380	0.378340
9	7	0	-4.525583	1.333378	-0.528442
10	6	0	-5.229885	3.525653	-1.150299
11	1	0	-5.429982	3.896817	-2.157594
12	1	0	-5.214353	4.365342	-0.450575
13	6	0	-3.988815	2.604802	-1.048934
14	1	0	-3.220089	2.981482	-0.368821
15	1	0	-3.511057	2.421310	-2.016537
16	6	0	-6.981341	-3.071153	0.775253
17	1	0	-7.326917	-3.347663	1.774090
18	1	0	-7.410563	-3.754261	0.039512
19	6	0	-5.446613	-2.909497	0.666202
20	1	0	-5.012698	-3.504313	-0.143551
21	1	0	-4.924976	-3.170908	1.591549
22	47	0	-3.139112	-0.554965	0.149452
23	6	0	5.221145	-0.940743	-0.112950
24	6	0	4.393900	0.141096	0.062569
25	6	0	4.939030	1.424446	0.292344
26	6	0	4.111034	2.561201	0.483814
27	6	0	6.368613	1.585529	0.329195
28	6	0	4.688549	3.791789	0.704540
29	1	0	3.034172	2.418051	0.450721
30	6	0	6.932951	2.876781	0.559087
31	6	0	6.102630	3.953479	0.743215
32	1	0	4.056762	4.662699	0.853674
33	1	0	8.010171	3.001089	0.587650
34	1	0	6.522487	4.938743	0.919459
35	6	0	4.849691	-2.331450	-0.345831
36	6	0	5.810584	-3.287793	-0.730891
37	6	0	3.507967	-2.729708	-0.182158
38	6	0	5.432059	-4.607717	-0.951220
39	1	0	6.846337	-2.995962	-0.863761
40	6	0	3.139779	-4.052714	-0.401316
41	1	0	2.749439	-2.021264	0.131972
42	6	0	4.098063	-4.993778	-0.787447
43	1	0	6.178275	-5.336812	-1.252168
44	1	0	2.102534	-4.337655	-0.259650
45	1	0	3.808094	-6.026535	-0.957720
46	6	0	8.645403	0.386762	0.119161
47	1	0	9.054120	1.030414	-0.668120
48	1	0	9.054358	0.732753	1.075269
49	1	0	8.978153	-0.637794	-0.054736
50	8	0	6.578839	-0.730667	-0.073585
51	6	0	7.152338	0.446976	0.129913

52	7	0	-0.311287	-1.617743	0.551512
53	7	0	0.255488	-2.582960	0.807064
54	6	0	-1.000079	-0.558907	0.285180
55	1	0	3.312205	0.040493	0.017696
56	15	0	-0.085675	0.878933	-0.085533
57	8	0	1.407613	0.830766	0.111913
58	8	0	-0.538994	1.295944	-1.585922
59	8	0	-0.775032	2.120580	0.726813
60	6	0	0.089192	2.423703	-2.214391
61	1	0	1.178888	2.327646	-2.181055
62	1	0	-0.245981	2.425997	-3.253282
63	1	0	-0.213586	3.356298	-1.726131
64	6	0	-0.621545	2.156211	2.152232
65	1	0	-1.123852	3.060851	2.500646
66	1	0	-1.088171	1.276415	2.609814
67	1	0	0.437286	2.193495	2.429045

INT3'A

Zero-point correction= 0.527478 (Hartree/Particle)
Thermal correction to Energy= 0.567247
Thermal correction to Enthalpy= 0.568191
Thermal correction to Gibbs Free Energy= 0.445490
E(sov) = -2165.91631177 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.021977	-0.511080	-0.844482
2	6	0	2.728374	-2.555926	-0.862939
3	6	0	2.536232	-3.910415	-0.499884
4	6	0	1.727256	-1.904279	-1.661576
5	6	0	1.409866	-4.585885	-0.918007
6	1	0	3.286289	-4.407203	0.107775
7	6	0	0.574667	-2.629632	-2.079801
8	6	0	0.424626	-3.945543	-1.714083
9	1	0	1.271826	-5.625764	-0.637135
10	1	0	-0.180448	-2.141831	-2.684975
11	1	0	-0.450037	-4.502603	-2.034010
12	6	0	5.110897	0.405851	-0.520476
13	6	0	4.905981	1.798440	-0.563463
14	6	0	6.373276	-0.098492	-0.151765
15	6	0	5.947161	2.662381	-0.235708
16	1	0	3.932084	2.196965	-0.826924
17	6	0	7.407154	0.774033	0.171827
18	1	0	6.557339	-1.168726	-0.148291
19	6	0	7.196563	2.155696	0.131402

20	1	0	5.779704	3.734706	-0.261972
21	1	0	8.380247	0.377474	0.444783
22	1	0	8.005790	2.834753	0.383144
23	6	0	1.126959	0.270110	-2.942377
24	1	0	1.453151	0.098834	-3.977640
25	1	0	0.066503	0.029280	-2.865902
26	1	0	1.279262	1.327321	-2.709971
27	8	0	3.049053	0.053917	-1.624559
28	6	0	1.947147	-0.564937	-2.020627
29	6	0	3.871953	-1.818696	-0.470516
30	1	0	4.622701	-2.283016	0.157315
31	6	0	-5.655870	-0.156749	0.267440
32	1	0	-6.482575	-0.744958	-0.148536
33	1	0	-6.098008	0.379415	1.118904
34	6	0	-4.624151	-1.108893	0.796838
35	8	0	-5.146209	-1.993856	1.674096
36	6	0	-5.252645	0.860048	-0.759630
37	8	0	-6.318119	1.408236	-1.376549
38	7	0	-4.089932	1.289726	-1.083352
39	7	0	-3.377845	-1.183598	0.529796
40	6	0	-4.021451	-2.767779	2.189548
41	1	0	-3.895568	-2.502488	3.243124
42	1	0	-4.282738	-3.824364	2.109252
43	6	0	-2.837889	-2.326749	1.299446
44	1	0	-2.531956	-3.108924	0.594001
45	1	0	-1.954707	-2.005743	1.856566
46	6	0	-5.812399	2.437078	-2.273374
47	1	0	-6.175058	2.208928	-3.277488
48	1	0	-6.224683	3.394261	-1.945873
49	6	0	-4.276934	2.330983	-2.115781
50	1	0	-3.819015	3.266229	-1.780685
51	1	0	-3.776169	2.024131	-3.039804
52	47	0	-2.020158	0.702347	-0.209096
53	15	0	0.602389	0.421692	1.803841
54	8	0	-0.127836	-0.814409	2.212402
55	8	0	2.209127	0.265713	1.591441
56	8	0	0.615895	1.571717	2.958764
57	6	0	3.029235	-0.059345	2.732252
58	1	0	2.701330	-1.000895	3.184065
59	1	0	4.050802	-0.159548	2.360954
60	1	0	2.983695	0.743171	3.472155
61	6	0	-0.578585	1.834933	3.708623
62	1	0	-0.992975	0.907412	4.113977
63	1	0	-0.293496	2.503843	4.522662
64	1	0	-1.324845	2.331477	3.077137
65	6	0	0.035369	1.110295	0.284687
66	7	0	0.716474	2.079303	-0.228078

67	7	0	1.305484	2.911563	-0.762214

TS3A

Zero-point correction= 0.526636 (Hartree/Particle)
Thermal correction to Energy= 0.565413
Thermal correction to Enthalpy= 0.566357
Thermal correction to Gibbs Free Energy= 0.447861
E(sov) = -2165.91665705 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.906848	0.280052	-0.783839
2	6	0	3.196544	-1.999916	-1.202932
3	6	0	3.450785	-3.388907	-1.237302
4	6	0	1.921977	-1.518645	-1.645070
5	6	0	2.468676	-4.265048	-1.656279
6	1	0	4.423981	-3.756646	-0.925803
7	6	0	0.920592	-2.443362	-2.044181
8	6	0	1.192977	-3.792808	-2.045233
9	1	0	2.672038	-5.331609	-1.677794
10	1	0	-0.060433	-2.086882	-2.333704
11	1	0	0.426937	-4.501037	-2.343344
12	6	0	4.767108	1.382838	-0.361797
13	6	0	4.468327	2.707858	-0.730420
14	6	0	5.921527	1.130875	0.404253
15	6	0	5.319669	3.746566	-0.365867
16	1	0	3.576778	2.919678	-1.307927
17	6	0	6.767137	2.173910	0.765201
18	1	0	6.153589	0.123022	0.733398
19	6	0	6.473377	3.484101	0.375384
20	1	0	5.081786	4.763438	-0.662901
21	1	0	7.653853	1.966213	1.356189
22	1	0	7.137453	4.296382	0.655409
23	6	0	0.671527	0.600669	-2.463298
24	1	0	0.995199	0.694906	-3.510129
25	1	0	-0.277980	0.067688	-2.442058
26	1	0	0.530159	1.603648	-2.057511
27	8	0	2.708851	0.697836	-1.317037
28	6	0	1.733137	-0.120329	-1.697378
29	6	0	4.165730	-1.059243	-0.759599
30	1	0	5.130284	-1.410638	-0.413636
31	6	0	-5.516899	0.650895	-0.259677
32	1	0	-6.291379	0.680815	-1.036052
33	1	0	-6.076281	0.656539	0.686050
34	6	0	-4.801706	-0.664605	-0.368423

35	8	0	-5.648743	-1.711747	-0.289596
36	6	0	-4.737506	1.931278	-0.338841
37	8	0	-5.540111	3.005882	-0.462513
38	7	0	-3.475435	2.135287	-0.269479
39	7	0	-3.556825	-0.907830	-0.523234
40	6	0	-4.822768	-2.914752	-0.305188
41	1	0	-4.915419	-3.388908	0.675702
42	1	0	-5.223619	-3.580796	-1.071002
43	6	0	-3.403942	-2.377651	-0.600658
44	1	0	-3.061622	-2.641894	-1.608405
45	1	0	-2.641624	-2.703045	0.111208
46	6	0	-4.683591	4.183967	-0.462761
47	1	0	-4.867044	4.725899	-1.392684
48	1	0	-4.976330	4.806112	0.385734
49	6	0	-3.257746	3.594793	-0.346447
50	1	0	-2.730222	3.933827	0.550202
51	1	0	-2.631029	3.827417	-1.213121
52	47	0	-1.770154	0.583859	0.002209
53	15	0	0.311389	-1.259709	1.639979
54	8	0	-0.562406	-2.330485	1.072434
55	8	0	1.887020	-1.613522	1.752327
56	8	0	0.002045	-0.924442	3.204298
57	6	0	2.277973	-2.736758	2.569491
58	1	0	1.757096	-3.643470	2.247947
59	1	0	3.353859	-2.858454	2.432621
60	1	0	2.059476	-2.532712	3.620660
61	6	0	-1.358073	-0.799740	3.641405
62	1	0	-1.924418	-1.706272	3.408367
63	1	0	-1.324546	-0.648128	4.721668
64	1	0	-1.835893	0.068365	3.170795
65	6	0	0.246026	0.235223	0.705041
66	7	0	1.023051	1.221809	1.033086
67	7	0	1.710963	2.121455	1.208743

INT4A

Zero-point correction= 0.528015 (Hartree/Particle)
Thermal correction to Energy= 0.567111
Thermal correction to Enthalpy= 0.568055
Thermal correction to Gibbs Free Energy= 0.446498
E(sov) = -2165.93183908 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.893773	-0.767787	-0.734351
2	6	0	1.567910	-1.245607	-1.235504

3	6	0	0.558872	-2.196576	-1.475030
4	6	0	1.369927	0.087069	-1.673593
5	6	0	-0.604089	-1.845209	-2.157859
6	1	0	0.710856	-3.222867	-1.151542
7	6	0	0.221687	0.427906	-2.382802
8	6	0	-0.778120	-0.528105	-2.627263
9	1	0	-1.354266	-2.600329	-2.377057
10	1	0	0.081111	1.440173	-2.746587
11	1	0	-1.632327	-0.275018	-3.249603
12	6	0	5.278394	-1.067826	-0.340237
13	6	0	6.195868	-0.025502	-0.119072
14	6	0	5.712847	-2.396867	-0.180309
15	6	0	7.504151	-0.305271	0.270052
16	1	0	5.875914	1.002470	-0.243834
17	6	0	7.019186	-2.671767	0.212366
18	1	0	5.034455	-3.217816	-0.390611
19	6	0	7.919796	-1.627132	0.440496
20	1	0	8.199479	0.511259	0.442098
21	1	0	7.340678	-3.702993	0.326450
22	1	0	8.940723	-1.843972	0.741301
23	6	0	2.593355	2.245495	-2.301424
24	1	0	2.771975	1.845315	-3.302822
25	1	0	1.701888	2.877141	-2.315655
26	1	0	3.449111	2.868738	-2.026764
27	8	0	3.750379	0.466153	-1.310506
28	6	0	2.442800	1.096847	-1.297198
29	6	0	2.826241	-1.596861	-0.617334
30	1	0	2.939408	-2.566631	-0.149128
31	6	0	-5.757198	-0.885875	-0.165784
32	1	0	-5.982183	-1.354549	-1.135138
33	1	0	-6.705764	-0.870791	0.377608
34	6	0	-4.815729	-1.792142	0.578933
35	8	0	-5.462471	-2.781421	1.224828
36	6	0	-5.347675	0.538785	-0.419723
37	8	0	-6.401500	1.376059	-0.472756
38	7	0	-4.182814	1.023946	-0.633445
39	7	0	-3.536875	-1.773439	0.636564
40	6	0	-4.444650	-3.644979	1.807381
41	1	0	-4.656058	-3.732454	2.874428
42	1	0	-4.534151	-4.626502	1.335722
43	6	0	-3.120861	-2.913189	1.479853
44	1	0	-2.413954	-3.541640	0.930414
45	1	0	-2.611677	-2.538018	2.373944
46	6	0	-5.881970	2.689024	-0.830875
47	1	0	-6.310958	2.961566	-1.798024
48	1	0	-6.217828	3.396152	-0.070448
49	6	0	-4.349337	2.473688	-0.865516

50	1	0	-3.823705	3.030028	-0.082562
51	1	0	-3.906287	2.748047	-1.827477
52	47	0	-2.129388	-0.163337	-0.402326
53	15	0	0.922654	1.278151	1.323091
54	8	0	-0.444689	1.055563	0.750671
55	8	0	1.516505	0.073098	2.194223
56	8	0	0.983594	2.491045	2.384026
57	6	0	0.840247	-0.371914	3.391291
58	1	0	-0.193293	-0.651701	3.165811
59	1	0	1.394292	-1.242666	3.742272
60	1	0	0.861236	0.416033	4.148046
61	6	0	0.242060	3.707514	2.158083
62	1	0	-0.817888	3.484825	2.013560
63	1	0	0.381299	4.316427	3.051647
64	1	0	0.633569	4.241292	1.285893
65	6	0	2.193148	1.654781	0.132517
66	7	0	3.144458	2.438990	0.587496
67	7	0	3.984866	3.121657	0.934318

INT2-com

Zero-point correction= 0.554431 (Hartree/Particle)
Thermal correction to Energy= 0.603445
Thermal correction to Enthalpy= 0.604389
Thermal correction to Gibbs Free Energy= 0.458221
E(sov) = -3127.63065178 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.878039	-1.977932	-1.006245
2	1	0	-4.687525	-1.149885	-1.700160
3	1	0	-5.523191	-2.691631	-1.526730
4	6	0	-3.562419	-2.641428	-0.687230
5	8	0	-2.973874	-3.211176	-1.766797
6	6	0	-5.599508	-1.453742	0.199430
7	8	0	-6.738451	-2.089525	0.516498
8	7	0	-5.255378	-0.455778	0.929790
9	7	0	-2.983852	-2.687259	0.444911
10	6	0	-1.747878	-3.832519	-1.264312
11	1	0	-1.849892	-4.912834	-1.398134
12	1	0	-0.915852	-3.456988	-1.858395
13	6	0	-1.704587	-3.391516	0.220401
14	1	0	-0.877254	-2.704506	0.426858
15	1	0	-1.619425	-4.236842	0.910335
16	6	0	-7.288556	-1.426767	1.690929
17	1	0	-8.282677	-1.059552	1.426245

18	1	0	-7.373463	-2.174373	2.482121
19	6	0	-6.265250	-0.305776	1.995287
20	1	0	-5.788551	-0.424960	2.973100
21	1	0	-6.703486	0.695978	1.952323
22	47	0	-3.268200	0.484422	0.963035
23	6	0	-0.923681	2.388402	0.305198
24	6	0	-1.313569	1.298281	1.030010
25	6	0	-0.299203	0.670930	1.835564
26	6	0	-0.576054	-0.454981	2.648907
27	6	0	1.051123	1.160388	1.833027
28	6	0	0.419293	-1.060687	3.392832
29	1	0	-1.589727	-0.845583	2.663621
30	6	0	2.063204	0.524882	2.603092
31	6	0	1.745424	-0.575416	3.367967
32	1	0	0.179652	-1.929446	4.000920
33	1	0	3.090886	0.874473	2.565471
34	1	0	2.523631	-1.076397	3.934177
35	6	0	-1.727007	3.249489	-0.586409
36	6	0	-1.508386	4.637567	-0.625037
37	6	0	-2.712346	2.703319	-1.425171
38	6	0	-2.276467	5.455060	-1.452141
39	1	0	-0.740359	5.075729	0.004042
40	6	0	-3.477673	3.522220	-2.254215
41	1	0	-2.850350	1.626610	-1.445592
42	6	0	-3.267556	4.902722	-2.266523
43	1	0	-2.100083	6.527165	-1.459469
44	1	0	-4.227859	3.079364	-2.904231
45	1	0	-3.862981	5.541384	-2.913080
46	6	0	2.681812	2.887114	0.807075
47	1	0	3.250510	2.976105	1.735338
48	1	0	3.270895	2.231330	0.147281
49	1	0	2.569374	3.865019	0.334216
50	8	0	0.379857	2.862949	0.356190
51	6	0	1.345211	2.275470	1.023508
52	7	0	2.154781	-3.084470	-1.227185
53	7	0	1.990817	-4.196512	-1.429264
54	6	0	2.298914	-1.817793	-0.974581
55	15	0	1.541743	-0.609463	-2.030444
56	8	0	1.244657	0.684916	-1.357489
57	8	0	2.380956	-0.458127	-3.404638
58	8	0	0.269121	-1.455902	-2.584995
59	6	0	3.484109	0.479327	-3.460051
60	1	0	3.102471	1.502399	-3.403458
61	1	0	4.187443	0.306928	-2.641645
62	1	0	3.966413	0.310684	-4.424592
63	6	0	-0.538747	-0.895258	-3.633912
64	1	0	0.003901	-0.916374	-4.582929

65	1	0	-1.433468	-1.518100	-3.696432
66	1	0	-0.822978	0.134371	-3.392729
67	16	0	5.190795	0.022869	0.827649
68	8	0	5.189393	0.951772	1.982884
69	8	0	4.543184	-1.290856	1.083898
70	8	0	4.807577	0.646136	-0.467768
71	1	0	3.024391	-1.544498	-0.200056
72	6	0	6.984753	-0.401742	0.599163
73	9	0	7.475759	-0.994191	1.697745
74	9	0	7.704592	0.704607	0.357716
75	9	0	7.141942	-1.240238	-0.438372

TS2

Zero-point correction= 0.554276 (Hartree/Particle)
Thermal correction to Energy= 0.602021
Thermal correction to Enthalpy= 0.602965
Thermal correction to Gibbs Free Energy= 0.462540
E(sov) = -3127.61351666 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.557565	-0.267625	-0.750835
2	1	0	-6.373616	0.450558	-1.561714
3	1	0	-7.646374	-0.339417	-0.658691
4	6	0	-6.031270	-1.609408	-1.169678
5	8	0	-6.965501	-2.410956	-1.719714
6	6	0	-5.998293	0.306222	0.520421
7	8	0	-6.481573	1.543142	0.795760
8	7	0	-5.165874	-0.229845	1.320386
9	7	0	-4.827953	-2.046295	-1.124923
10	6	0	-6.285820	-3.619778	-2.160645
11	1	0	-6.776268	-4.469410	-1.681344
12	1	0	-6.408147	-3.691983	-3.244178
13	6	0	-4.821802	-3.401589	-1.710429
14	1	0	-4.110052	-3.441682	-2.540179
15	1	0	-4.498552	-4.124404	-0.954697
16	6	0	-5.811931	1.969133	2.018496
17	1	0	-5.219108	2.854781	1.779131
18	1	0	-6.584362	2.225408	2.747614
19	6	0	-4.952982	0.739411	2.411674
20	1	0	-5.265427	0.289433	3.360310
21	1	0	-3.888264	0.977085	2.486192
22	47	0	-3.008019	-1.156028	-0.161440
23	6	0	-0.810937	0.807250	0.734762
24	6	0	-1.110493	-0.501562	0.542914

25	6	0	-0.099045	-1.468765	0.958412
26	6	0	-0.339640	-2.859597	0.915874
27	6	0	1.172500	-1.043478	1.433923
28	6	0	0.629032	-3.778527	1.293066
29	1	0	-1.311377	-3.197955	0.563915
30	6	0	2.157711	-1.979749	1.795967
31	6	0	1.889260	-3.339957	1.724368
32	1	0	0.415634	-4.842813	1.236558
33	1	0	3.147250	-1.650657	2.091479
34	1	0	2.668416	-4.050517	1.980583
35	6	0	-1.648046	1.994416	0.454747
36	6	0	-1.593123	3.123795	1.293181
37	6	0	-2.502550	2.040133	-0.662079
38	6	0	-2.394971	4.238495	1.045663
39	1	0	-0.915590	3.123231	2.139964
40	6	0	-3.302623	3.156240	-0.909322
41	1	0	-2.509542	1.203244	-1.353729
42	6	0	-3.258792	4.260470	-0.052944
43	1	0	-2.337934	5.096299	1.710800
44	1	0	-3.946715	3.172486	-1.785200
45	1	0	-3.875606	5.133199	-0.250078
46	6	0	2.400262	0.965780	2.512102
47	1	0	1.940436	0.819800	3.496761
48	1	0	3.370974	0.469841	2.490751
49	1	0	2.543072	2.033985	2.335796
50	8	0	0.380136	1.221633	1.351301
51	6	0	1.452653	0.401785	1.470671
52	7	0	2.174346	-0.168034	-1.117297
53	7	0	1.785330	-0.958524	-1.812168
54	6	0	2.551813	0.704382	-0.154095
55	15	0	2.601746	2.440977	-0.738533
56	8	0	2.961298	3.384513	0.346747
57	8	0	3.552291	2.447132	-2.035863
58	8	0	1.153164	2.563851	-1.419449
59	6	0	4.994219	2.346213	-1.888446
60	1	0	5.336680	2.968893	-1.058311
61	1	0	5.273058	1.302160	-1.730722
62	1	0	5.414802	2.710099	-2.826824
63	6	0	0.712285	3.840588	-1.929055
64	1	0	1.228247	4.063741	-2.867327
65	1	0	-0.360240	3.743569	-2.097852
66	1	0	0.902119	4.628944	-1.195924
67	16	0	5.453849	-1.413795	0.100498
68	8	0	5.436758	-2.776215	0.652799
69	8	0	4.847941	-1.226234	-1.242380
70	8	0	5.030248	-0.339463	1.061613
71	1	0	3.539696	0.376985	0.241797

72	6	0	7.251378	-1.027633	-0.165721
73	9	0	7.792571	-1.882329	-1.044040
74	9	0	7.934026	-1.107704	0.983750
75	9	0	7.396677	0.221615	-0.653444

INT3

Zero-point correction= 0.555292 (Hartree/Particle)
Thermal correction to Energy= 0.603159
Thermal correction to Enthalpy= 0.604103
Thermal correction to Gibbs Free Energy= 0.463839
E(sov) = -3127.61461987 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.403494	-0.263094	-0.873596
2	1	0	-6.128387	0.435630	-1.675363
3	1	0	-7.497813	-0.288322	-0.856848
4	6	0	-5.902447	-1.631544	-1.233187
5	8	0	-6.846484	-2.445482	-1.746949
6	6	0	-5.904766	0.300775	0.427538
7	8	0	-6.351788	1.559634	0.663460
8	7	0	-5.142598	-0.261194	1.277396
9	7	0	-4.705144	-2.081891	-1.165373
10	6	0	-6.182863	-3.684279	-2.124330
11	1	0	-6.684904	-4.501686	-1.602757
12	1	0	-6.305707	-3.810345	-3.202917
13	6	0	-4.715985	-3.463612	-1.683880
14	1	0	-4.004366	-3.553688	-2.509933
15	1	0	-4.402614	-4.152863	-0.893456
16	6	0	-5.744650	1.966400	1.924676
17	1	0	-5.117074	2.837130	1.723109
18	1	0	-6.552282	2.240906	2.608012
19	6	0	-4.942747	0.713942	2.365321
20	1	0	-5.304919	0.287390	3.306981
21	1	0	-3.873879	0.917409	2.476661
22	47	0	-2.898645	-1.179000	-0.196748
23	6	0	-0.770568	0.839067	0.740969
24	6	0	-1.053270	-0.476484	0.582906
25	6	0	-0.067656	-1.427910	1.112643
26	6	0	-0.345556	-2.806284	1.203941
27	6	0	1.204717	-0.991220	1.559064
28	6	0	0.593705	-3.713117	1.684322
29	1	0	-1.323893	-3.152971	0.878090
30	6	0	2.156661	-1.906390	2.021911
31	6	0	1.855709	-3.266445	2.083380

32	1	0	0.349374	-4.771285	1.731733
33	1	0	3.151005	-1.575643	2.299297
34	1	0	2.613635	-3.966302	2.420587
35	6	0	-1.626320	1.999183	0.403219
36	6	0	-1.622214	3.146379	1.219919
37	6	0	-2.448173	2.007452	-0.739032
38	6	0	-2.440823	4.238279	0.928135
39	1	0	-0.970575	3.175124	2.086254
40	6	0	-3.264790	3.100811	-1.031329
41	1	0	-2.417781	1.157971	-1.414645
42	6	0	-3.271864	4.221942	-0.195782
43	1	0	-2.422887	5.108858	1.579133
44	1	0	-3.882687	3.085963	-1.926139
45	1	0	-3.902657	5.076110	-0.427112
46	6	0	2.398316	1.042181	2.569704
47	1	0	1.887532	0.839919	3.515223
48	1	0	3.387253	0.581396	2.584035
49	1	0	2.514940	2.120383	2.443520
50	8	0	0.386132	1.292745	1.393248
51	6	0	1.529976	0.482145	1.436203
52	7	0	2.008587	-0.129355	-0.980355
53	7	0	1.706082	-0.836081	-1.785362
54	6	0	2.416622	0.710612	0.059853
55	15	0	2.564495	2.453984	-0.606129
56	8	0	3.005525	3.409961	0.433488
57	8	0	3.489037	2.301598	-1.904580
58	8	0	1.121162	2.624580	-1.273436
59	6	0	4.940389	2.233253	-1.810864
60	1	0	5.291793	2.737201	-0.907986
61	1	0	5.236749	1.184915	-1.810988
62	1	0	5.322808	2.743087	-2.696359
63	6	0	0.694661	3.922272	-1.749764
64	1	0	1.204485	4.155041	-2.688928
65	1	0	-0.380531	3.843006	-1.906390
66	1	0	0.907412	4.688677	-1.000681
67	16	0	5.323493	-1.390849	0.007333
68	8	0	5.294256	-2.732543	0.602219
69	8	0	4.629214	-1.214296	-1.295699
70	8	0	5.000710	-0.265300	0.952896
71	1	0	3.455748	0.358571	0.316412
72	6	0	7.115306	-1.090378	-0.386070
73	9	0	7.553543	-1.986991	-1.278505
74	9	0	7.864599	-1.182279	0.718704
75	9	0	7.289126	0.140833	-0.909458

TS3

Zero-point correction= 0.550780 (Hartree/Particle)
Thermal correction to Energy= 0.598144
Thermal correction to Enthalpy= 0.599089
Thermal correction to Gibbs Free Energy= 0.460682
E(sov) = -3127.59677562 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.250812	-0.070513	-1.001059
2	1	0	-5.776966	0.584857	-1.743701
3	1	0	-7.331572	0.041197	-1.129829
4	6	0	-5.872483	-1.493022	-1.292324
5	8	0	-6.882301	-2.268694	-1.732670
6	6	0	-5.858848	0.421155	0.365559
7	8	0	-6.228121	1.706015	0.595125
8	7	0	-5.231356	-0.221946	1.265759
9	7	0	-4.709298	-2.023537	-1.210885
10	6	0	-6.318340	-3.579246	-2.020474
11	1	0	-6.863765	-4.313200	-1.423601
12	1	0	-6.478048	-3.782075	-3.082348
13	6	0	-4.828022	-3.433224	-1.628326
14	1	0	-4.146125	-3.631242	-2.460747
15	1	0	-4.543481	-4.085834	-0.797001
16	6	0	-5.738143	2.025397	1.929792
17	1	0	-5.053524	2.870658	1.836419
18	1	0	-6.599879	2.310501	2.539480
19	6	0	-5.048908	0.713666	2.390227
20	1	0	-5.498402	0.292817	3.295943
21	1	0	-3.978515	0.845664	2.575222
22	47	0	-2.873592	-1.188560	-0.254455
23	6	0	-0.748263	0.780129	0.777648
24	6	0	-1.042517	-0.527487	0.579053
25	6	0	-0.077556	-1.501360	1.109126
26	6	0	-0.389991	-2.871492	1.208491
27	6	0	1.202076	-1.091292	1.559624
28	6	0	0.518944	-3.797943	1.709761
29	1	0	-1.374023	-3.196235	0.877088
30	6	0	2.119292	-2.026049	2.050062
31	6	0	1.783901	-3.378087	2.126166
32	1	0	0.245995	-4.848740	1.766518
33	1	0	3.111427	-1.714719	2.356809
34	1	0	2.513050	-4.093038	2.495155
35	6	0	-1.594378	1.955120	0.465782
36	6	0	-1.606331	3.066629	1.329728
37	6	0	-2.385067	2.015690	-0.696147
38	6	0	-2.410994	4.175062	1.062633

39	1	0	-0.975322	3.054683	2.211738
40	6	0	-3.187083	3.125863	-0.964526
41	1	0	-2.337905	1.196078	-1.406941
42	6	0	-3.211040	4.211134	-0.083292
43	1	0	-2.405371	5.018271	1.749179
44	1	0	-3.779478	3.153519	-1.876195
45	1	0	-3.830872	5.078239	-0.295672
46	6	0	2.437316	0.920270	2.558453
47	1	0	1.913305	0.746941	3.502412
48	1	0	3.410390	0.429522	2.592874
49	1	0	2.596213	1.991577	2.422071
50	8	0	0.404390	1.200838	1.449117
51	6	0	1.560899	0.378795	1.421712
52	7	0	1.919129	-0.193204	-0.979761
53	7	0	1.666218	-0.900463	-1.814427
54	6	0	2.349274	0.605380	0.032228
55	15	0	2.578751	2.325022	-0.587186
56	8	0	3.203170	3.220064	0.416219
57	8	0	3.371172	2.151356	-1.979306
58	8	0	1.113030	2.682335	-1.131144
59	6	0	4.817016	2.114134	-2.037442
60	1	0	5.256113	2.487405	-1.109661
61	1	0	5.128862	1.085582	-2.220672
62	1	0	5.114435	2.754426	-2.870669
63	6	0	0.812931	4.028383	-1.556061
64	1	0	1.288240	4.228263	-2.521279
65	1	0	-0.271897	4.077379	-1.649636
66	1	0	1.157004	4.748997	-0.809546
67	16	0	5.329789	-1.432755	-0.158400
68	8	0	5.350898	-2.678595	0.600899
69	8	0	4.794362	-1.416962	-1.526059
70	8	0	4.750684	-0.239839	0.665538
71	1	0	3.670080	0.124692	0.301205
72	6	0	7.104827	-0.882424	-0.271558
73	9	0	7.794390	-1.791971	-0.965022
74	9	0	7.631959	-0.765208	0.947425
75	9	0	7.194055	0.298154	-0.900028

INT4

Zero-point correction= 0.555561 (Hartree/Particle)
Thermal correction to Energy= 0.603371
Thermal correction to Enthalpy= 0.604316
Thermal correction to Gibbs Free Energy= 0.464492
E(sov) = -3127.60736495 A.U.

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	4.343882	-0.736904	-1.066218
2	1	0	3.642198	-0.304757	-1.793579
3	1	0	5.323038	-0.753229	-1.553663
4	6	0	4.410605	0.178302	0.120035
5	8	0	5.517901	0.943088	0.175770
6	6	0	3.912800	-2.148710	-0.779649
7	8	0	4.008820	-2.961956	-1.865596
8	7	0	3.467791	-2.623303	0.313442
9	7	0	3.528061	0.344535	1.032178
10	6	0	5.324881	1.878208	1.276825
11	1	0	6.212806	1.831392	1.910119
12	1	0	5.221533	2.875156	0.843620
13	6	0	4.029137	1.380699	1.955244
14	1	0	3.284390	2.172454	2.060278
15	1	0	4.204309	0.933003	2.939860
16	6	0	3.557253	-4.272446	-1.421594
17	1	0	2.736141	-4.579400	-2.071379
18	1	0	4.396412	-4.966294	-1.528241
19	6	0	3.127369	-4.032294	0.048640
20	1	0	3.654081	-4.680736	0.756438
21	1	0	2.052090	-4.172713	0.197081
22	47	0	1.530348	-0.633102	1.221605
23	6	0	-1.260212	-1.821593	0.573605
24	6	0	-0.521436	-1.101191	1.451972
25	6	0	-1.237861	-0.613636	2.641763
26	6	0	-0.558592	-0.200622	3.804555
27	6	0	-2.653092	-0.558412	2.659832
28	6	0	-1.241543	0.253890	4.929384
29	1	0	0.527950	-0.250793	3.807829
30	6	0	-3.335882	-0.089657	3.784479
31	6	0	-2.636947	0.315983	4.922631
32	1	0	-0.685981	0.562908	5.811436
33	1	0	-4.420454	-0.038221	3.782419
34	1	0	-3.178144	0.678106	5.792518
35	6	0	-0.805863	-2.520715	-0.650215
36	6	0	-1.372538	-3.760166	-1.002499
37	6	0	0.153689	-1.962005	-1.512705
38	6	0	-0.966462	-4.433490	-2.154053
39	1	0	-2.138284	-4.189108	-0.364900
40	6	0	0.552765	-2.632269	-2.670801
41	1	0	0.550124	-0.975300	-1.294716
42	6	0	-0.000084	-3.875230	-2.995686
43	1	0	-1.413279	-5.393827	-2.399616
44	1	0	1.289327	-2.175929	-3.327651
45	1	0	0.304768	-4.392267	-3.902308

46	6	0	-4.763644	-1.571772	1.626708
47	1	0	-4.696366	-2.382149	2.358208
48	1	0	-5.444000	-0.804480	2.005641
49	1	0	-5.170576	-1.954661	0.690325
50	8	0	-2.630489	-2.057185	0.771781
51	6	0	-3.363702	-0.997656	1.389508
52	7	0	-2.692807	1.225564	0.544999
53	7	0	-2.073952	2.173777	0.738372
54	6	0	-3.436082	0.186592	0.361136
55	15	0	-4.147666	0.042127	-1.292493
56	8	0	-5.295284	-0.893303	-1.402371
57	8	0	-4.466068	1.574727	-1.726816
58	8	0	-2.854526	-0.261885	-2.191360
59	6	0	-5.725314	2.155388	-1.343619
60	1	0	-6.554105	1.505480	-1.636201
61	1	0	-5.757781	2.327879	-0.261681
62	1	0	-5.793821	3.111465	-1.865484
63	6	0	-3.003837	-0.769656	-3.533235
64	1	0	-3.239590	0.052098	-4.216680
65	1	0	-2.043147	-1.214725	-3.793188
66	1	0	-3.790851	-1.527048	-3.569076
67	16	0	1.451018	2.964220	-0.744494
68	8	0	2.819127	3.344397	-0.428760
69	8	0	1.138605	1.786723	-1.543269
70	8	0	0.638462	2.975049	0.636055
71	1	0	-0.251547	2.527835	0.560600
72	6	0	0.653874	4.418625	-1.599656
73	9	0	1.176651	4.535528	-2.819081
74	9	0	0.875554	5.532435	-0.907511
75	9	0	-0.659303	4.200638	-1.691060

TS4

Zero-point correction= 0.552594 (Hartree/Particle)
Thermal correction to Energy= 0.599885
Thermal correction to Enthalpy= 0.600829
Thermal correction to Gibbs Free Energy= 0.461880
E(sov) = -3127.61202449 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.465226	-0.773389	0.583111
2	1	0	-5.595107	-0.523222	1.643897
3	1	0	-6.455988	-1.110581	0.250977
4	6	0	-5.144808	0.497059	-0.148252
5	8	0	-6.168755	1.379575	-0.099486

6	6	0	-4.512589	-1.928379	0.486868
7	8	0	-4.774958	-2.891447	1.407083
8	7	0	-3.559409	-2.113666	-0.338487
9	7	0	-4.075347	0.862001	-0.744629
10	6	0	-5.715480	2.592160	-0.765067
11	1	0	-6.404737	2.796330	-1.587908
12	1	0	-5.763547	3.407203	-0.039054
13	6	0	-4.277577	2.246932	-1.217995
14	1	0	-3.518246	2.887381	-0.762733
15	1	0	-4.154161	2.282718	-2.305015
16	6	0	-3.743399	-3.904857	1.232322
17	1	0	-3.117599	-3.899757	2.128746
18	1	0	-4.240118	-4.872525	1.133198
19	6	0	-2.988329	-3.440633	-0.036536
20	1	0	-3.152312	-4.101470	-0.895350
21	1	0	-1.911232	-3.354335	0.123847
22	47	0	-2.017205	-0.108061	-0.882999
23	6	0	0.698863	-1.335476	-0.145652
24	6	0	0.121862	-0.499315	-1.060800
25	6	0	0.718000	-0.525707	-2.412532
26	6	0	0.036827	0.007740	-3.522565
27	6	0	1.981791	-1.117549	-2.644917
28	6	0	0.569953	-0.049723	-4.807392
29	1	0	-0.933591	0.471515	-3.357525
30	6	0	2.513246	-1.178071	-3.935096
31	6	0	1.812745	-0.648586	-5.020302
32	1	0	0.016954	0.373829	-5.641858
33	1	0	3.484596	-1.633366	-4.102722
34	1	0	2.239393	-0.696893	-6.018298
35	6	0	0.214119	-1.651646	1.223026
36	6	0	0.593197	-2.861300	1.836124
37	6	0	-0.621220	-0.778304	1.944543
38	6	0	0.116901	-3.203356	3.102846
39	1	0	1.268961	-3.527878	1.313787
40	6	0	-1.083139	-1.116360	3.215260
41	1	0	-0.890146	0.184049	1.524379
42	6	0	-0.727543	-2.336350	3.799446
43	1	0	0.419980	-4.146725	3.550187
44	1	0	-1.712374	-0.414507	3.757044
45	1	0	-1.088110	-2.596797	4.791214
46	6	0	3.635400	-2.836508	-1.701520
47	1	0	3.040130	-3.639141	-2.147869
48	1	0	4.450884	-2.576164	-2.381354
49	1	0	4.069597	-3.179934	-0.760483
50	8	0	1.810903	-2.095869	-0.432885
51	6	0	2.744000	-1.618514	-1.429263
52	7	0	3.616087	0.694308	-1.367384

53	7	0	3.688499	1.704821	-1.888510
54	6	0	3.574314	-0.477406	-0.790443
55	15	0	4.321025	-0.598580	0.830109
56	8	0	4.769611	-1.963481	1.211943
57	8	0	5.486745	0.535415	0.844104
58	8	0	3.229868	0.105307	1.783379
59	6	0	6.798968	0.187658	0.372468
60	1	0	7.154950	-0.724429	0.859024
61	1	0	6.794909	0.045041	-0.714360
62	1	0	7.449180	1.027510	0.624218
63	6	0	3.423339	0.080099	3.210793
64	1	0	4.315397	0.653217	3.483365
65	1	0	2.537469	0.547016	3.640220
66	1	0	3.516635	-0.950099	3.564518
67	16	0	-0.218945	3.171510	0.291216
68	8	0	-0.174282	4.496143	-0.307037
69	8	0	-1.494670	2.609998	0.754558
70	8	0	0.567644	2.149649	-0.605907
71	1	0	0.187675	1.147513	-0.632786
72	6	0	0.885519	3.226097	1.791434
73	9	0	0.414124	4.144336	2.640198
74	9	0	2.129219	3.541717	1.442796
75	9	0	0.881420	2.032328	2.396576

3a+L6Ag

Zero-point correction= 0.556921 (Hartree/Particle)
Thermal correction to Energy= 0.604949
Thermal correction to Enthalpy= 0.605893
Thermal correction to Gibbs Free Energy= 0.463792
E(sov) = -3127.68044228 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.911811	3.409916	-1.291788
2	1	0	-0.865599	4.390750	-1.779520
3	1	0	-0.173432	3.459305	-0.478420
4	6	0	-2.264574	3.259240	-0.660503
5	8	0	-2.579999	4.311169	0.132172
6	6	0	-0.432969	2.386158	-2.280068
7	8	0	0.644127	2.818187	-2.973894
8	7	0	-0.856489	1.204060	-2.528043
9	7	0	-3.102384	2.302733	-0.753204
10	6	0	-3.853979	3.984666	0.759075
11	1	0	-3.684234	3.923187	1.837014
12	1	0	-4.547977	4.800791	0.544724

13	6	0	-4.246676	2.631019	0.118403
14	1	0	-5.156759	2.696999	-0.487598
15	1	0	-4.372574	1.826693	0.847598
16	6	0	1.109950	1.691145	-3.773648
17	1	0	1.232086	2.043029	-4.799499
18	1	0	2.071884	1.374279	-3.365769
19	6	0	0.001669	0.633453	-3.586538
20	1	0	0.396936	-0.332396	-3.264850
21	1	0	-0.600559	0.477813	-4.488590
22	47	0	-2.397669	0.052852	-1.297894
23	6	0	1.257256	-0.698155	-0.186759
24	6	0	0.483846	-0.417815	0.889569
25	6	0	0.530104	0.909001	1.481351
26	6	0	-0.489836	1.380463	2.329200
27	6	0	1.607432	1.766066	1.156808
28	6	0	-0.438988	2.676497	2.837754
29	1	0	-1.329032	0.729788	2.559478
30	6	0	1.643454	3.065387	1.670023
31	6	0	0.622195	3.524905	2.507117
32	1	0	-1.228702	3.026266	3.497619
33	1	0	2.474347	3.723599	1.434696
34	1	0	0.664399	4.533896	2.907406
35	6	0	1.225314	-1.921529	-1.007182
36	6	0	2.271196	-2.191215	-1.911242
37	6	0	0.152635	-2.830983	-0.917381
38	6	0	2.241731	-3.340189	-2.702380
39	1	0	3.110458	-1.507237	-1.974602
40	6	0	0.137089	-3.978848	-1.706208
41	1	0	-0.674433	-2.646508	-0.239722
42	6	0	1.177160	-4.238284	-2.604074
43	1	0	3.058537	-3.535343	-3.392802
44	1	0	-0.698348	-4.668230	-1.621772
45	1	0	1.156413	-5.133055	-3.220725
46	6	0	3.444338	2.200789	-0.576802
47	1	0	2.721277	2.736646	-1.199404
48	1	0	3.985308	2.922856	0.040593
49	1	0	4.165653	1.683473	-1.212472
50	8	0	2.149590	0.240548	-0.656490
51	6	0	2.721624	1.173448	0.302264
52	7	0	3.544093	0.333346	2.472075
53	7	0	3.404334	0.290443	3.601487
54	6	0	3.739305	0.409682	1.181000
55	15	0	5.056352	-0.612738	0.527737
56	8	0	5.407197	-0.315247	-0.887014
57	8	0	6.289416	-0.487450	1.578612
58	8	0	4.545349	-2.097273	0.871825
59	6	0	7.197245	0.619495	1.451866

60	1	0	7.602687	0.671299	0.437790
61	1	0	6.691495	1.561319	1.694532
62	1	0	7.999963	0.443592	2.169968
63	6	0	5.337113	-3.239308	0.488665
64	1	0	6.254819	-3.278258	1.082912
65	1	0	4.721495	-4.115830	0.693615
66	1	0	5.579713	-3.196835	-0.576880
67	16	0	-3.370469	-1.656416	1.147280
68	8	0	-3.579681	-0.286059	1.667234
69	8	0	-3.359254	-1.717203	-0.366838
70	8	0	-2.295341	-2.441780	1.775749
71	1	0	-0.216194	-1.148588	1.279122
72	6	0	-4.946441	-2.562752	1.534764
73	9	0	-5.994459	-1.913171	1.009001
74	9	0	-5.111606	-2.639065	2.860669
75	9	0	-4.911424	-3.801133	1.031138

TS2-C

Zero-point correction= 0.522076 (Hartree/Particle)
Thermal correction to Energy= 0.560786
Thermal correction to Enthalpy= 0.561730
Thermal correction to Gibbs Free Energy= 0.442168
E(sov) = -2165.84029319 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.449034	0.216567	1.050644
2	1	0	5.836002	1.196529	1.361072
3	1	0	6.306526	-0.460611	1.153927
4	6	0	4.408430	-0.204799	2.044918
5	8	0	4.919270	-0.317006	3.286253
6	6	0	5.096861	0.298293	-0.404315
7	8	0	6.153541	0.658321	-1.159067
8	7	0	3.982042	0.083613	-0.993088
9	7	0	3.162165	-0.448797	1.884018
10	6	0	3.823515	-0.697593	4.166792
11	1	0	4.099933	-1.635086	4.653251
12	1	0	3.716397	0.086102	4.919955
13	6	0	2.614775	-0.816516	3.207854
14	1	0	1.798087	-0.137017	3.469385
15	1	0	2.206236	-1.830957	3.164663
16	6	0	5.690374	0.713874	-2.539258
17	1	0	5.850744	1.731690	-2.901074
18	1	0	6.300286	0.019610	-3.120865
19	6	0	4.199469	0.310489	-2.437559

20	1	0	3.969220	-0.605965	-2.989631
21	1	0	3.522280	1.093940	-2.790432
22	47	0	1.850643	-0.420312	-0.077386
23	6	0	-1.025565	0.379060	-0.998603
24	6	0	-0.129398	-0.701512	-0.835001
25	6	0	-0.693858	-2.005049	-1.152659
26	6	0	0.134441	-3.136415	-1.298209
27	6	0	-2.097779	-2.163164	-1.326589
28	6	0	-0.399095	-4.378508	-1.623599
29	1	0	1.205828	-3.014344	-1.162320
30	6	0	-2.628399	-3.419292	-1.612546
31	6	0	-1.781751	-4.520713	-1.773785
32	1	0	0.253332	-5.237514	-1.746917
33	1	0	-3.699237	-3.551157	-1.728809
34	1	0	-2.205710	-5.491541	-2.013070
35	6	0	-0.607221	1.813594	-1.018443
36	6	0	-0.893045	2.604246	-2.142014
37	6	0	0.072857	2.387610	0.065446
38	6	0	-0.477707	3.936107	-2.188552
39	1	0	-1.435383	2.171585	-2.976272
40	6	0	0.479535	3.722376	0.018762
41	1	0	0.259800	1.796819	0.958370
42	6	0	0.210315	4.499032	-1.110273
43	1	0	-0.693909	4.534809	-3.068968
44	1	0	0.992351	4.158514	0.871496
45	1	0	0.525030	5.537995	-1.146106
46	6	0	-4.325199	-0.946705	-1.779024
47	1	0	-4.226502	-1.199770	-2.838681
48	1	0	-4.973038	-1.681540	-1.294796
49	1	0	-4.790275	0.036729	-1.694187
50	8	0	-2.232590	0.180413	-1.699190
51	6	0	-2.947550	-0.916332	-1.134121
52	7	0	-2.890542	-1.608440	1.256751
53	7	0	-2.784077	-2.477330	1.973295
54	6	0	-2.979818	-0.565567	0.427891
55	1	0	-1.596844	0.008654	0.212993
56	15	0	-4.010214	0.747653	1.213100
57	8	0	-3.429742	1.246120	2.482425
58	8	0	-4.243315	1.827160	0.056124
59	8	0	-5.403732	-0.049157	1.293590
60	6	0	-3.795183	3.204234	0.173190
61	1	0	-3.303618	3.366261	1.133864
62	1	0	-3.106484	3.398365	-0.648928
63	1	0	-4.679794	3.838393	0.088708
64	6	0	-6.542811	0.568234	1.944544
65	1	0	-6.876876	1.435666	1.368313
66	1	0	-7.325662	-0.189851	1.961281

67	1	0	-6.281646	0.864108	2.963529

INT3-C

Zero-point correction= 0.527584 (Hartree/Particle)
Thermal correction to Energy= 0.566479
Thermal correction to Enthalpy= 0.567423
Thermal correction to Gibbs Free Energy= 0.447606
E(sov) = -2165.86470947 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.291463	-1.149691	0.813147
2	1	0	5.908989	-0.862435	1.672117
3	1	0	5.933991	-1.815424	0.219564
4	6	0	4.135066	-1.956121	1.325197
5	8	0	4.524317	-2.904336	2.196708
6	6	0	5.023514	0.083924	0.003237
7	8	0	6.125866	0.839391	-0.153742
8	7	0	3.940509	0.479869	-0.552262
9	7	0	2.888987	-1.874788	1.043626
10	6	0	3.328987	-3.640057	2.589675
11	1	0	3.468911	-4.681060	2.290414
12	1	0	3.247149	-3.580325	3.676540
13	6	0	2.192020	-2.915877	1.829546
14	1	0	1.466737	-2.442117	2.498210
15	1	0	1.643752	-3.580146	1.155068
16	6	0	5.748396	1.978338	-0.981254
17	1	0	5.971546	2.884881	-0.415339
18	1	0	6.364031	1.949727	-1.882825
19	6	0	4.239639	1.752788	-1.242467
20	1	0	4.005727	1.654644	-2.306964
21	1	0	3.608857	2.546163	-0.830361
22	47	0	1.773495	-0.387738	-0.381859
23	6	0	-0.993945	0.902672	-0.130934
24	6	0	-0.195081	0.041223	-1.029566
25	6	0	-0.849380	-0.463670	-2.191660
26	6	0	-0.090770	-1.139645	-3.184138
27	6	0	-2.262795	-0.324773	-2.372549
28	6	0	-0.688506	-1.640117	-4.328978
29	1	0	0.979249	-1.240888	-3.025007
30	6	0	-2.851840	-0.865907	-3.511203
31	6	0	-2.073392	-1.506772	-4.483276
32	1	0	-0.098260	-2.142384	-5.088604
33	1	0	-3.922846	-0.794070	-3.664490
34	1	0	-2.558957	-1.912069	-5.366689

35	6	0	-0.251735	2.143448	0.343076
36	6	0	0.168024	3.108051	-0.584010
37	6	0	-0.007493	2.340006	1.706712
38	6	0	0.841324	4.250135	-0.150398
39	1	0	-0.051752	2.972465	-1.639921
40	6	0	0.673095	3.482265	2.137799
41	1	0	-0.374192	1.611787	2.425011
42	6	0	1.100660	4.435650	1.211771
43	1	0	1.152425	5.000973	-0.871762
44	1	0	0.854055	3.633352	3.198329
45	1	0	1.619735	5.328295	1.549558
46	6	0	-4.274010	1.148611	-1.828946
47	1	0	-3.936703	1.884026	-2.565798
48	1	0	-5.008594	0.484069	-2.291025
49	1	0	-4.766065	1.665759	-1.003623
50	8	0	-2.266225	1.345106	-0.635400
51	6	0	-3.077650	0.359855	-1.276586
52	7	0	-3.779391	-1.900245	-0.568480
53	7	0	-3.981524	-2.973333	-0.900105
54	6	0	-3.538530	-0.670570	-0.212894
55	1	0	-1.168534	0.263138	0.760946
56	15	0	-3.793137	-0.227939	1.513088
57	8	0	-2.556947	-0.052137	2.334310
58	8	0	-4.741299	1.074900	1.496440
59	8	0	-4.759283	-1.435516	1.940562
60	6	0	-4.276823	2.345739	2.012431
61	1	0	-3.804012	2.215754	2.987653
62	1	0	-3.567741	2.792146	1.311625
63	1	0	-5.166867	2.969768	2.101726
64	6	0	-5.103225	-1.626745	3.331490
65	1	0	-5.789920	-0.839509	3.655195
66	1	0	-5.598622	-2.596125	3.388669
67	1	0	-4.202846	-1.623997	3.951053

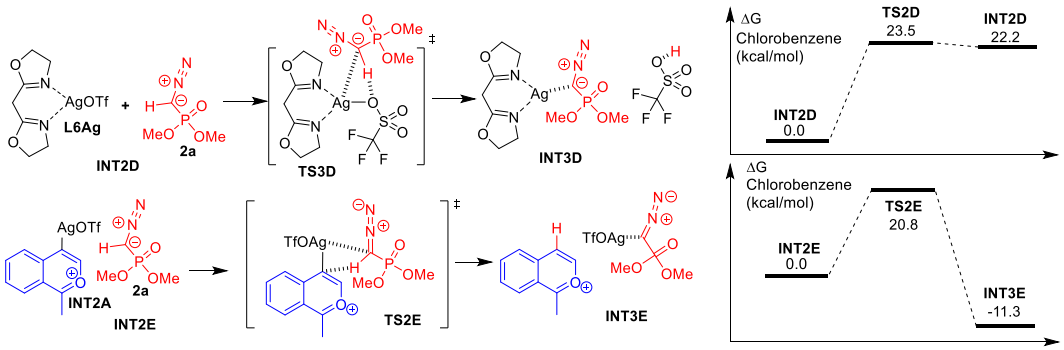
TS3-C

Zero-point correction= 0.523328 (Hartree/Particle)
Thermal correction to Energy= 0.562284
Thermal correction to Enthalpy= 0.563228
Thermal correction to Gibbs Free Energy= 0.443859
E(sov) = -2165.82724075 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.808618	-0.406115	0.327370
2	1	0	6.607267	0.026810	0.939139

3	1	0	6.326484	-1.058837	-0.390342
4	6	0	4.966799	-1.271980	1.218532
5	8	0	5.711898	-1.963264	2.101073
6	6	0	5.152090	0.705427	-0.437211
7	8	0	6.045009	1.597127	-0.913399
8	7	0	3.915759	0.885848	-0.702280
9	7	0	3.698773	-1.456590	1.231271
10	6	0	4.803344	-2.812040	2.859091
11	1	0	5.085592	-3.850409	2.670732
12	1	0	4.941735	-2.582920	3.917238
13	6	0	3.409553	-2.431390	2.306210
14	1	0	2.766946	-1.963899	3.058944
15	1	0	2.870758	-3.288619	1.891848
16	6	0	5.286228	2.588898	-1.664888
17	1	0	5.492383	3.565985	-1.222927
18	1	0	5.648785	2.572387	-2.695148
19	6	0	3.818249	2.121419	-1.506416
20	1	0	3.340298	1.896353	-2.464728
21	1	0	3.190535	2.847838	-0.981652
22	47	0	2.009573	-0.464867	-0.032809
23	6	0	-0.856591	0.734729	-0.590459
24	6	0	-0.049426	-0.368330	-0.641416
25	6	0	-0.782525	-1.624420	-1.221507
26	6	0	0.010205	-2.706445	-1.769414
27	6	0	-2.161341	-1.509200	-1.681812
28	6	0	-0.517537	-3.595335	-2.678053
29	1	0	1.039797	-2.789598	-1.432924
30	6	0	-2.649550	-2.396561	-2.625966
31	6	0	-1.843143	-3.433478	-3.117141
32	1	0	0.087862	-4.407467	-3.067735
33	1	0	-3.670426	-2.312044	-2.980608
34	1	0	-2.258985	-4.130543	-3.838826
35	6	0	-0.343416	2.089924	-0.276790
36	6	0	-0.733897	3.190329	-1.062431
37	6	0	0.513013	2.307725	0.816750
38	6	0	-0.250770	4.466208	-0.780401
39	1	0	-1.410201	3.036387	-1.896662
40	6	0	0.985490	3.589371	1.102634
41	1	0	0.773950	1.476745	1.465208
42	6	0	0.612363	4.670935	0.300772
43	1	0	-0.551873	5.304362	-1.402351
44	1	0	1.629174	3.744848	1.964044
45	1	0	0.977754	5.668928	0.525448
46	6	0	-4.155839	0.047341	-1.982458
47	1	0	-3.776897	0.258736	-2.985907
48	1	0	-4.937365	-0.713279	-2.030463
49	1	0	-4.595282	0.959525	-1.576712

50	8	0	-2.161932	0.796555	-0.992863
51	6	0	-3.001570	-0.396974	-1.073862
52	7	0	-2.999798	-1.752877	0.980168
53	7	0	-2.554342	-2.627415	1.561284
54	6	0	-3.530794	-0.756878	0.320937
55	1	0	-0.809477	-1.795236	-0.099996
56	15	0	-4.839005	0.078566	1.254504
57	8	0	-4.741343	-0.206473	2.705403
58	8	0	-4.783409	1.631317	0.822392
59	8	0	-6.155743	-0.404967	0.471301
60	6	0	-3.979886	2.569889	1.573406
61	1	0	-2.951994	2.550838	1.201651
62	1	0	-4.417374	3.553699	1.397733
63	1	0	-4.007951	2.329961	2.638645
64	6	0	-7.454091	0.033076	0.941922
65	1	0	-7.566889	1.108690	0.781397
66	1	0	-8.188386	-0.513049	0.349397
67	1	0	-7.573089	-0.207796	2.001275



INT2D

Zero-point correction= 0.321384 (Hartree/Particle)
Thermal correction to Energy= 0.355352
Thermal correction to Enthalpy= 0.356296
Thermal correction to Gibbs Free Energy= 0.246468
E(sov) = -2435.41490455 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.278687	-0.756007	1.072002
2	1	0	-4.198061	-1.029286	1.598476
3	1	0	-3.390340	0.294634	0.754013
4	6	0	-2.138858	-0.780006	2.044313
5	8	0	-2.451265	-0.205658	3.227007
6	6	0	-3.180944	-1.576181	-0.177800
7	8	0	-4.390737	-1.885243	-0.694757

8	7	0	-2.147001	-1.943174	-0.839474
9	7	0	-0.945296	-1.209152	1.887899
10	6	0	-1.200540	-0.087745	3.964324
11	1	0	-0.938737	0.973547	3.991979
12	1	0	-1.375776	-0.453183	4.977891
13	6	0	-0.209060	-0.935475	3.137481
14	1	0	0.041169	-1.887407	3.620639
15	1	0	0.722795	-0.417503	2.901774
16	6	0	-4.154923	-2.542723	-1.969243
17	1	0	-4.661320	-3.510256	-1.943450
18	1	0	-4.597794	-1.920340	-2.750920
19	6	0	-2.612891	-2.638387	-2.053497
20	1	0	-2.205859	-2.136589	-2.935774
21	1	0	-2.250057	-3.671697	-2.049388
22	47	0	0.046534	-1.501337	-0.224912
23	15	0	-1.167205	2.573854	-0.155246
24	8	0	-2.543480	2.007851	-0.159691
25	8	0	-0.363722	2.315259	1.204229
26	8	0	-1.066177	4.187314	-0.246988
27	6	0	0.896944	2.963205	1.510246
28	1	0	0.749262	4.043539	1.572326
29	1	0	1.207808	2.563878	2.475527
30	1	0	1.654102	2.709092	0.765396
31	6	0	-1.690937	4.868113	-1.345720
32	1	0	-2.766589	4.668899	-1.359195
33	1	0	-1.512982	5.933378	-1.190372
34	1	0	-1.241878	4.558067	-2.296287
35	6	0	-0.166095	1.915725	-1.481319
36	1	0	0.923743	1.922035	-1.490341
37	7	0	-0.751865	1.230632	-2.420358
38	7	0	-1.278629	0.639638	-3.240706
39	16	0	2.842405	-0.023475	-0.169297
40	8	0	2.907966	1.317969	-0.789218
41	8	0	2.493762	-0.067062	1.264967
42	8	0	2.082352	-1.031026	-1.003199
43	6	0	4.576039	-0.685247	-0.268122
44	9	0	5.403010	0.105579	0.426449
45	9	0	4.625333	-1.919017	0.250199
46	9	0	4.988623	-0.733526	-1.538907

TS3D

Zero-point correction= 0.320100 (Hartree/Particle)
Thermal correction to Energy= 0.353671
Thermal correction to Enthalpy= 0.354615
Thermal correction to Gibbs Free Energy= 0.245610
E(sov) = -2435.37664647 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.338092	-0.894349	0.875158
2	1	0	-5.282761	-1.444013	0.869785
3	1	0	-4.337320	-0.278775	1.785243
4	6	0	-3.206882	-1.879993	0.952276
5	8	0	-3.590044	-3.161588	1.104436
6	6	0	-4.307884	0.027641	-0.315331
7	8	0	-5.497292	0.633734	-0.553403
8	7	0	-3.313765	0.301755	-1.061667
9	7	0	-1.950322	-1.634237	0.926853
10	6	0	-2.372916	-3.957057	1.218280
11	1	0	-2.387876	-4.440690	2.198156
12	1	0	-2.402062	-4.717620	0.435529
13	6	0	-1.235625	-2.922695	1.045975
14	1	0	-0.635063	-3.091564	0.148281
15	1	0	-0.551586	-2.886472	1.897696
16	6	0	-5.264615	1.548357	-1.664250
17	1	0	-5.992941	1.315512	-2.444297
18	1	0	-5.435535	2.564809	-1.299566
19	6	0	-3.792810	1.271565	-2.065956
20	1	0	-3.167415	2.168099	-2.044484
21	1	0	-3.702362	0.829704	-3.064051
22	47	0	-0.952383	0.255855	0.280377
23	15	0	1.495854	2.807161	0.642544
24	8	0	1.794611	4.214158	0.279045
25	8	0	1.188404	2.680209	2.233911
26	8	0	2.762105	1.772750	0.430464
27	6	0	1.097381	1.434704	2.926049
28	1	0	1.874391	0.735059	2.603343
29	1	0	1.216456	1.657664	3.989618
30	1	0	0.113372	0.976354	2.763590
31	6	0	4.074506	2.240110	0.793095
32	1	0	4.174130	2.294806	1.883015
33	1	0	4.783310	1.513014	0.395955
34	1	0	4.257714	3.226848	0.360311
35	6	0	0.242346	1.949246	-0.263727
36	1	0	1.763553	0.443635	-0.915985
37	7	0	-0.220183	2.618571	-1.278807
38	7	0	-0.664201	3.154530	-2.187520
39	16	0	2.167417	-1.687309	-0.702018
40	8	0	2.006584	-0.322199	-1.513777
41	8	0	1.821780	-1.512121	0.706844
42	8	0	1.589400	-2.767387	-1.486761
43	6	0	4.018247	-1.899766	-0.793617

44	9	0	4.624797	-0.911416	-0.134322
45	9	0	4.329960	-3.064956	-0.224075
46	9	0	4.413073	-1.900669	-2.062885

INT3D

Zero-point correction= 0.321412 (Hartree/Particle)
Thermal correction to Energy= 0.355024
Thermal correction to Enthalpy= 0.355968
Thermal correction to Gibbs Free Energy= 0.246573
E(sov) = -2435.37964558 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.191363	1.142216	0.867292
2	1	0	5.096359	1.751716	0.928208
3	1	0	4.211359	0.453922	1.722991
4	6	0	2.992548	2.039096	0.987742
5	8	0	3.277038	3.345029	1.143513
6	6	0	4.239888	0.323917	-0.396912
7	8	0	5.473410	-0.166893	-0.674988
8	7	0	3.269212	0.038902	-1.169140
9	7	0	1.758462	1.695497	0.987903
10	6	0	2.003955	4.042461	1.283857
11	1	0	2.003460	4.529919	2.261920
12	1	0	1.955285	4.799684	0.498662
13	6	0	0.947341	2.922051	1.138094
14	1	0	0.310178	3.047380	0.259679
15	1	0	0.296072	2.827027	2.011111
16	6	0	5.311440	-1.001122	-1.859237
17	1	0	6.021216	-0.650572	-2.612008
18	1	0	5.556724	-2.028907	-1.578497
19	6	0	3.822814	-0.803917	-2.246872
20	1	0	3.271500	-1.746382	-2.300561
21	1	0	3.699675	-0.288653	-3.205688
22	47	0	0.964213	-0.291760	0.391043
23	15	0	-1.288486	-3.011515	0.507446
24	8	0	-1.621798	-4.370850	0.019007
25	8	0	-1.416320	-2.933828	2.122923
26	8	0	-2.459595	-1.884380	0.055908
27	6	0	-1.210186	-1.730793	2.869429
28	1	0	-1.768148	-0.892254	2.440039
29	1	0	-1.567131	-1.930792	3.882770
30	1	0	-0.143850	-1.480604	2.902946
31	6	0	-3.835286	-2.325422	0.142400
32	1	0	-4.087803	-2.548201	1.182761

33	1	0	-4.448607	-1.499683	-0.219571
34	1	0	-3.978749	-3.215274	-0.473509
35	6	0	0.191659	-2.237590	-0.017484
36	1	0	-2.222752	-0.613414	-0.811733
37	7	0	0.913926	-2.963420	-0.813938
38	7	0	1.602763	-3.553958	-1.513649
39	16	0	-2.299278	1.571253	-0.605757
40	8	0	-2.200611	0.216602	-1.419073
41	8	0	-2.086694	1.350705	0.824130
42	8	0	-1.569781	2.608736	-1.319851
43	6	0	-4.109337	1.958721	-0.821873
44	9	0	-4.846191	0.975624	-0.289419
45	9	0	-4.380558	3.099908	-0.188598
46	9	0	-4.402136	2.081429	-2.112818

INT2E

Zero-point correction= 0.378405 (Hartree/Particle)
Thermal correction to Energy= 0.415974
Thermal correction to Enthalpy= 0.416918
Thermal correction to Gibbs Free Energy= 0.299077
E(sov) = -2594.80846736 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.188167	-0.249798	0.127260
2	6	0	3.239261	0.325819	0.328447
3	6	0	2.020726	0.849435	-0.051433
4	6	0	2.048665	2.169964	-0.603076
5	6	0	0.853170	2.824664	-1.019460
6	6	0	3.284554	2.900339	-0.750577
7	6	0	0.892852	4.092880	-1.553214
8	1	0	-0.094323	2.309770	-0.889235
9	6	0	3.295905	4.216356	-1.305688
10	6	0	2.119083	4.796491	-1.702482
11	1	0	-0.032001	4.570305	-1.864996
12	1	0	4.235183	4.750081	-1.410408
13	1	0	2.118828	5.796144	-2.126937
14	6	0	3.545803	-0.968791	0.959930
15	6	0	4.613791	-1.077551	1.873118
16	6	0	2.779064	-2.112903	0.678812
17	6	0	4.884273	-2.289218	2.502154
18	1	0	5.216092	-0.205181	2.105746
19	6	0	3.049548	-3.322552	1.315050
20	1	0	1.974141	-2.078537	-0.045169
21	6	0	4.100182	-3.414476	2.229199

22	1	0	5.701911	-2.352878	3.215079
23	1	0	2.420264	-4.177199	1.090114
24	1	0	4.308217	-4.356561	2.729126
25	6	0	5.845426	2.839278	-0.401181
26	1	0	6.122624	3.074763	-1.435089
27	1	0	5.920153	3.765486	0.180124
28	1	0	6.559149	2.115261	-0.003837
29	8	0	4.412317	1.058985	0.171172
30	6	0	4.460252	2.273369	-0.334325
31	7	0	-4.379036	2.214833	2.951117
32	7	0	-5.311143	2.223980	3.604710
33	6	0	-3.329687	2.208224	2.175971
34	1	0	-2.400117	2.552025	2.611643
35	15	0	-3.382591	1.491695	0.548013
36	8	0	-2.039022	1.574637	-0.099525
37	8	0	-4.069086	0.082000	0.805170
38	8	0	-4.554998	2.238951	-0.293609
39	6	0	-4.410375	-0.813132	-0.286415
40	1	0	-3.638452	-0.794372	-1.055046
41	1	0	-4.447180	-1.812504	0.143839
42	1	0	-5.381122	-0.517641	-0.692896
43	6	0	-4.284794	3.513728	-0.891247
44	1	0	-5.180193	3.789235	-1.451363
45	1	0	-4.091412	4.268878	-0.119941
46	1	0	-3.426769	3.449800	-1.566672
47	16	0	-1.310198	-3.124561	-0.241743
48	8	0	-0.024945	-3.728189	0.148617
49	8	0	-2.537800	-3.902265	-0.047443
50	8	0	-1.466278	-1.680219	0.194423
51	6	0	-1.158946	-2.929649	-2.087303
52	9	0	-2.239534	-2.315959	-2.601705
53	9	0	-0.076278	-2.178902	-2.392870
54	9	0	-1.023030	-4.116846	-2.686153

TS2E

Zero-point correction= 0.376143 (Hartree/Particle)
Thermal correction to Energy= 0.413152
Thermal correction to Enthalpy= 0.414096
Thermal correction to Gibbs Free Energy= 0.296810
E(sov) = -2594.77312661 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.398924	-1.382295	-0.486166
2	6	0	-0.419823	2.410893	0.860606

3	6	0	-0.972471	1.493689	0.005032
4	6	0	-1.715811	2.055121	-1.082469
5	6	0	-2.355875	1.216532	-2.041094
6	6	0	-1.861485	3.481563	-1.257147
7	6	0	-3.058802	1.753802	-3.096530
8	1	0	-2.288164	0.139934	-1.916426
9	6	0	-2.594616	4.013327	-2.361178
10	6	0	-3.176960	3.160258	-3.263982
11	1	0	-3.532960	1.092650	-3.816806
12	1	0	-2.686184	5.088098	-2.484865
13	1	0	-3.732901	3.556646	-4.108673
14	6	0	0.399045	2.150702	2.057320
15	6	0	0.258098	2.918793	3.227444
16	6	0	1.344568	1.111802	2.036316
17	6	0	1.024934	2.630895	4.354599
18	1	0	-0.464341	3.729221	3.256323
19	6	0	2.115935	0.831880	3.162681
20	1	0	1.520761	0.555581	1.123319
21	6	0	1.952354	1.584864	4.327739
22	1	0	0.897118	3.222642	5.257142
23	1	0	2.850122	0.033585	3.109564
24	1	0	2.550620	1.365940	5.208029
25	6	0	-1.316423	5.813466	-0.280172
26	1	0	-0.846974	6.230765	-1.178542
27	1	0	-2.349663	6.177265	-0.248125
28	1	0	-0.782869	6.185432	0.596507
29	8	0	-0.593667	3.796693	0.699749
30	6	0	-1.270624	4.315533	-0.300742
31	7	0	-1.063672	-1.755116	2.214590
32	7	0	-0.743345	-2.004960	3.269888
33	6	0	-1.402274	-1.439644	0.969210
34	1	0	-1.376408	-0.325538	0.740590
35	15	0	-2.643670	-2.445424	0.157531
36	8	0	-2.891231	-1.983105	-1.234735
37	8	0	-2.057453	-3.919919	0.396445
38	8	0	-3.973890	-2.504389	1.086412
39	6	0	-2.784842	-5.074319	-0.075413
40	1	0	-2.992354	-4.981147	-1.145061
41	1	0	-2.135639	-5.931840	0.102866
42	1	0	-3.717780	-5.185484	0.483875
43	6	0	-4.971124	-1.475601	0.953941
44	1	0	-5.837036	-1.812410	1.526177
45	1	0	-4.603707	-0.530893	1.370683
46	1	0	-5.242087	-1.335187	-0.095522
47	16	0	3.376493	-1.506805	-0.938511
48	8	0	2.960380	-1.396822	0.486982
49	8	0	4.430909	-2.461638	-1.275481

50	8	0	2.159319	-1.549423	-1.845853
51	6	0	4.071580	0.172771	-1.328957
52	9	0	4.403295	0.263749	-2.620699
53	9	0	3.153778	1.121816	-1.058130
54	9	0	5.157822	0.413799	-0.585699

INT3E

Zero-point correction= 0.380105 (Hartree/Particle)
Thermal correction to Energy= 0.417481
Thermal correction to Enthalpy= 0.418425
Thermal correction to Gibbs Free Energy= 0.299570
E(sov) = -2594.82698229 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	2.591587	1.785668	0.131828
2	6	0	-4.050167	-0.891657	0.373970
3	6	0	-2.681192	-0.863167	0.366201
4	6	0	-1.937687	-2.015898	0.019414
5	6	0	-0.523198	-2.013871	-0.023567
6	6	0	-2.649367	-3.229473	-0.296958
7	6	0	0.154579	-3.166018	-0.365618
8	1	0	0.023096	-1.103944	0.203163
9	6	0	-1.920046	-4.407011	-0.644191
10	6	0	-0.548199	-4.364814	-0.674941
11	1	0	1.240319	-3.121258	-0.389130
12	1	0	-2.451066	-5.322811	-0.882473
13	1	0	0.012647	-5.256185	-0.939971
14	6	0	-4.966055	0.206570	0.675357
15	6	0	-6.320183	-0.037196	0.975128
16	6	0	-4.487038	1.531572	0.670957
17	6	0	-7.171448	1.022020	1.273645
18	1	0	-6.699266	-1.053529	0.984322
19	6	0	-5.347484	2.583152	0.971644
20	1	0	-3.459305	1.760343	0.412929
21	6	0	-6.688128	2.334074	1.274796
22	1	0	-8.212965	0.823711	1.509720
23	1	0	-4.959554	3.596861	0.959673
24	1	0	-7.356001	3.158345	1.508598
25	6	0	-4.967419	-4.337031	-0.526246
26	1	0	-4.814473	-4.720968	-1.541047
27	1	0	-4.786877	-5.163214	0.170822
28	1	0	-6.004030	-4.010761	-0.426323
29	8	0	-4.680723	-2.075100	0.068004
30	6	0	-4.042232	-3.195265	-0.246804

31	7	0	5.473179	1.032989	0.588052
32	7	0	6.500195	1.503741	0.777827
33	6	0	4.288093	0.550527	0.376873
34	1	0	-2.141536	0.042076	0.629811
35	15	0	4.135736	-1.183386	0.242590
36	8	0	2.737855	-1.675427	0.020932
37	8	0	5.210319	-1.623617	-0.891758
38	8	0	4.846048	-1.901658	1.535830
39	6	0	5.400067	-3.011967	-1.187978
40	1	0	4.447581	-3.487351	-1.447450
41	1	0	6.075468	-3.057781	-2.045113
42	1	0	5.849888	-3.530239	-0.335046
43	6	0	4.158406	-1.859533	2.789297
44	1	0	4.771773	-2.413178	3.504152
45	1	0	4.042158	-0.825459	3.134790
46	1	0	3.170787	-2.326490	2.708013
47	16	0	-0.506241	2.507258	-0.085303
48	8	0	-0.520364	1.250880	0.708652
49	8	0	-1.614056	3.440778	0.153661
50	8	0	0.855002	3.137979	-0.159229
51	6	0	-0.763233	1.909058	-1.827498
52	9	0	-0.780596	2.922473	-2.693886
53	9	0	0.210438	1.053967	-2.179594
54	9	0	-1.941408	1.253322	-1.913203

---

12. References

[1] Desimoni, G.; Faita, G.; Jørgensen, K. A. *Chem. Rev.* **2011**, *111*, PR284.

[2] Gupta, A. K.; Vaishanv, N. K.; Kant, R.; Mohanan, K. *Org. Biomol. Chem*. **2017**, *15*, 6411.

[3] Matsuo, J.; Sasaki, S.; Hoshikawa, T.; Ishibashi, H. *Chem. Commun*. **2010**, *46*, 934.

[4] Zieliński, G. K.; Samojłowicz, C.; Wdowik, T.; Grela, K. *Org. Biomol. Chem.* **2015**, *13*, 2684

[5] Fu. B.; Du, D. M.; Wang, J, B.; *Tetrahedron: Asym*. **2004**, *15*, 119.

[6] Domin, D.; Benito-Garagorri, D.; Mereiter, K.; Fröhlich, J.; Kirchner, K. *Organometallics* **2005**, *24*, 3957.

[7] (a) Poh, J. S.; Makai, S.; von Keutz, T.; Tran, D. N.; Battilocchio, C.; Pasau, P.; Ley, S. V. *Angew. Chem. Int. Ed.* **2017**, *56*, 1864. (b) Madhukar, P.; Mahesh, P.; Dnyandeo, P.; Ghanshyam, W.; Mahesh Kumar, G.; Vinayak Assignee, G.; IN 2011CH04203

[8] Sakakura, A.; Kondo, R.; Ishihara, K. *Org. Lett*. **2005**, *10*, 1971.

[9] Yasui, E.; Wada, M.; Takamura, N. *Chem. Pharm. Bull*. **2007**, *55*, 1652.

[10] Parhi, B.; Gurjar, J.; Pramanik, S.; Midya, A.; Ghorai, P. *J. Org. Chem*. **2016**, *81*, 4654.

[11] Nicolle, S. M.; Moody, C. J. *Chem. Eur. J.* **2014**, *20*, 4420.

[12] Chen, J.; Wen, X.; Wang, Y.; Du, F.; Cai, L.; Peng, Y. *Org. Lett*. **2016**, *18*, 4336.

[13] (a) Satyanarayana, T.; Abraham, S.; Kagan, H. B. *Angew. Chem. Int. Ed*. **2009**, *48*, 456. (b) Blackmond, D. G. *Acc. Chem. Res*. **2000**, *33*, 402.

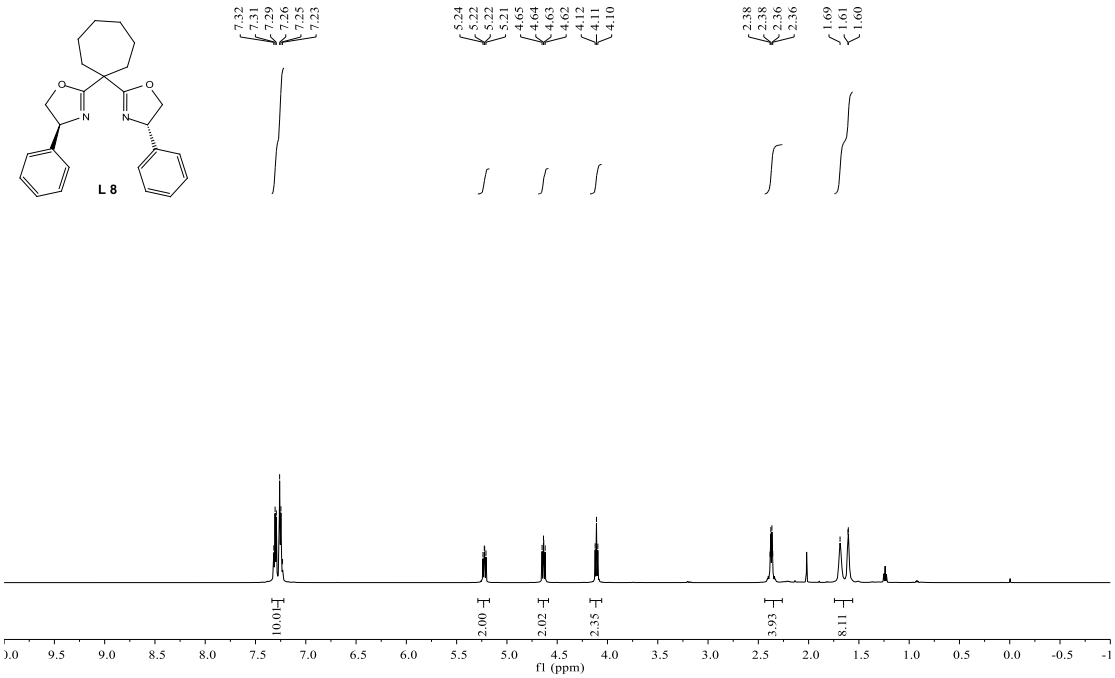
[14] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, 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. J.; Heyd, J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; 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 09, Gaussian, Inc.: Wallingford, CT, USA, **2009**.

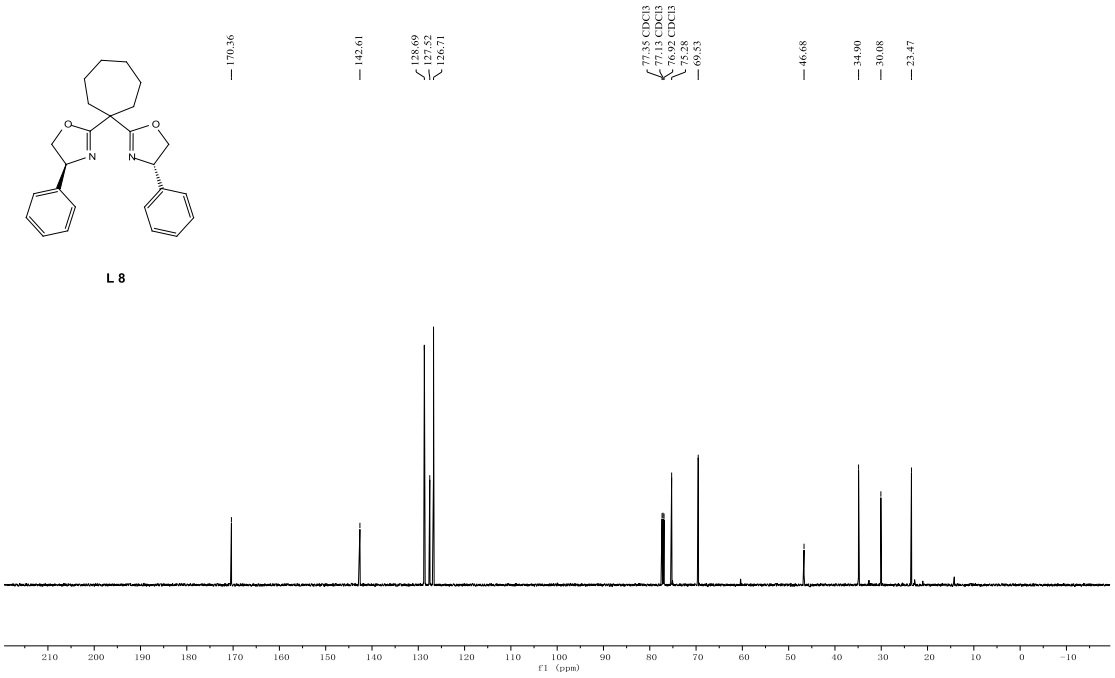
[15] Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363.

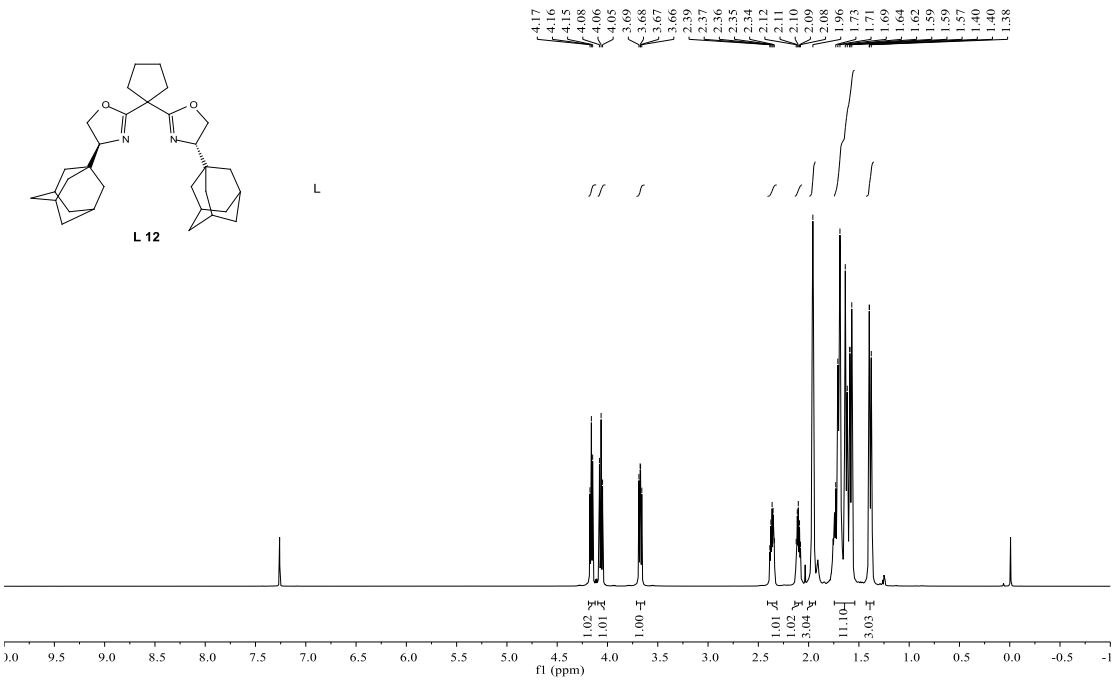
[16] Um, J. M.; DiRocco, D. A.; Noey, E. L.; Rovis, T.; Houk, K. N. *J. Am. Chem. Soc.* **2011,** *133*, 11249.

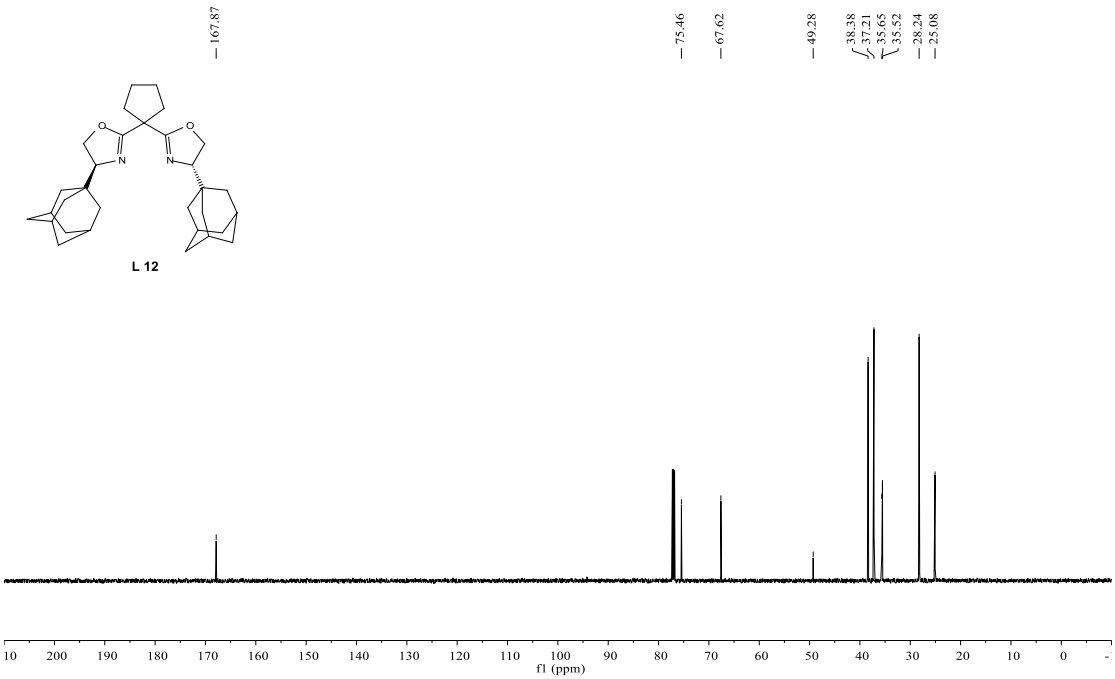
[17] (a) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B.* **2009**, *113*, 6378. (b) Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B.* **2011**, *115*, 14556.

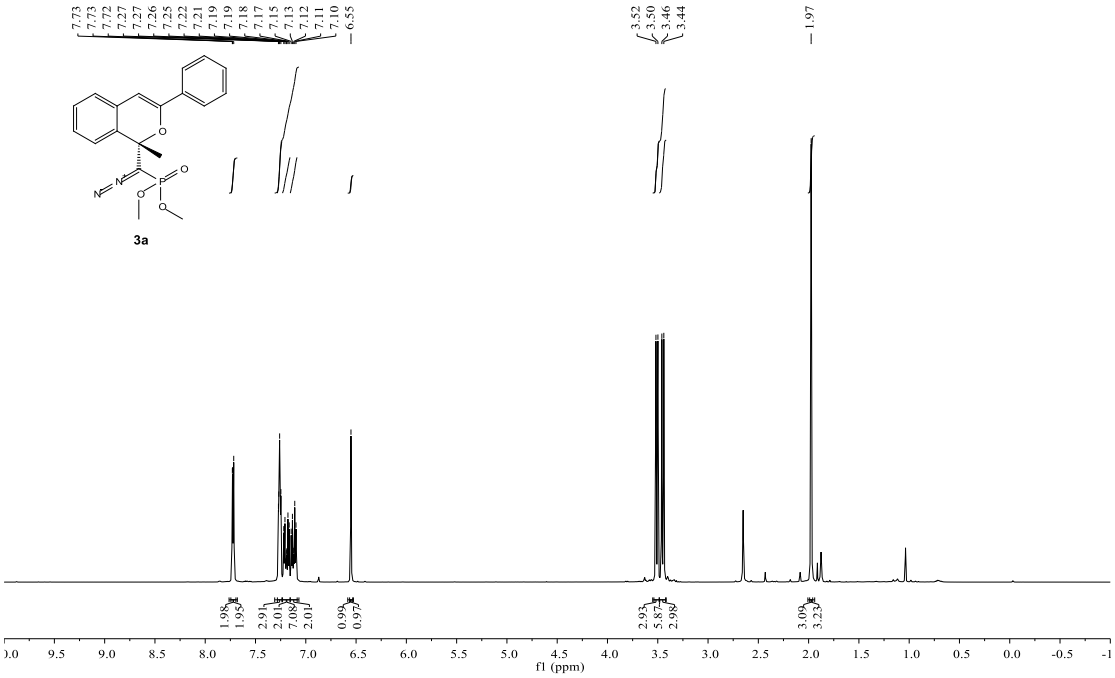
13. NMR spectra and HPLC for the catalysts, the tandem reaction products and derivatives



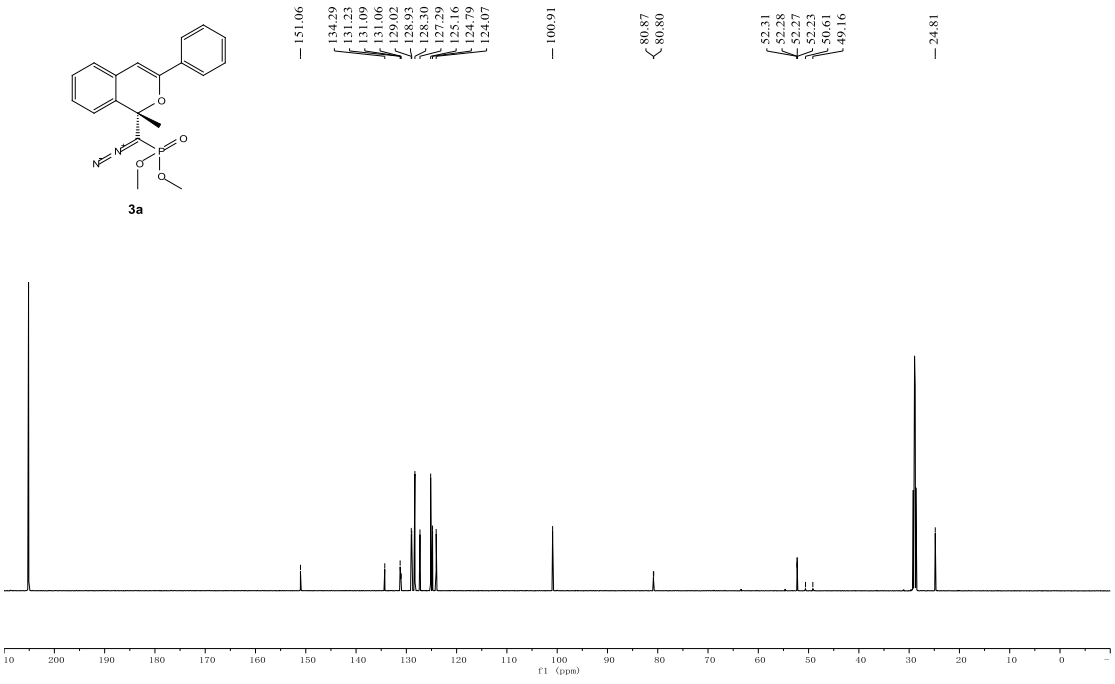



L 12
L
4.17
4.16
4.15
4.08
4.06
4.05
3.69
3.68
3.67
3.66
2.39
2.37
2.36
2.35
2.34
2.12
2.11
2.10
2.09
2.08
1.96
1.73
1.71
1.69
1.64
1.62
1.59
1.59
1.57
1.40
1.40
1.38
1.02
1.01
1.00
1.01
1.02
3.04
11.10
3.03
f1 (ppm)

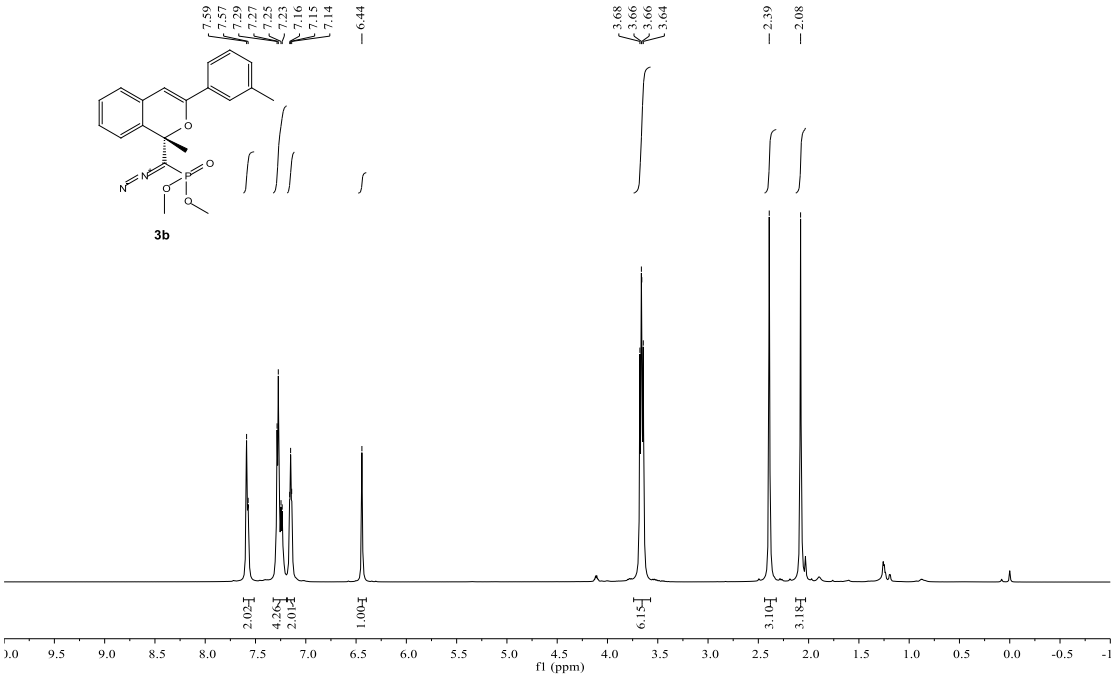

L 12
167.87
75.46
67.62
49.28
38.38
37.21
35.65
35.52
28.24
25.08
f1 (ppm)

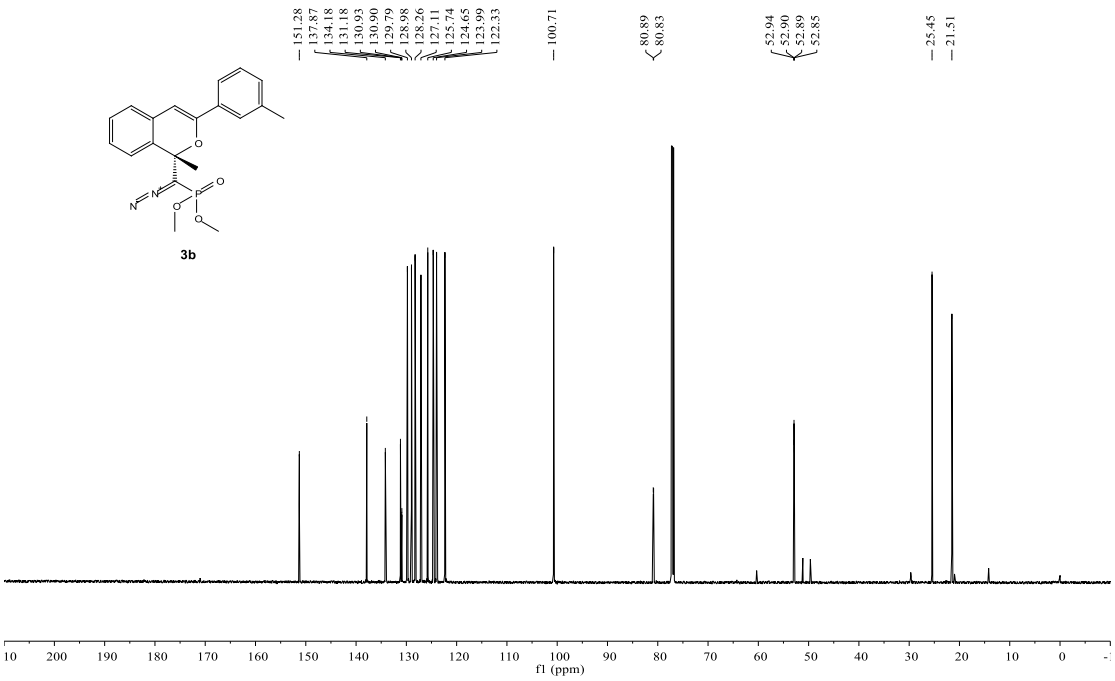

7.73
7.73
7.72
7.27
7.27
7.26
7.25
7.22
7.21
7.19
7.19
7.18
7.17
7.15
7.13
7.12
7.11
7.10
6.55
3.52
3.50
3.46
3.44
1.97
1.98
1.95
2.91
2.01
7.08
2.01
0.99
0.97
2.93
5.87
2.98
3.09
3.23
f1 (ppm)

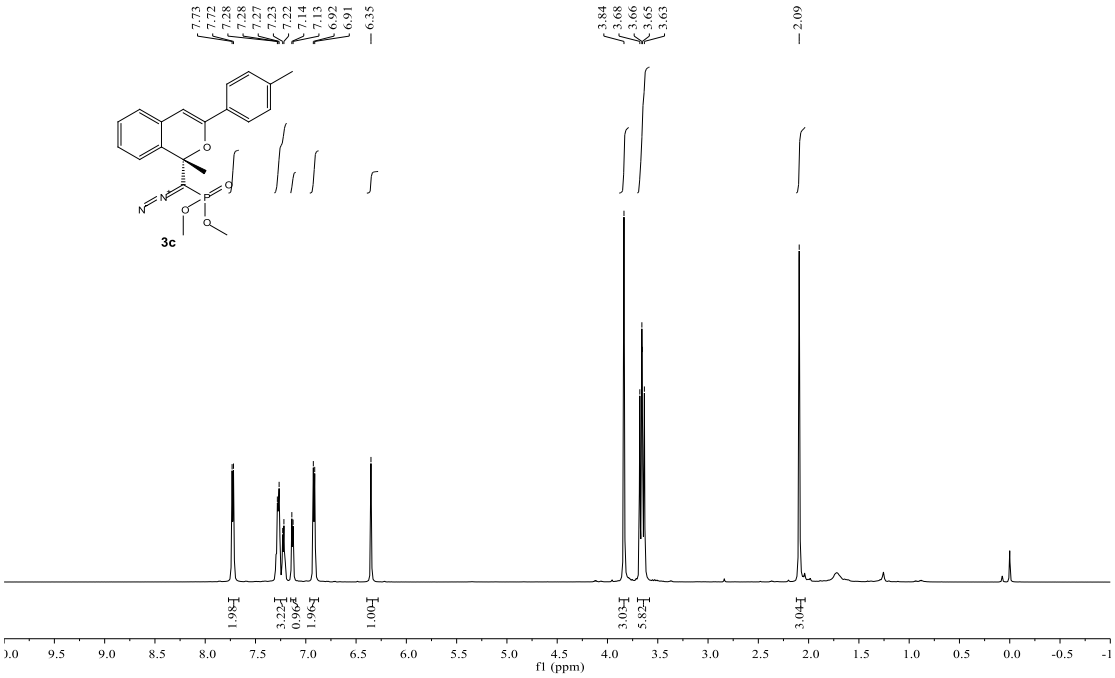
3a

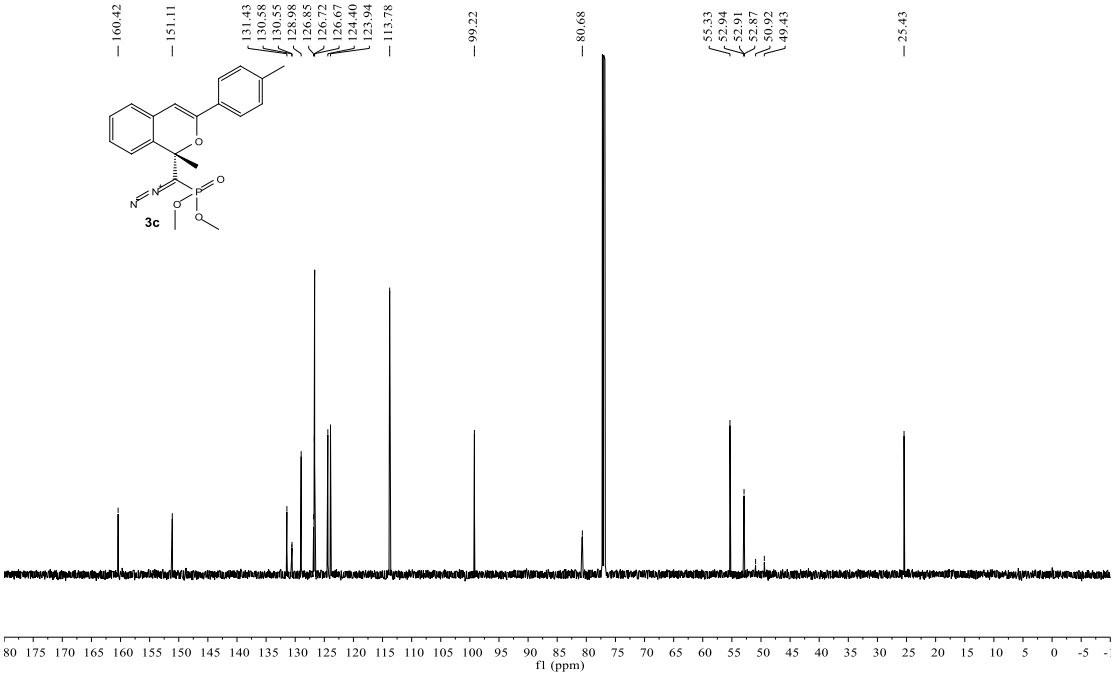

151.06
134.29
131.23
131.09
131.06
129.02
128.93
128.30
127.29
125.16
124.79
124.07
100.91
80.87
80.80
52.31
52.28
52.27
52.23
50.61
49.16
24.81
f1 (ppm)

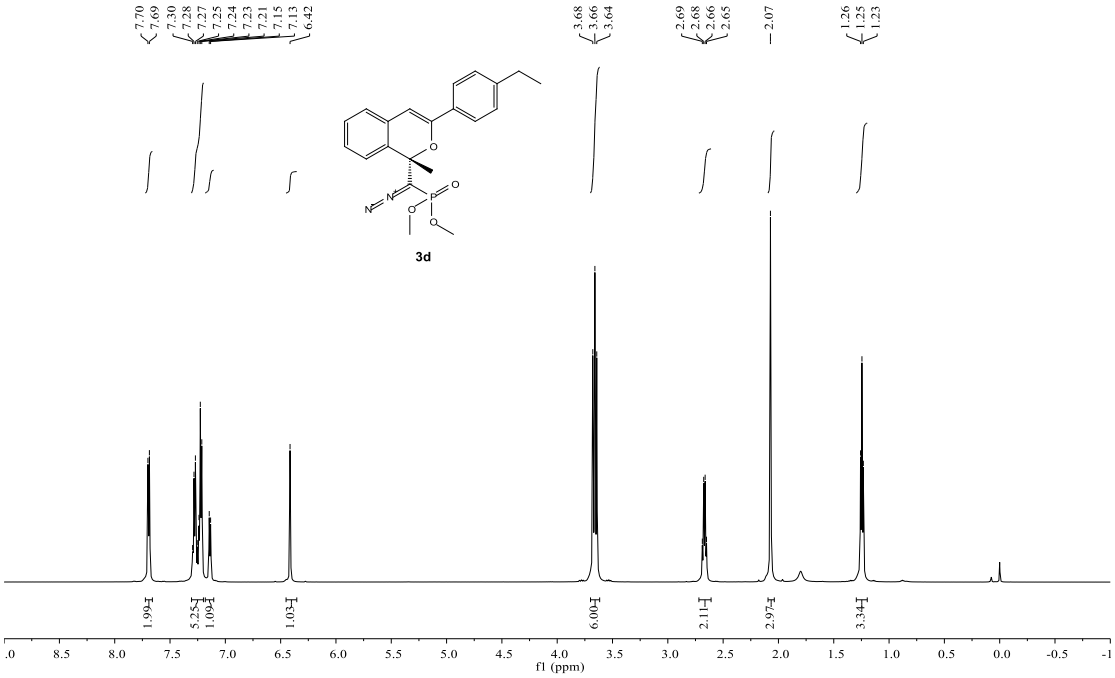
3a

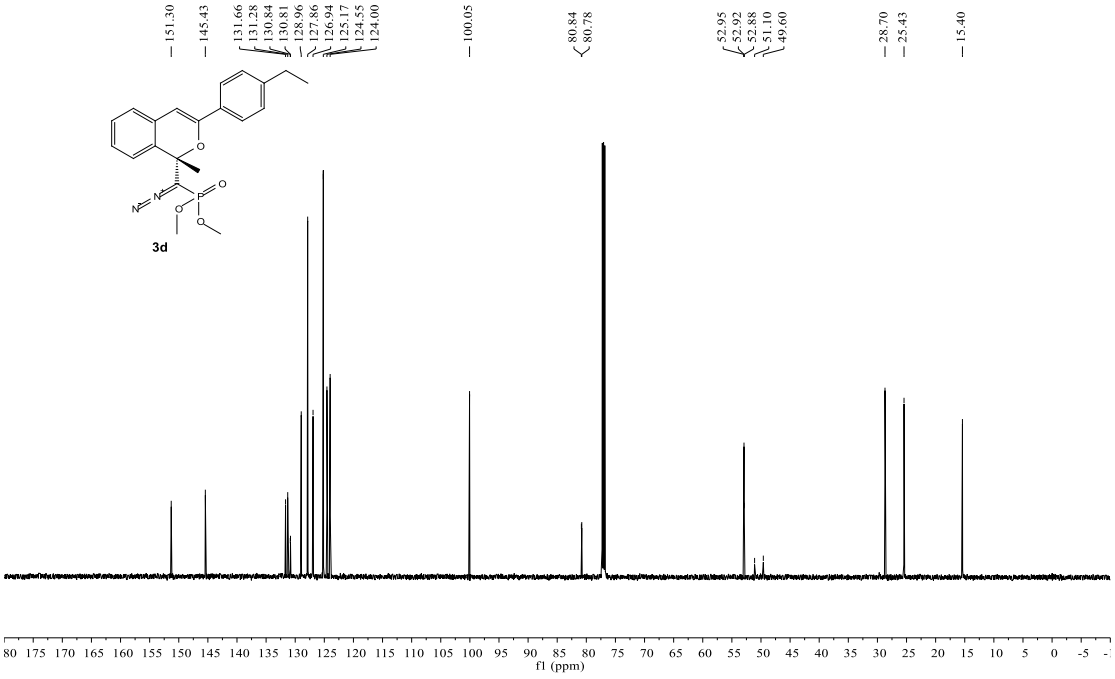

7.59
7.57
7.29
7.27
7.25
7.23
7.16
7.15
7.14
6.44
3.68
3.66
3.66
3.64
2.39
2.08
3b
2.02
4.26
2.01
1.00
6.15
3.10
3.18
f1 (ppm)

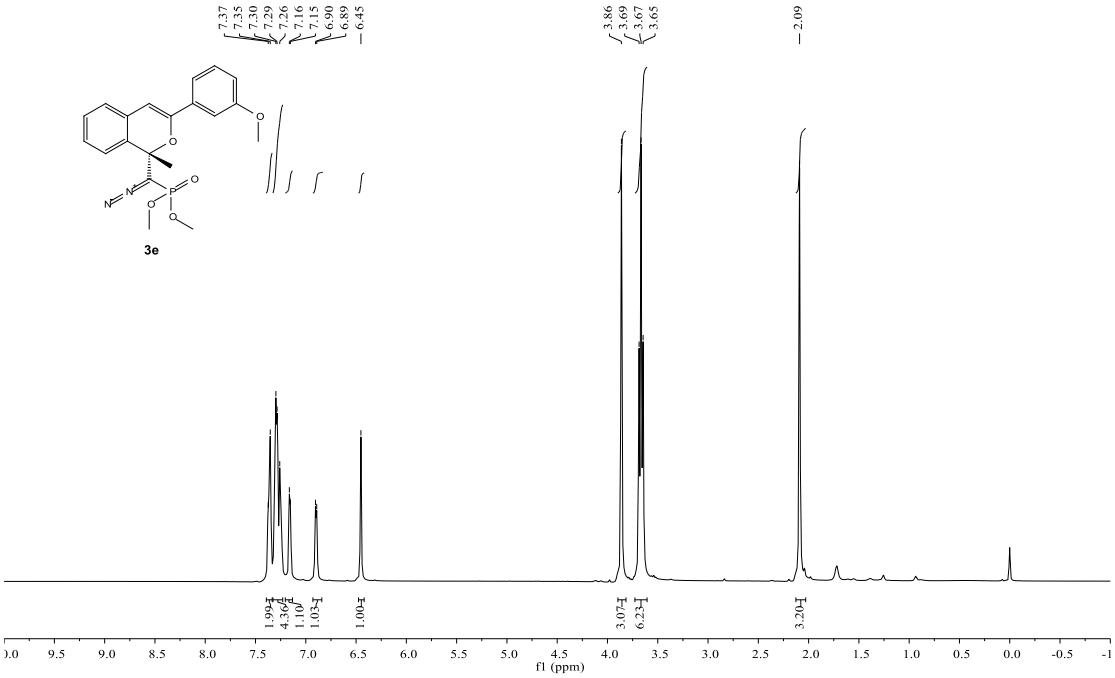

151.28
137.87
134.18
131.18
130.93
130.90
129.79
128.98
128.26
127.11
125.74
124.65
123.99
122.33
100.71
80.89
80.83
52.94
52.90
52.89
52.85
25.45
21.51
3b
f1 (ppm)

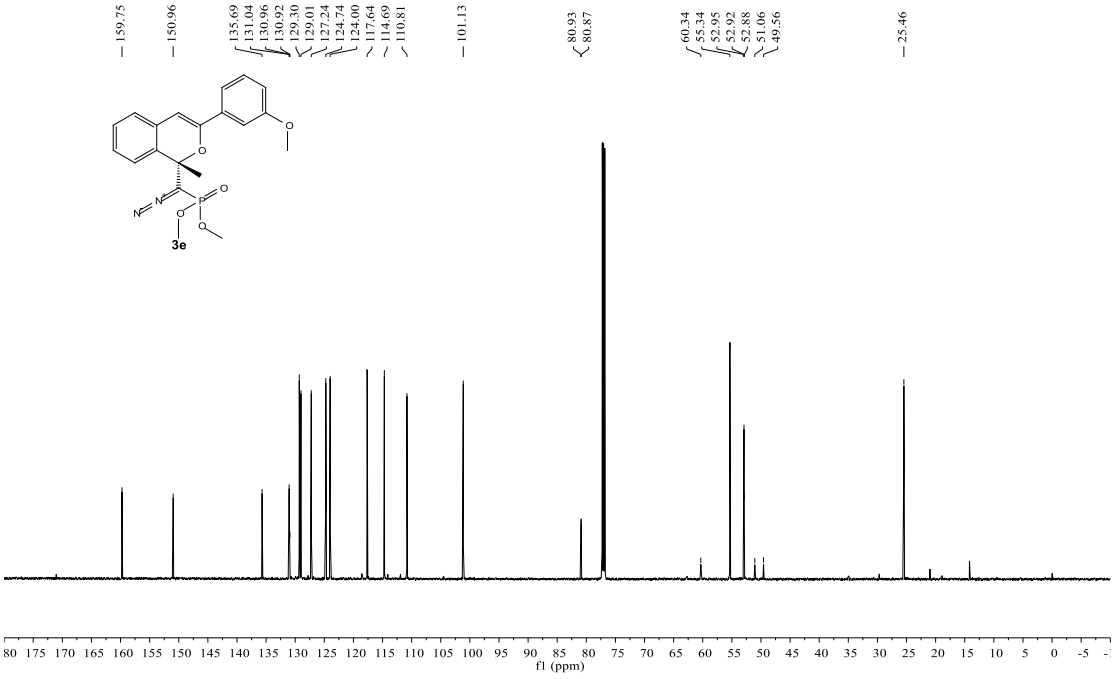

7.73
7.72
7.28
7.28
7.27
7.23
7.22
7.14
7.13
6.92
6.91
6.35
3.84
3.68
3.66
3.65
3.63
2.09
3c
1.98
3.22
0.96
1.96
1.00
3.03
5.82
3.04
f1 (ppm)

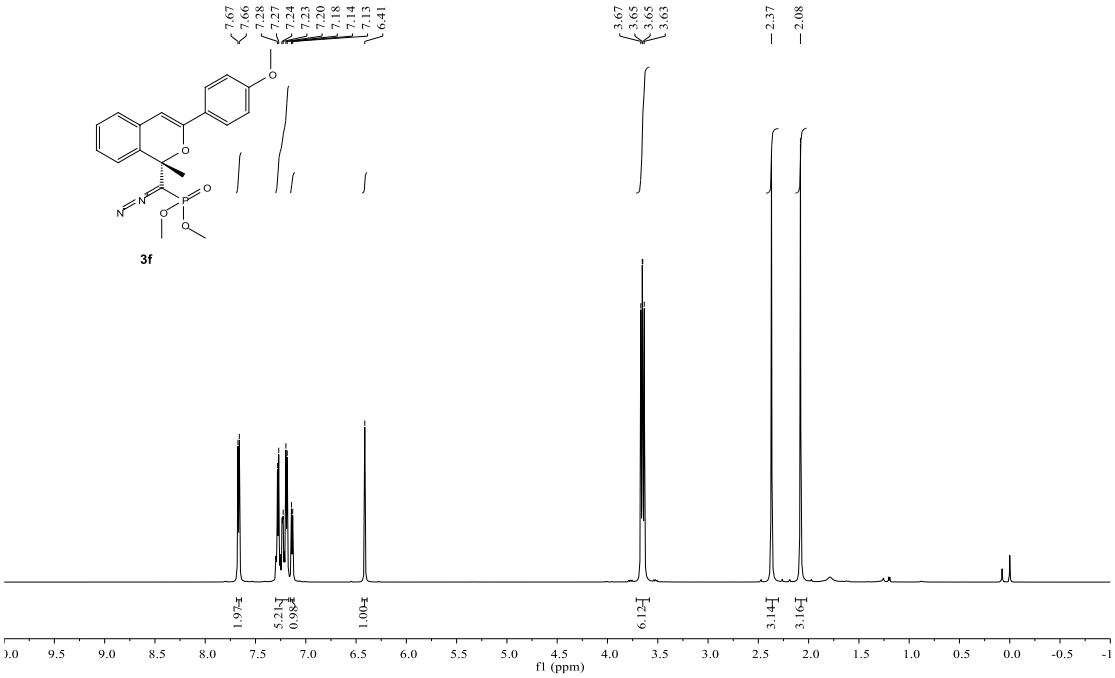

160.42
151.11
131.43
130.58
130.55
128.98
126.85
126.72
126.67
124.40
123.94
113.78
99.22
80.68
55.33
52.94
52.91
52.87
50.92
49.43
25.43
3c
f1 (ppm)

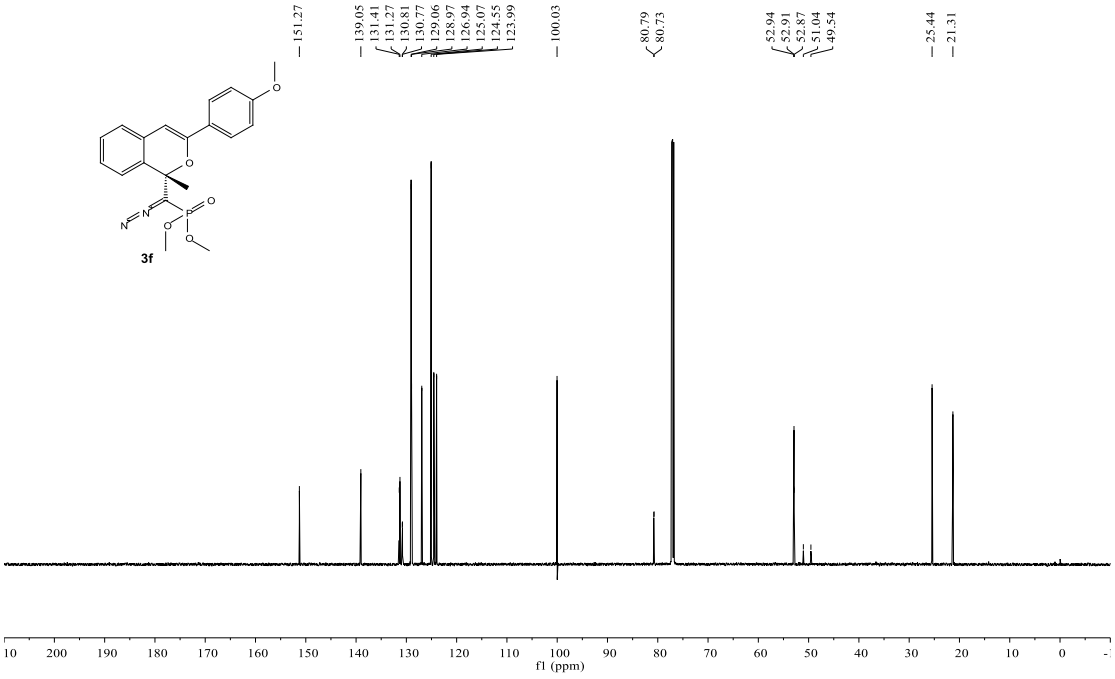

7.70
7.69
7.30
7.28
7.27
7.25
7.24
7.23
7.21
7.15
7.13
6.42
3.68
3.66
3.64
2.69
2.68
2.66
2.65
2.07
1.26
1.25
1.23
3d
1.99
5.25
1.09
1.03
6.00
2.11
2.97
3.34
f1 (ppm)

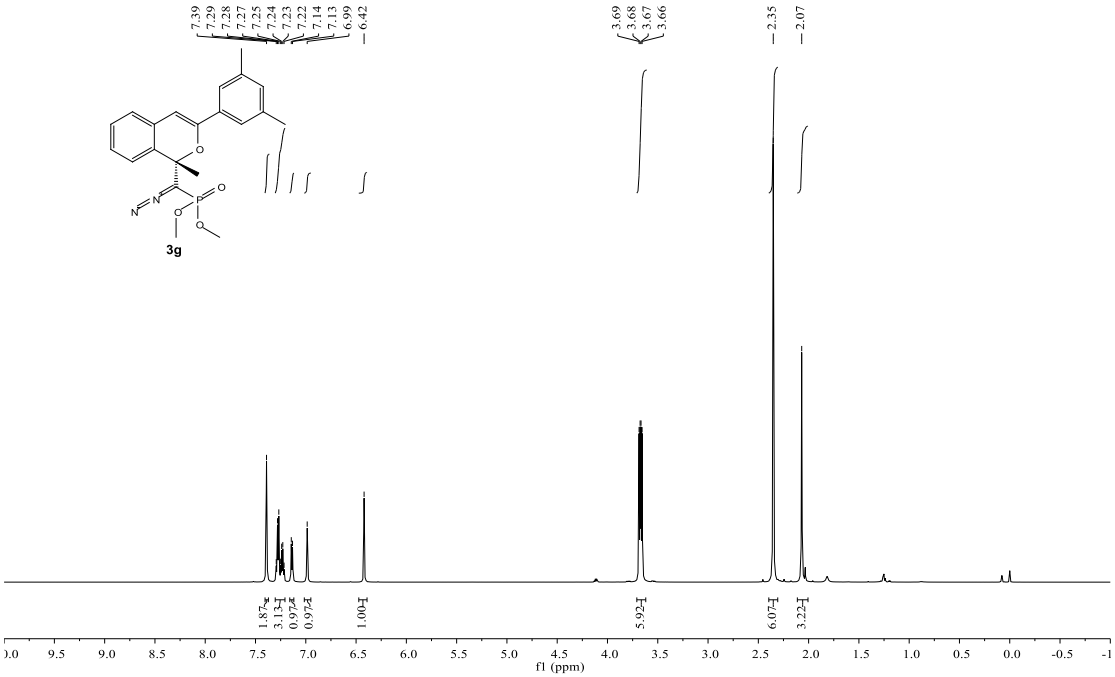

151.30
145.43
131.66
131.28
130.84
130.81
128.96
127.86
126.94
125.17
124.55
124.00
100.05
80.84
80.78
52.95
52.92
52.88
51.10
49.60
28.70
25.43
15.40
3d
f1 (ppm)

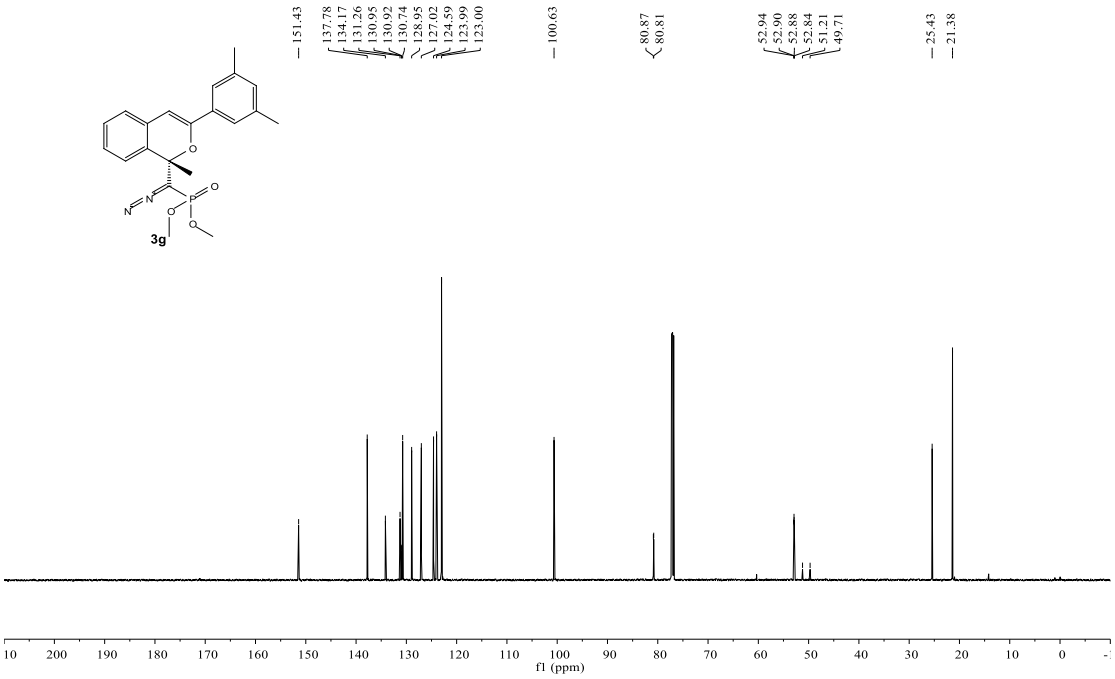

7.37
7.35
7.30
7.29
7.26
7.16
7.15
6.90
6.89
6.45
3.86
3.69
3.67
3.65
2.09
3e
1.99
4.36
1.10
1.03
1.00
3.07
6.23
3.20
f1 (ppm)

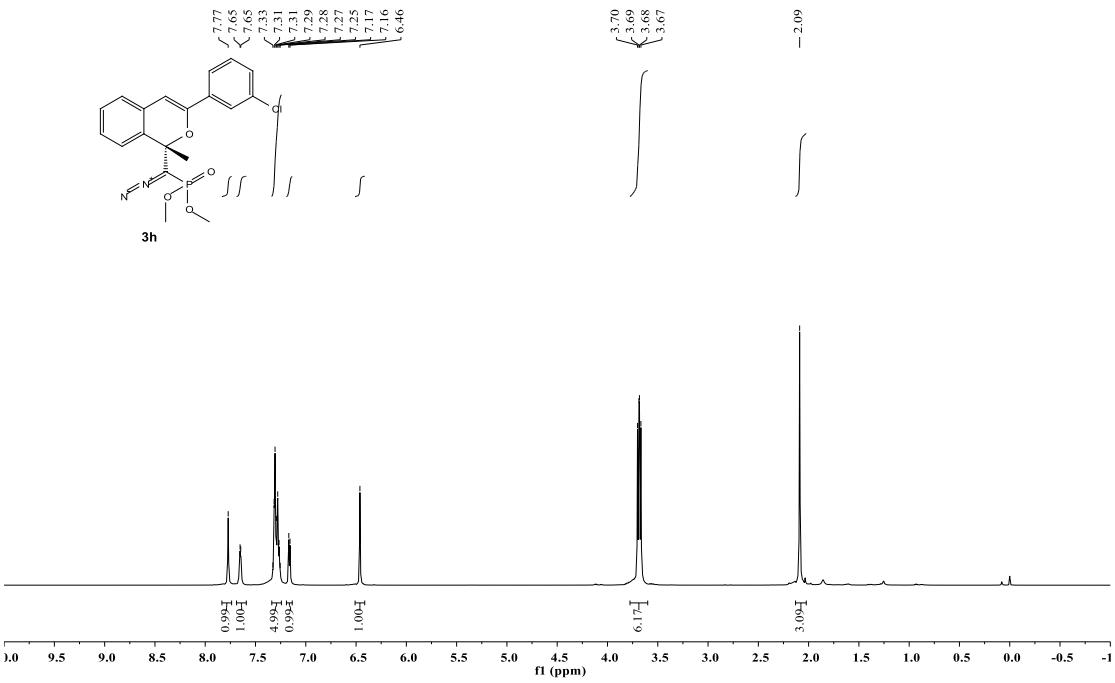

159.75
150.96
135.69
131.04
130.96
130.92
129.30
129.01
127.24
124.74
124.00
117.64
114.69
110.81
101.13
80.93
80.87
60.34
55.34
52.95
52.92
52.88
51.06
49.56
25.46
3e
f1 (ppm)

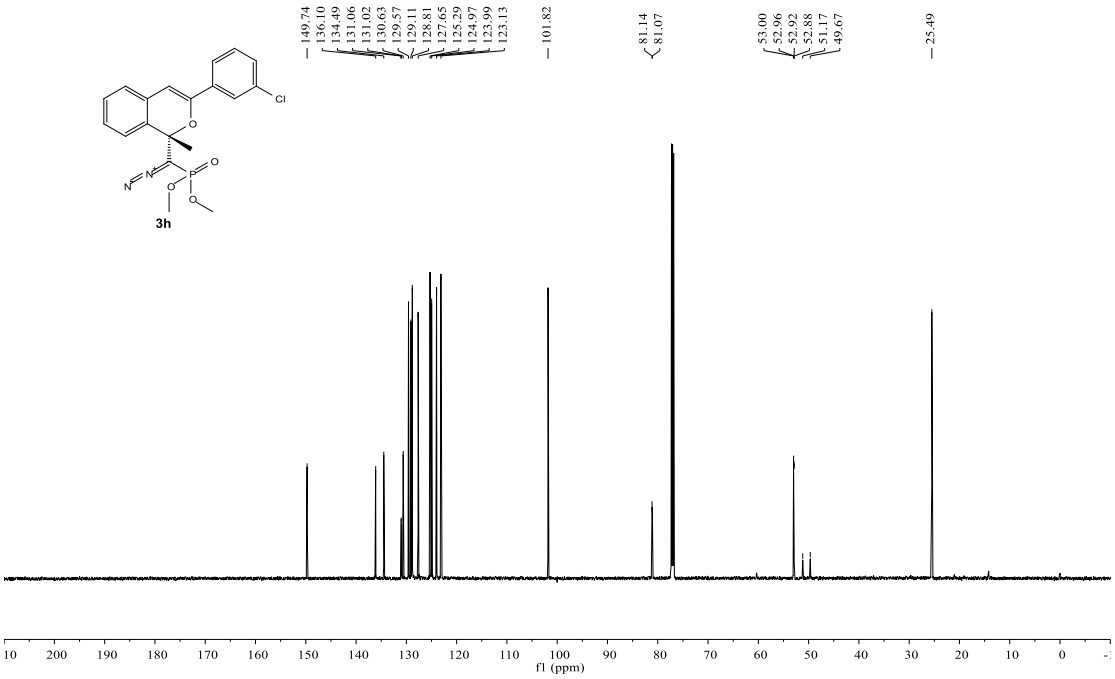

7.67
7.66
7.28
7.27
7.24
7.23
7.20
7.18
7.14
7.13
6.41
3.67
3.65
3.65
3.63
2.37
2.08
1.97
5.21
0.98
1.00
6.12
3.14
3.16
f1 (ppm)
3f

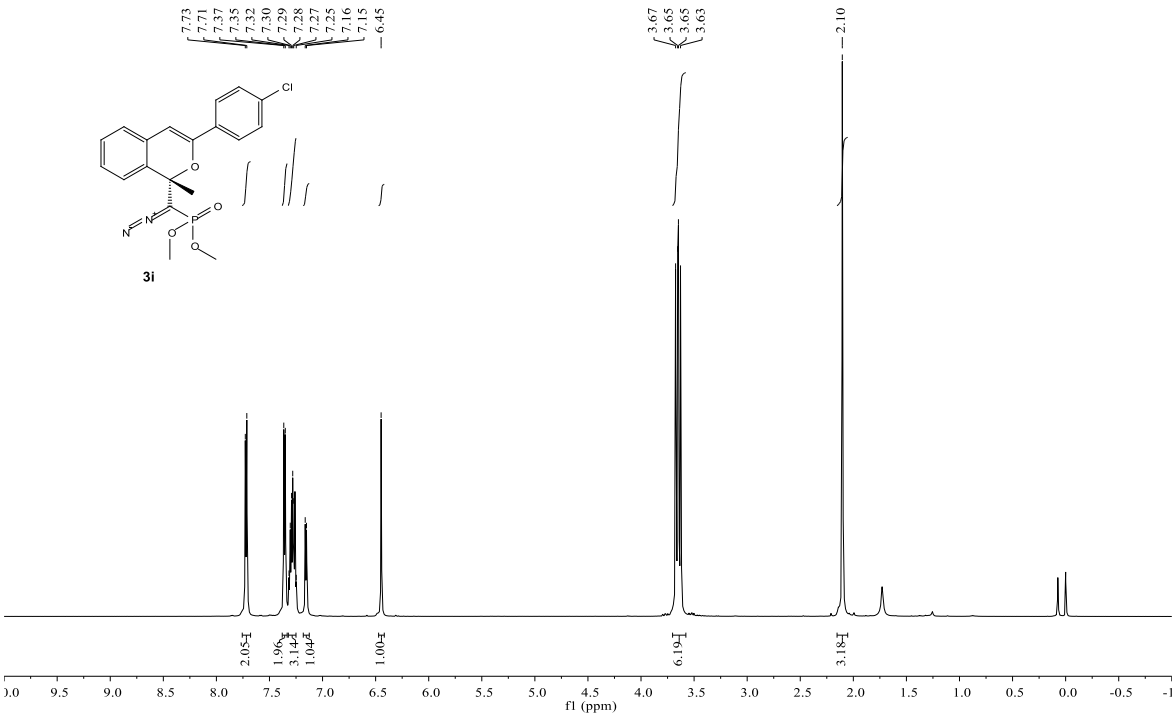

151.27
139.05
131.41
131.27
130.81
130.77
129.06
128.97
126.94
125.07
124.55
123.99
100.03
80.79
80.73
52.94
52.91
52.87
51.04
49.54
25.44
21.31
f1 (ppm)
3f

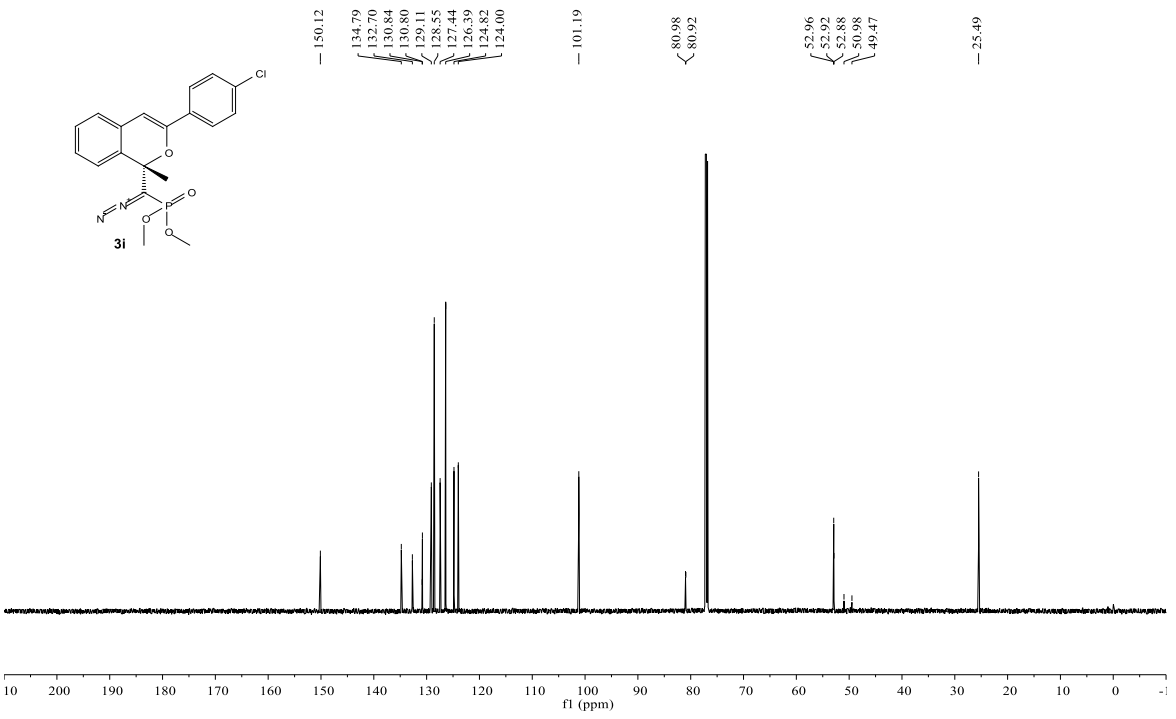

7.39
7.29
7.28
7.27
7.25
7.24
7.23
7.22
7.14
7.13
6.99
6.42
3.69
3.68
3.67
3.66
2.35
2.07
3g
1.87
3.13
0.97
0.97
1.00
5.92
6.07
3.22
f1 (ppm)

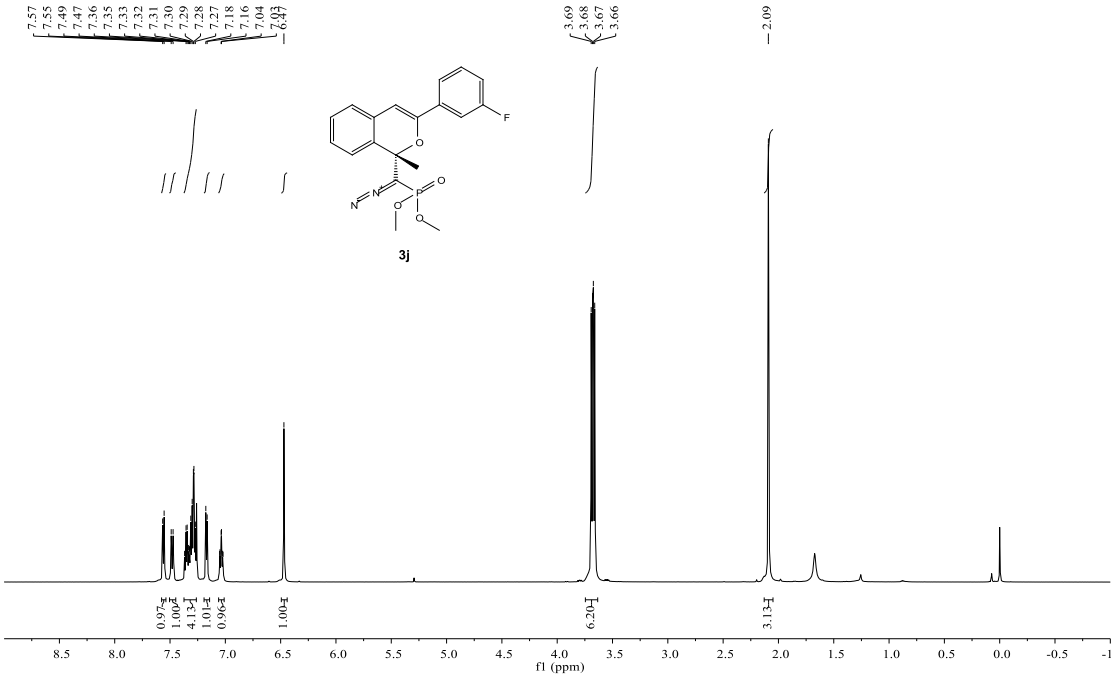

151.43
137.78
134.17
131.26
130.95
130.92
130.74
128.95
127.02
124.59
123.99
123.00
100.63
80.87
80.81
52.94
52.90
52.88
52.84
51.21
49.71
25.43
21.38
3g
f1 (ppm)

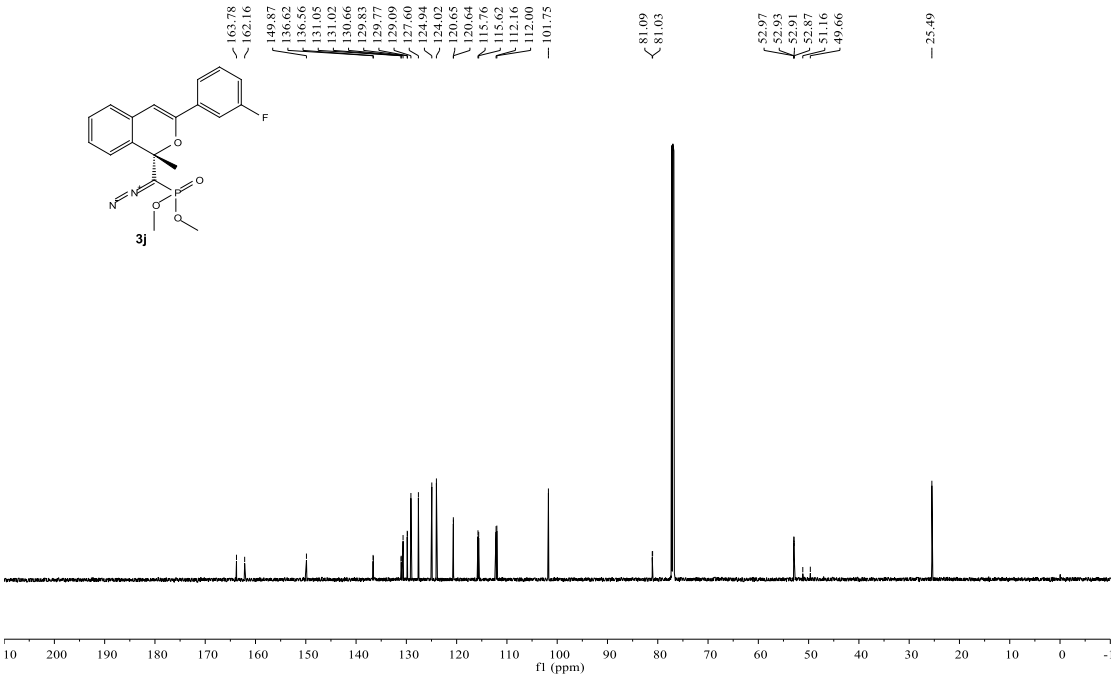

7.77
7.65
7.65
7.33
7.31
7.31
7.29
7.28
7.27
7.25
7.17
7.16
6.46
3.70
3.69
3.68
3.67
2.09
Cl
O
N
N
P
O
O
O
3h
0.99
1.00
4.99
0.99
1.00
6.17
3.09
f1 (ppm)

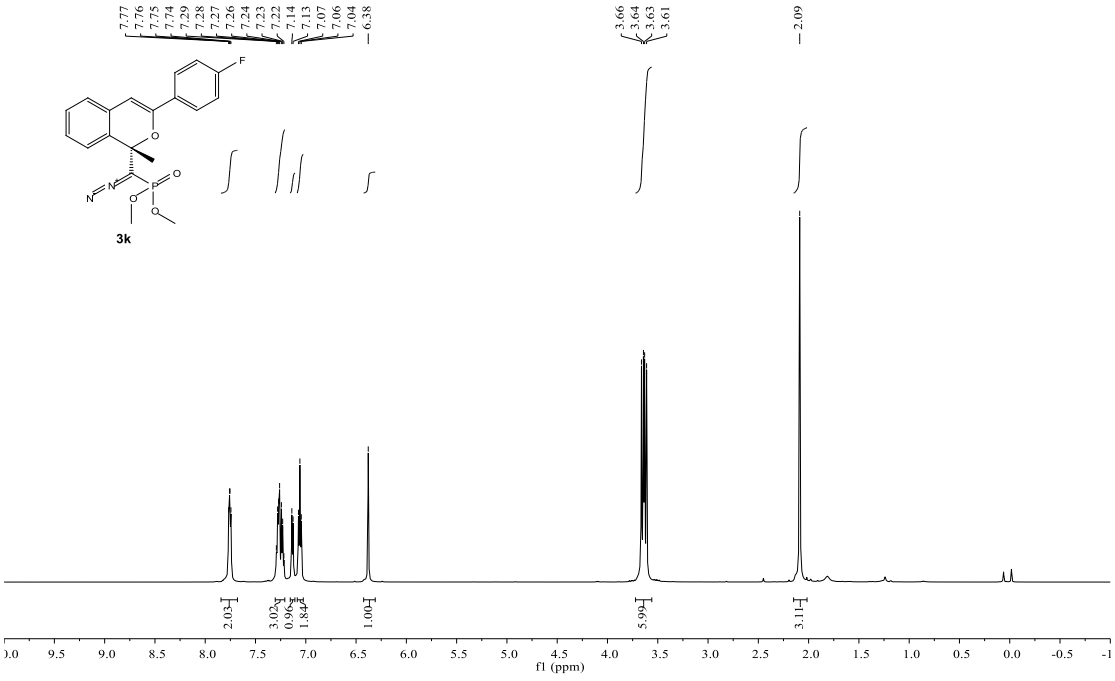

149.74
136.10
134.49
131.06
131.02
130.63
129.57
129.11
128.81
127.65
125.29
124.97
123.99
123.13
101.82
81.14
81.07
53.00
52.96
52.92
52.88
51.17
49.67
25.49
Cl
O
N
N
P
O
O
O
3h
f1 (ppm)

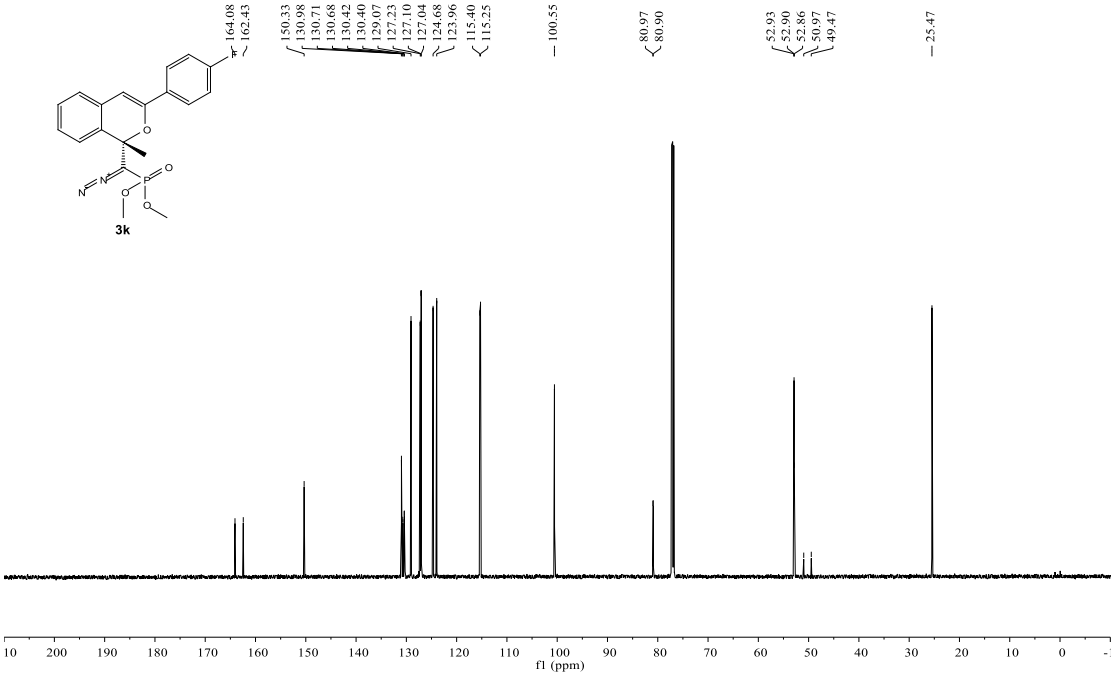

7.73
7.71
7.37
7.35
7.32
7.30
7.29
7.28
7.27
7.25
7.16
7.15
6.45
3.67
3.65
3.65
3.63
2.10
Cl
O
N
N
P
O
O
O
3i
2.05
1.96
3.14
1.04
1.00
6.19
3.18
f1 (ppm)

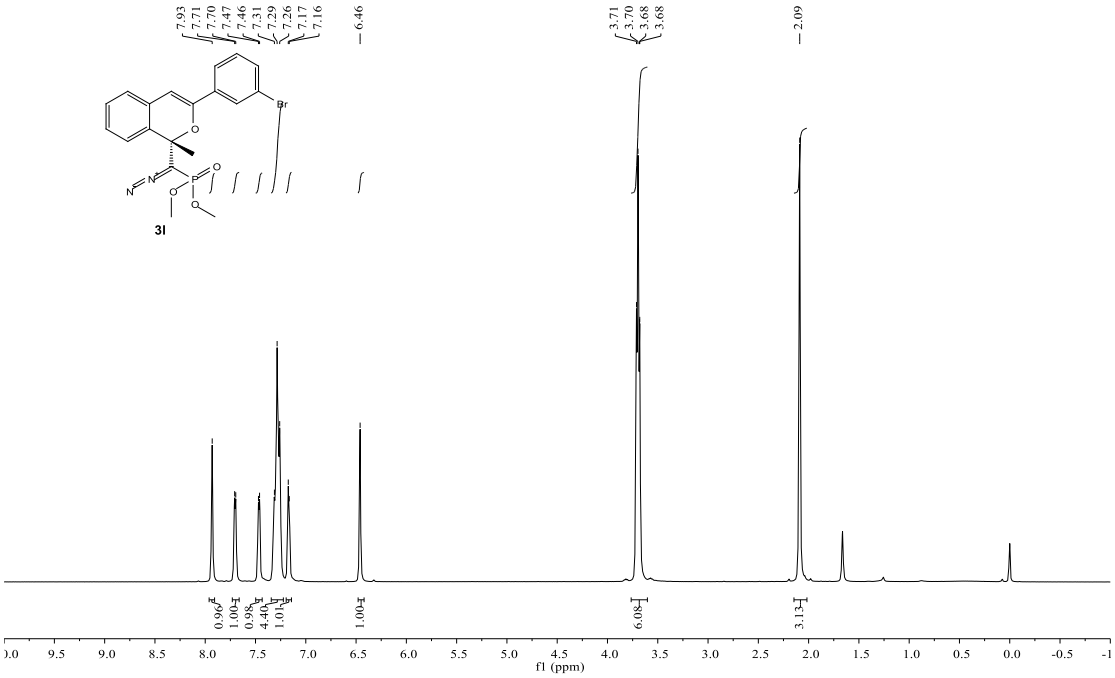

150.12
134.79
132.70
130.84
130.80
129.11
128.55
127.44
126.39
124.82
124.00
101.19
80.98
80.92
52.96
52.92
52.88
50.98
49.47
25.49
Cl
O
N
N
P
O
O
O
3i
f1 (ppm)

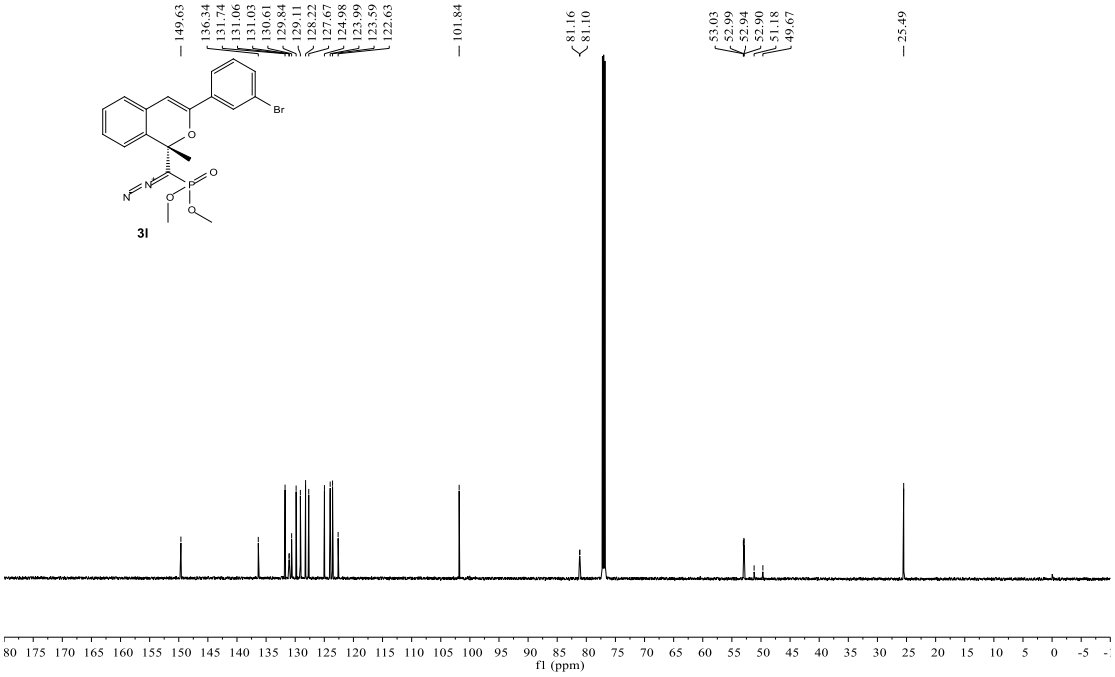

7.57
7.55
7.49
7.47
7.36
7.35
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.18
7.16
7.04
7.03
6.47
3.69
3.68
3.67
3.66
2.09
F
O
N
N
P
O
O
O
3j
0.97
1.00
4.13
1.01
0.96
1.00
6.20
3.13
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

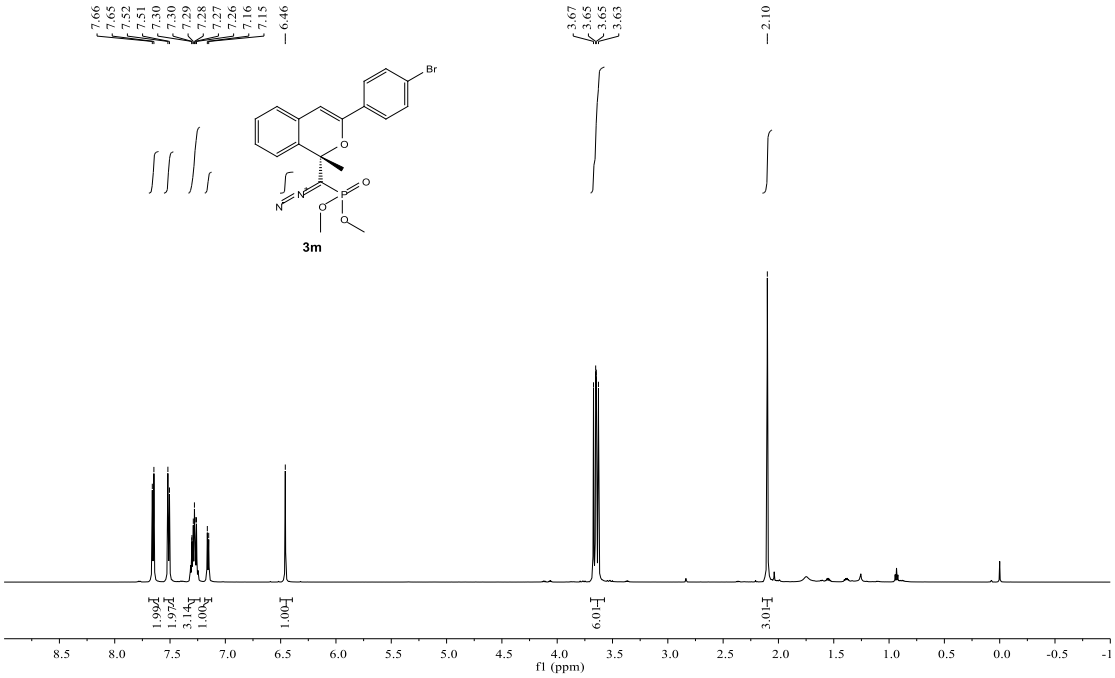

163.78
162.16
149.87
136.62
136.56
131.05
131.02
130.66
129.83
129.77
129.09
127.60
124.94
124.02
120.65
120.64
115.76
115.62
112.16
112.00
101.75
81.09
81.03
52.97
52.93
52.91
52.87
51.16
49.66
25.49
F
O
N
N
P
O
O
O
3j
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

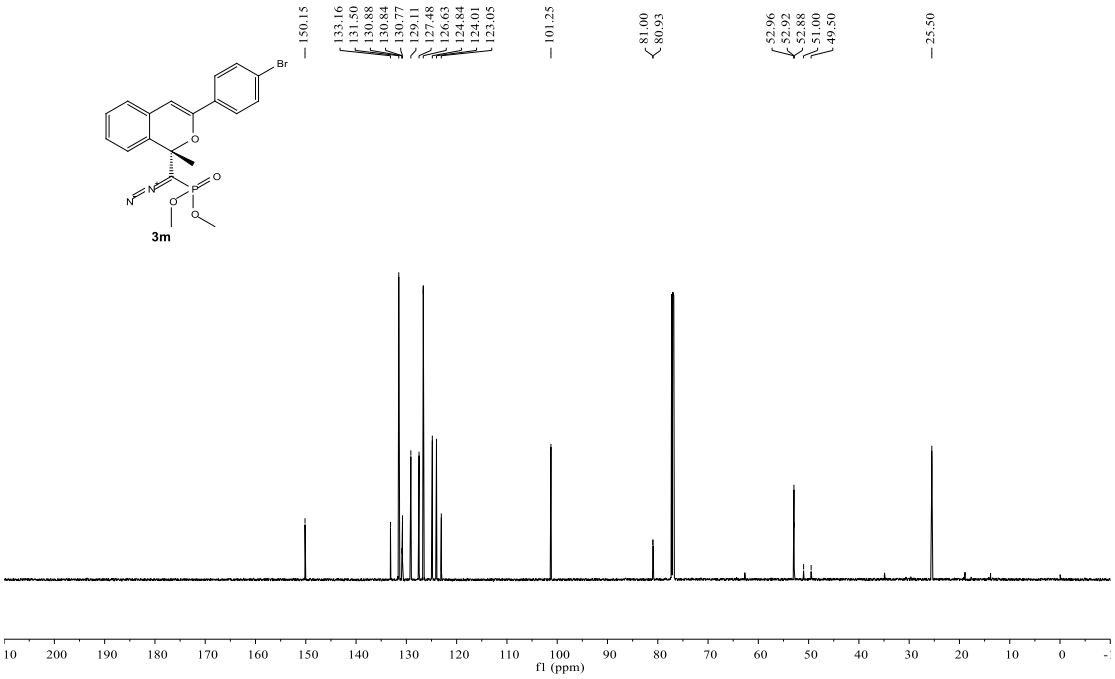

7.77
7.76
7.75
7.74
7.29
7.28
7.27
7.26
7.24
7.23
7.22
7.14
7.13
7.07
7.06
7.04
6.38
3.66
3.64
3.63
3.61
2.09
F
O
N
N
P
O
O
O
3k
2.03
3.02
0.96
1.84
1.00
5.99
3.11
f1 (ppm)

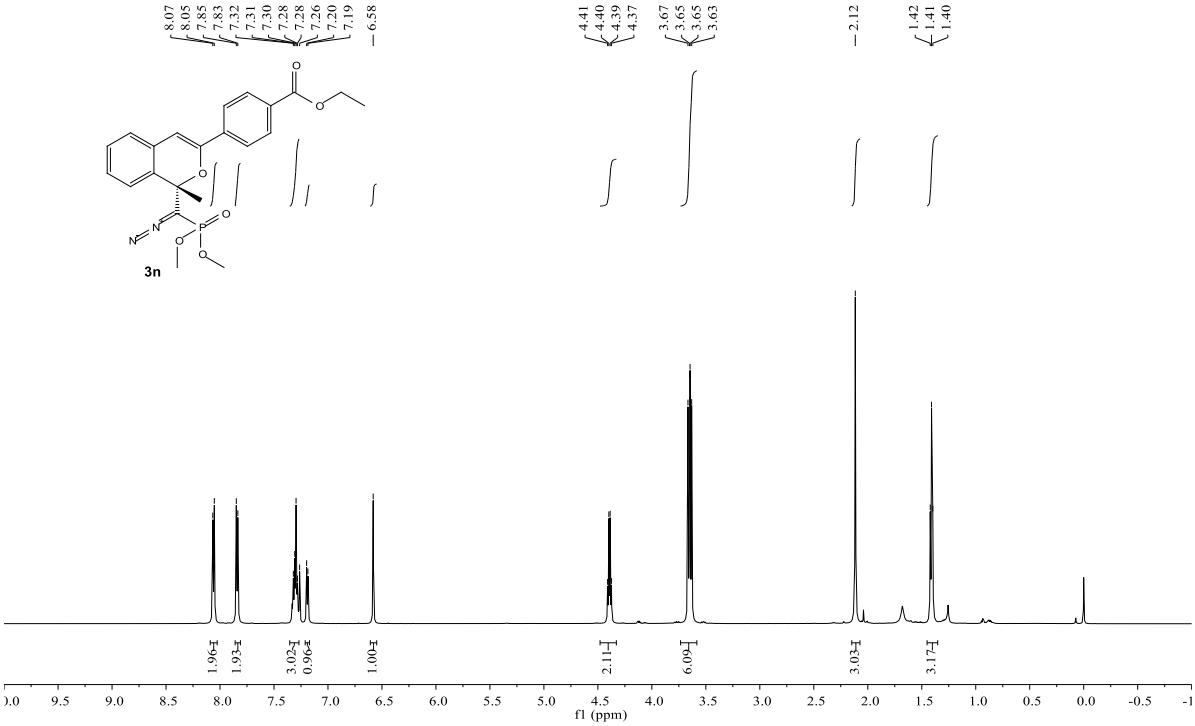

164.08
162.43
150.33
130.98
130.71
130.68
130.42
130.40
129.07
127.23
127.10
127.04
124.68
123.96
115.40
115.25
100.55
80.97
80.90
52.93
52.90
52.86
50.97
49.47
25.47
F
O
N
N
P
O
O
O
3k
f1 (ppm)

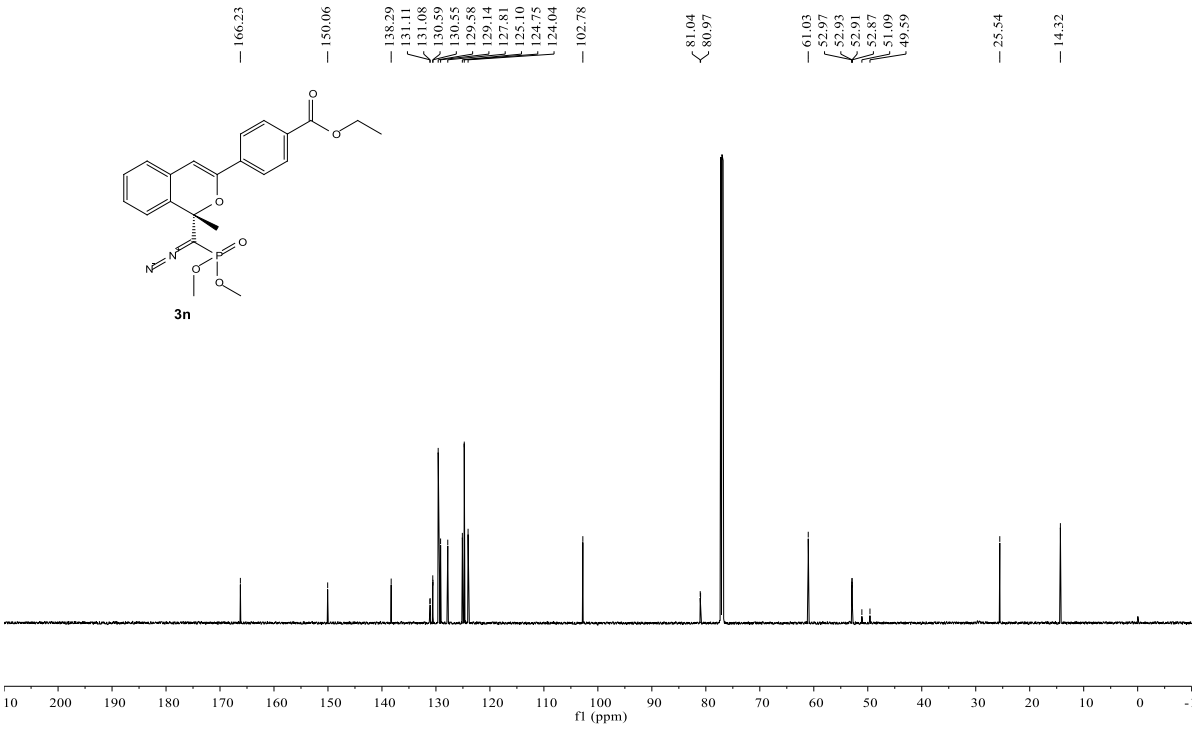

7.93
7.71
7.70
7.47
7.46
7.31
7.29
7.26
7.17
7.16
6.46
3.71
3.70
3.68
3.68
2.09
Br
O
N
N
P
O
O
O
3l
0.96
1.00
0.98
4.40
1.01
1.00
6.08
3.13
f1 (ppm)

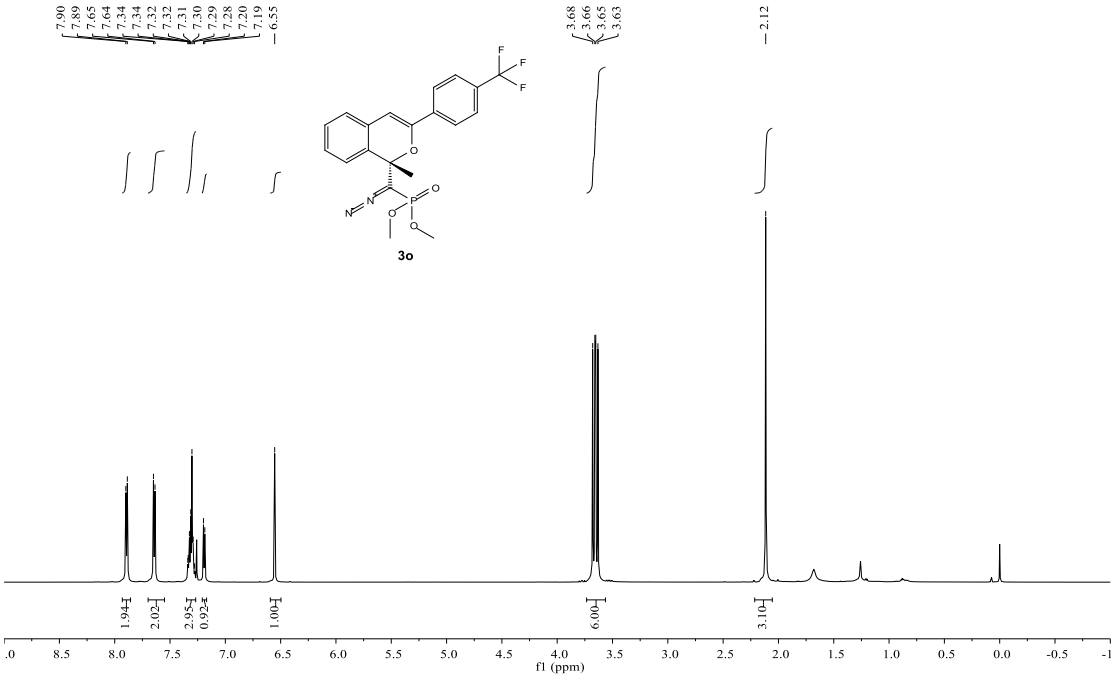

149.63
136.34
131.74
131.06
131.03
130.61
129.84
129.11
128.22
127.67
124.98
123.99
123.59
122.63
101.84
81.16
81.10
53.03
52.99
52.94
52.90
51.18
49.67
25.49
Br
O
N
N
P
O
O
O
3l
f1 (ppm)

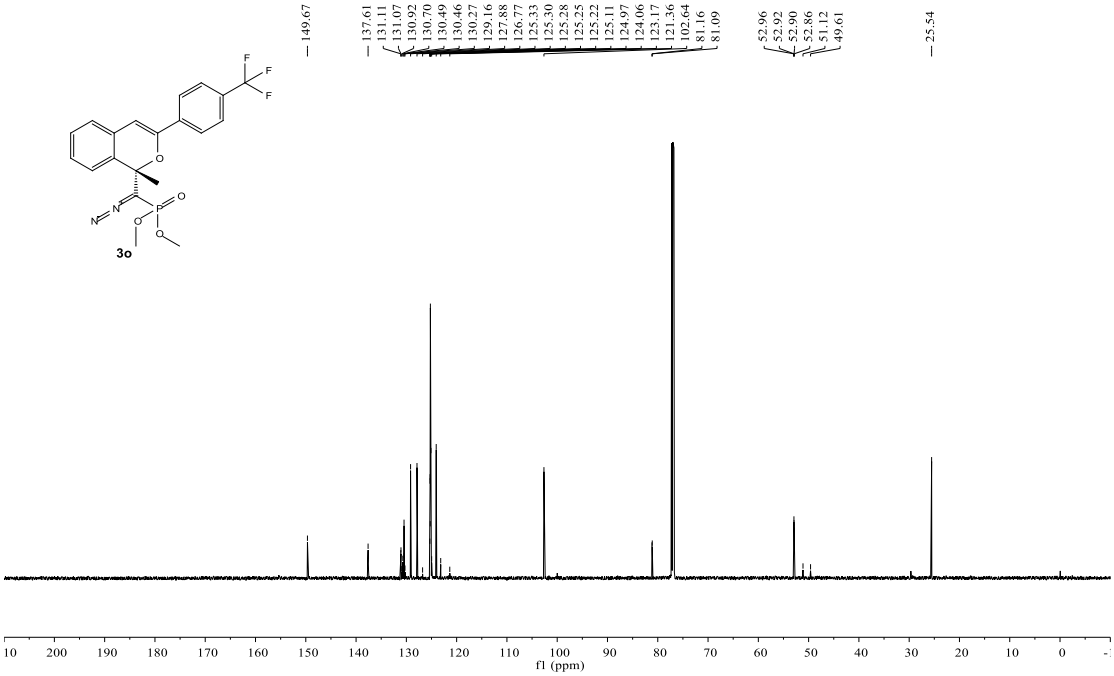

7.66
7.65
7.52
7.51
7.30
7.30
7.29
7.28
7.27
7.26
7.16
7.15
6.46
3.67
3.65
3.65
3.63
2.10
Br
O
N
N
P
O
O
O
3m
1.99
1.92
3.14
1.00
1.00
6.01
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

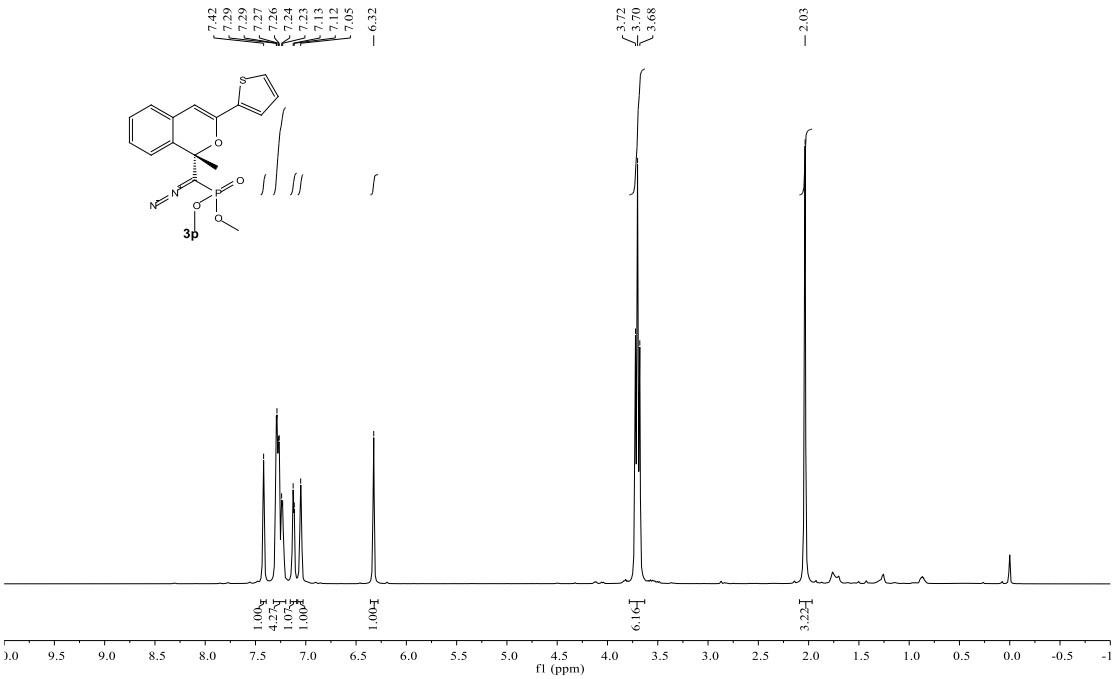

150.15
133.16
131.50
130.88
130.84
130.77
129.11
127.48
126.63
124.84
124.01
123.05
101.25
81.00
80.93
52.96
52.92
52.88
51.00
49.50
25.50
Br
O
N
N
P
O
O
O
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

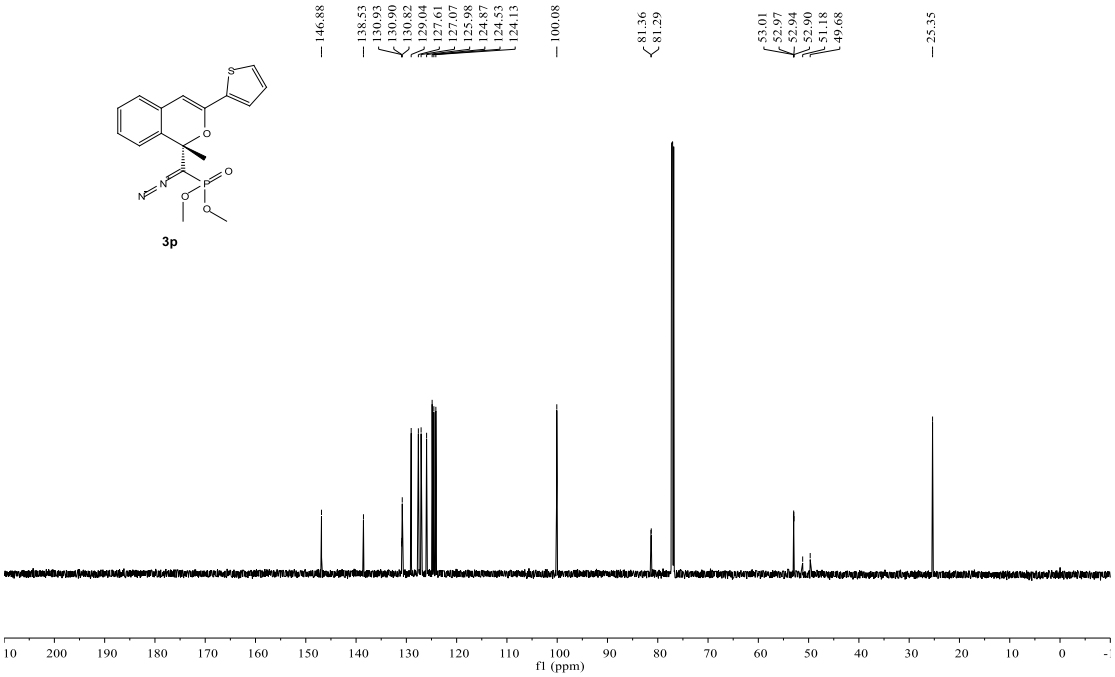

8.07
8.05
7.85
7.83
7.32
7.31
7.30
7.28
7.28
7.26
7.20
7.19
6.58
4.41
4.40
4.39
4.37
3.67
3.65
3.65
3.63
2.12
1.42
1.41
1.40
3n
1.96
1.93
3.02
0.96
1.00
2.11
6.09
3.03
3.17
f1 (ppm)

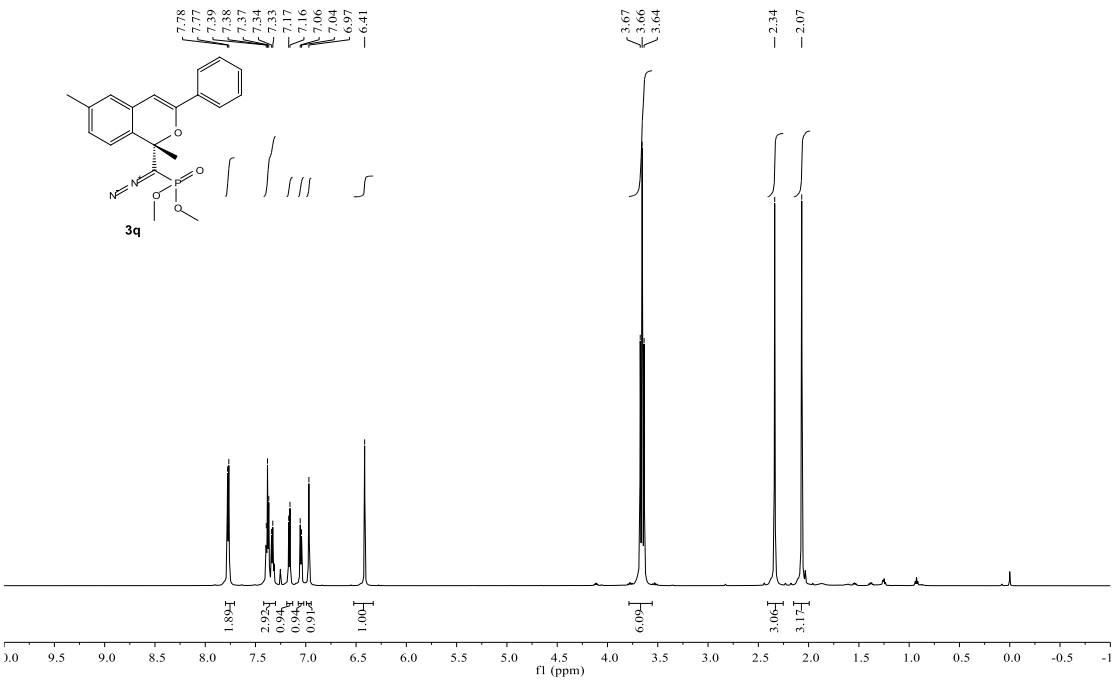

166.23
150.06
138.29
131.11
131.08
130.59
130.55
129.58
129.14
127.81
125.10
124.75
124.04
102.78
81.04
80.97
61.03
52.97
52.93
52.91
52.87
51.09
49.59
25.54
14.32
3n
f1 (ppm)

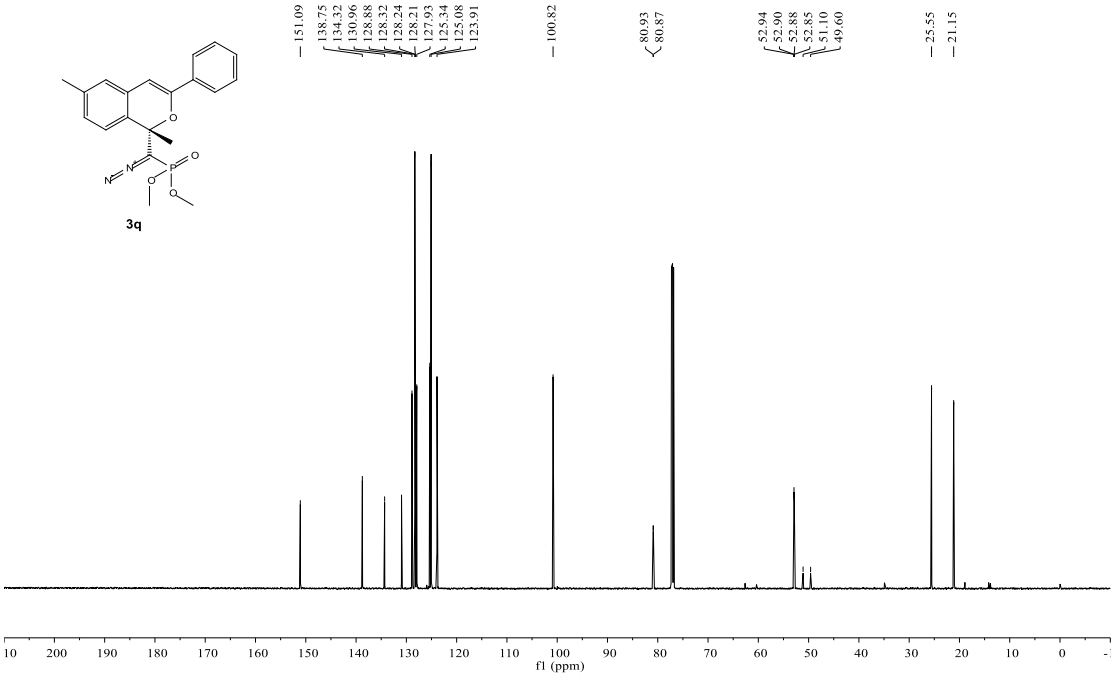

7.90
7.89
7.65
7.64
7.34
7.34
7.32
7.32
7.31
7.30
7.29
7.28
7.20
7.19
6.55
3.68
3.66
3.65
3.63
2.12
3o
1.94
2.02
2.95
0.92
1.00
6.00
3.10
f1 (ppm)

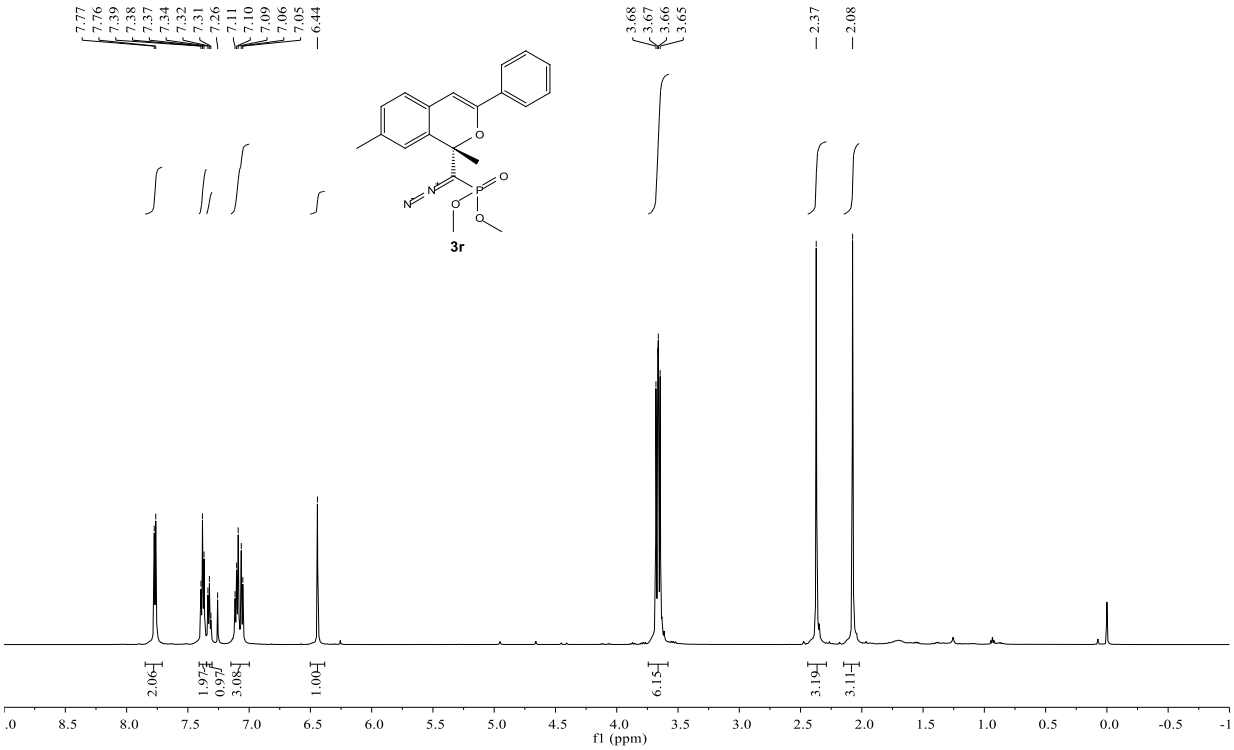

149.67
137.61
131.11
131.07
130.92
130.70
130.49
130.46
130.27
129.16
127.88
126.77
125.33
125.30
125.28
125.25
125.22
125.11
124.97
124.06
123.17
121.36
102.64
81.16
81.09
52.96
52.92
52.90
52.86
51.12
49.61
25.54
3o
f1 (ppm)

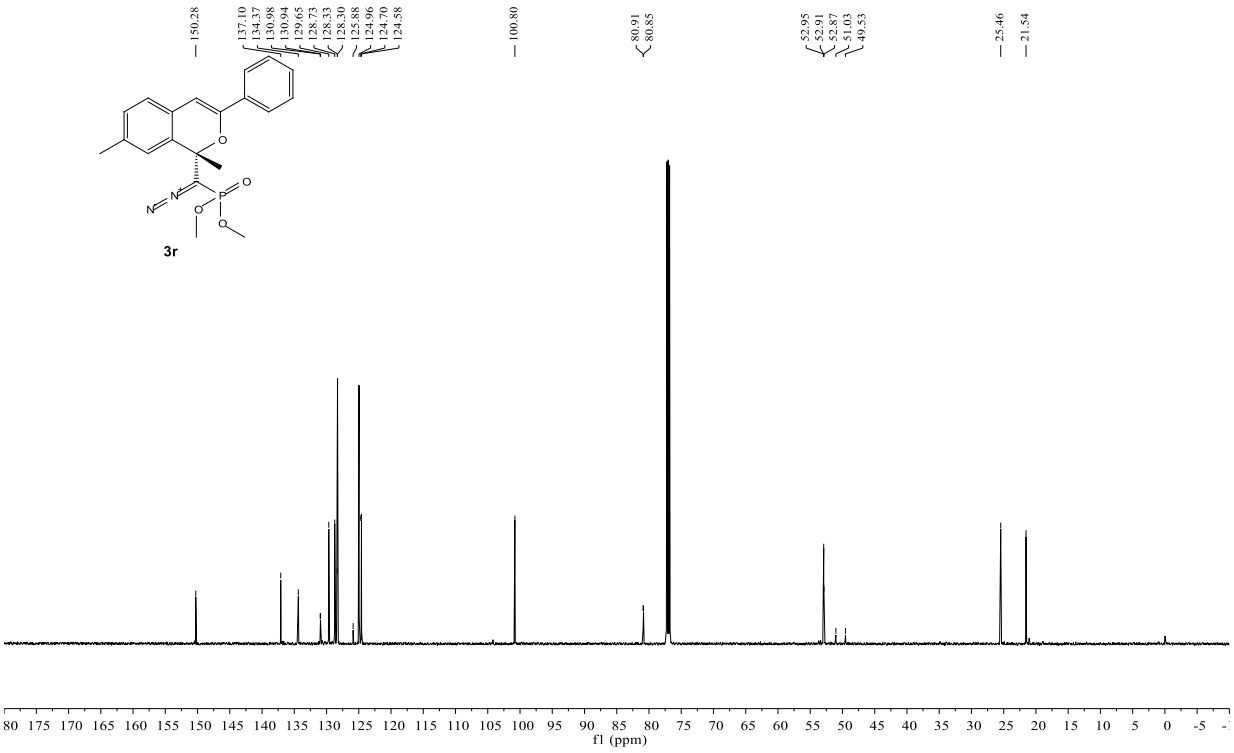

7.42
7.29
7.29
7.27
7.26
7.24
7.23
7.13
7.12
7.05
6.32
3.72
3.70
3.68
2.03
3p
1.00
4.27
1.07
1.00
1.00
6.16
3.22
f1 (ppm)

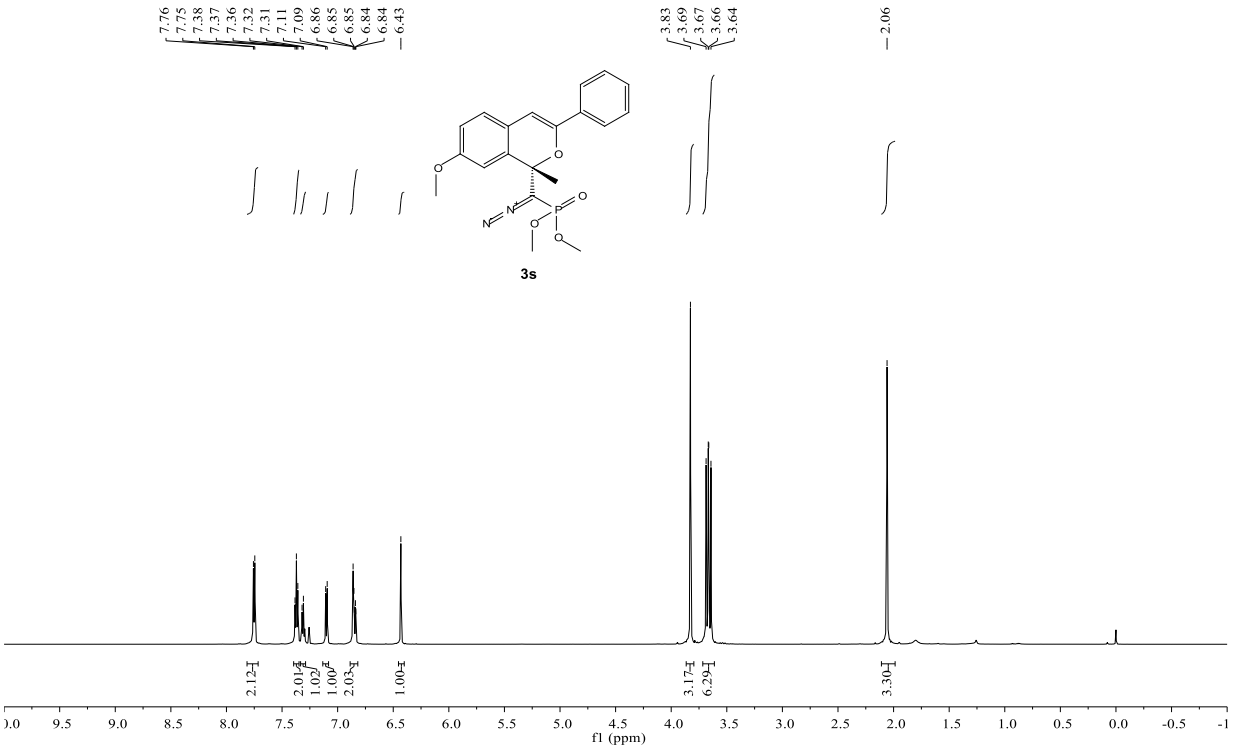

146.88
138.53
130.93
130.90
130.82
129.04
127.61
127.07
125.98
124.87
124.53
124.13
100.08
81.36
81.29
53.01
52.97
52.94
52.90
51.18
49.68
25.35
3p
f1 (ppm)

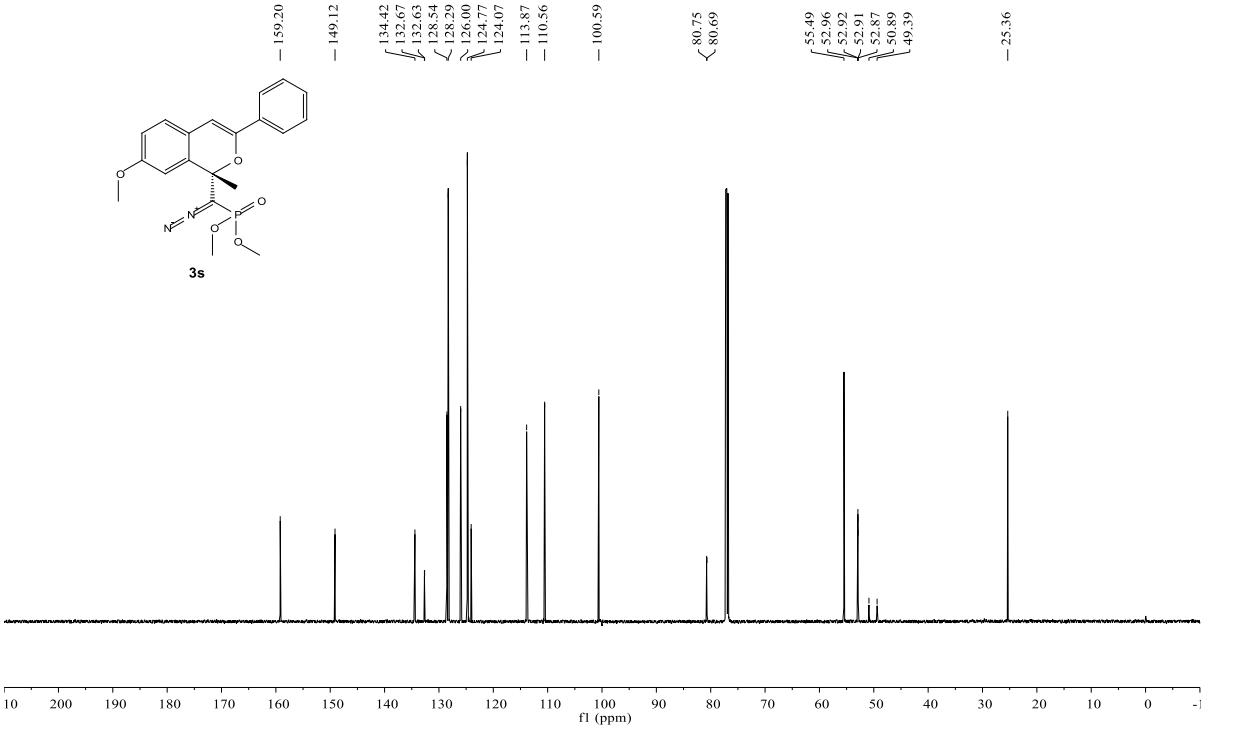

7.78
7.77
7.39
7.38
7.37
7.34
7.33
7.17
7.16
7.06
7.04
6.97
6.41
3.67
3.66
3.64
2.34
2.07
3q
1.89
2.92
0.94
0.94
0.91
1.00
6.09
3.06
3.17
f1 (ppm)

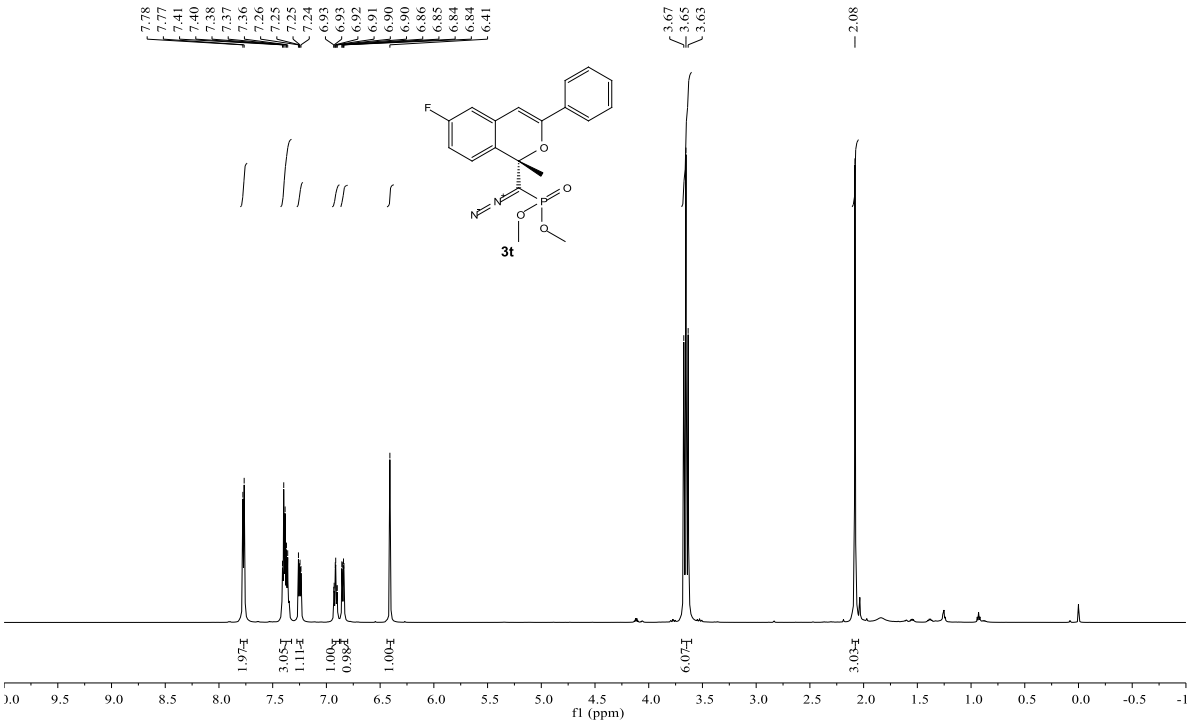

151.09
138.75
134.32
130.96
128.88
128.32
128.24
128.21
127.93
125.34
125.08
123.91
100.82
80.93
80.87
52.94
52.90
52.88
52.85
51.10
49.60
25.55
21.15
3q
f1 (ppm)

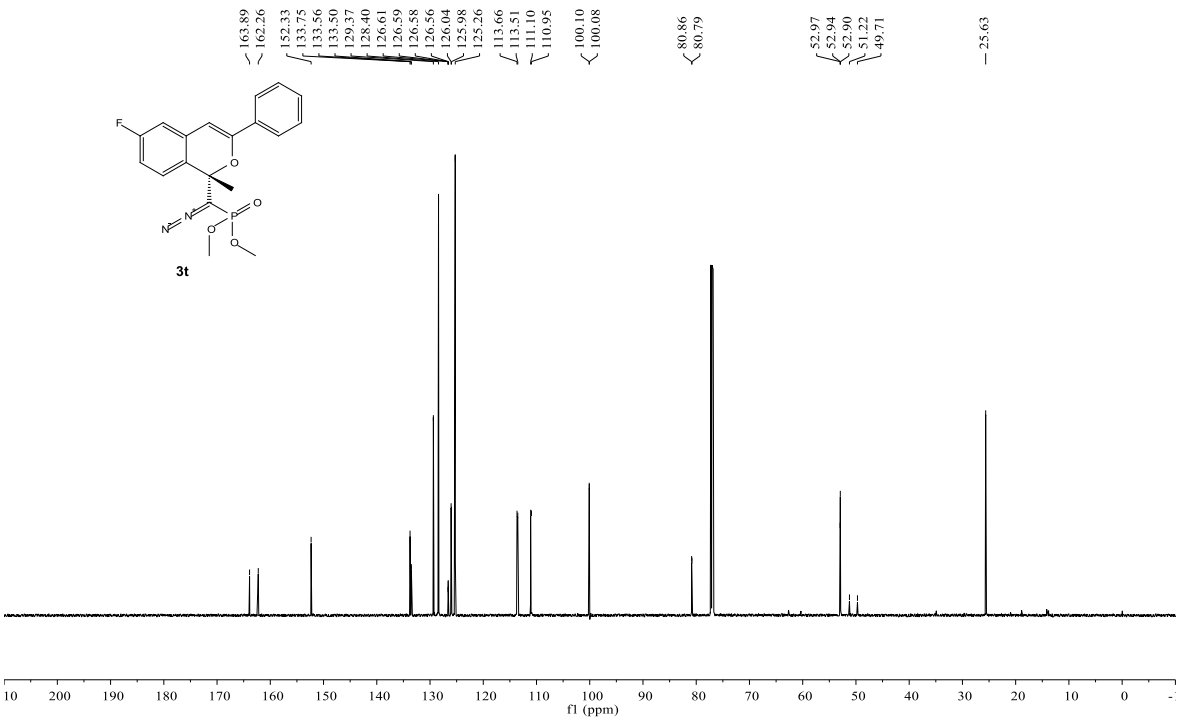

7.77
7.76
7.39
7.38
7.37
7.34
7.32
7.31
7.26
7.11
7.10
7.09
7.06
7.05
6.44
3.68
3.67
3.66
3.65
2.37
2.08
3r
2.06
1.97
0.97
3.08
1.00
6.15
3.19
3.11
f1 (ppm)

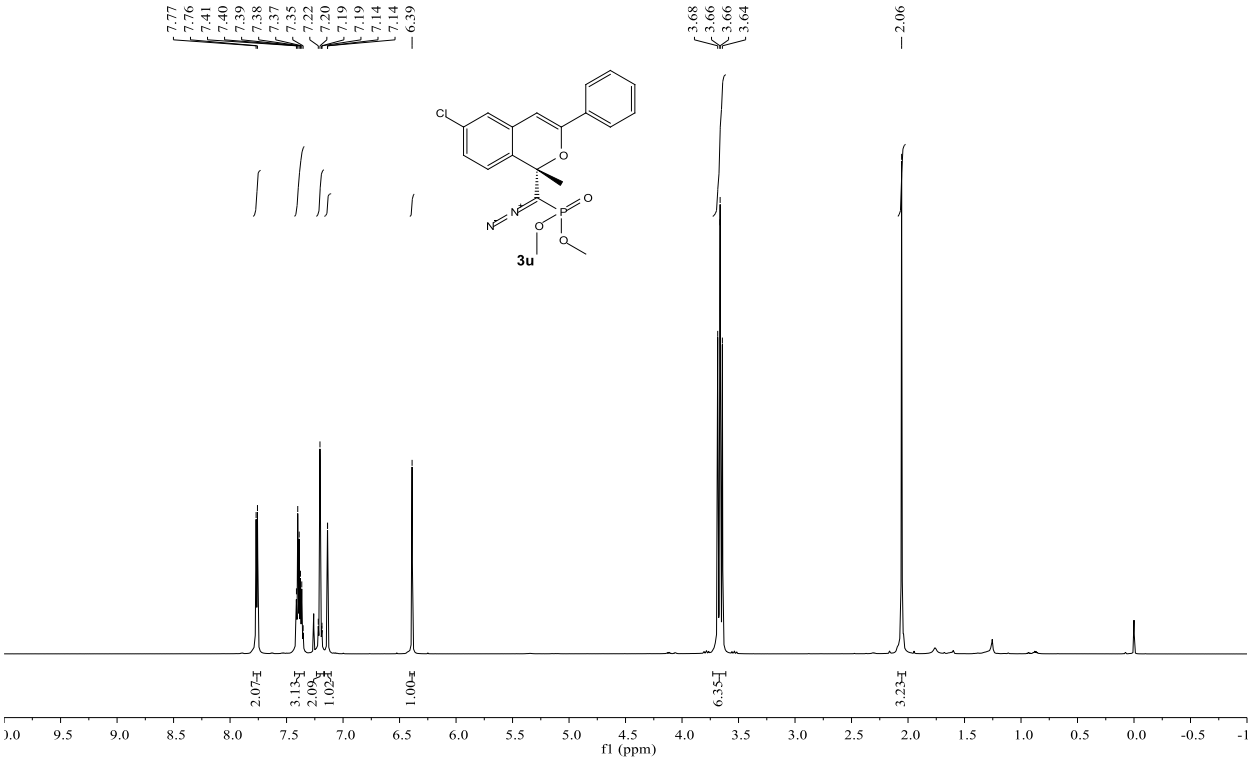

150.28
137.10
134.37
130.98
130.94
129.65
128.73
128.33
128.30
125.88
124.96
124.70
124.58
100.80
80.91
80.85
52.95
52.91
52.87
51.03
49.53
25.46
21.54
3r
f1 (ppm)

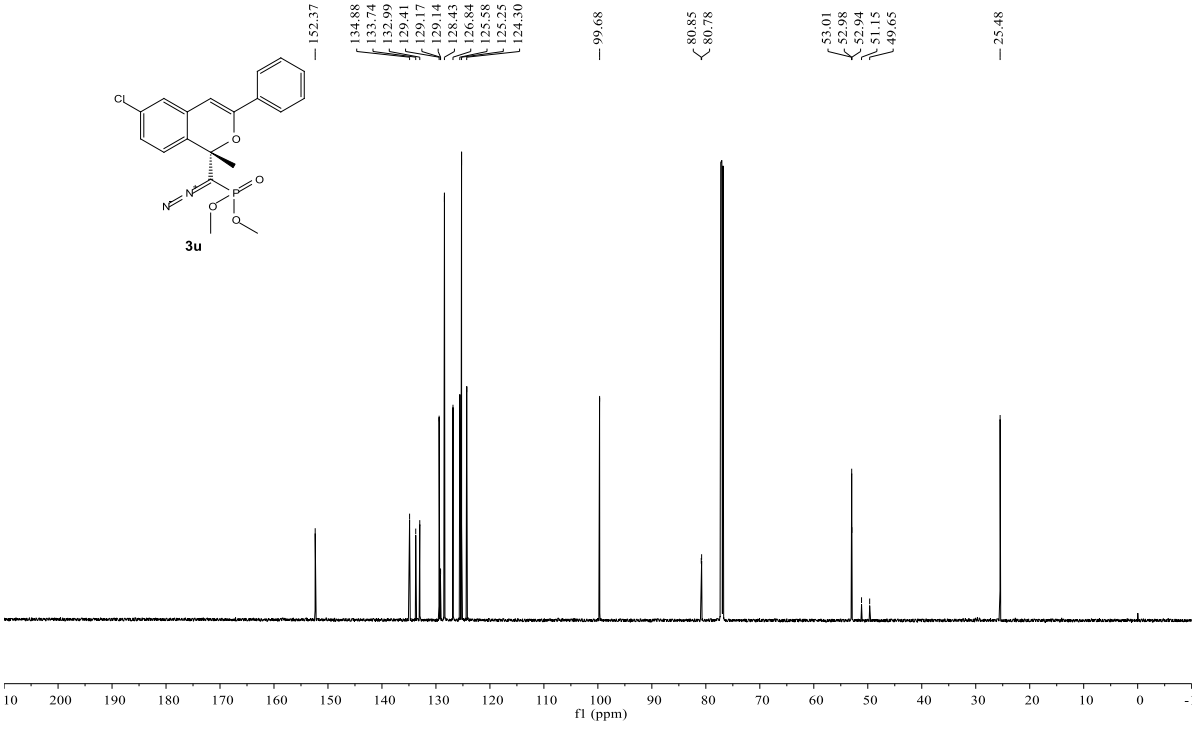

7.76
7.75
7.38
7.37
7.36
7.32
7.31
7.11
7.09
6.86
6.85
6.85
6.84
6.84
6.43
3.83
3.69
3.67
3.66
3.64
2.06
3s
2.12
2.01
1.02
1.00
2.03
1.00
3.17
6.29
3.30
f1 (ppm)

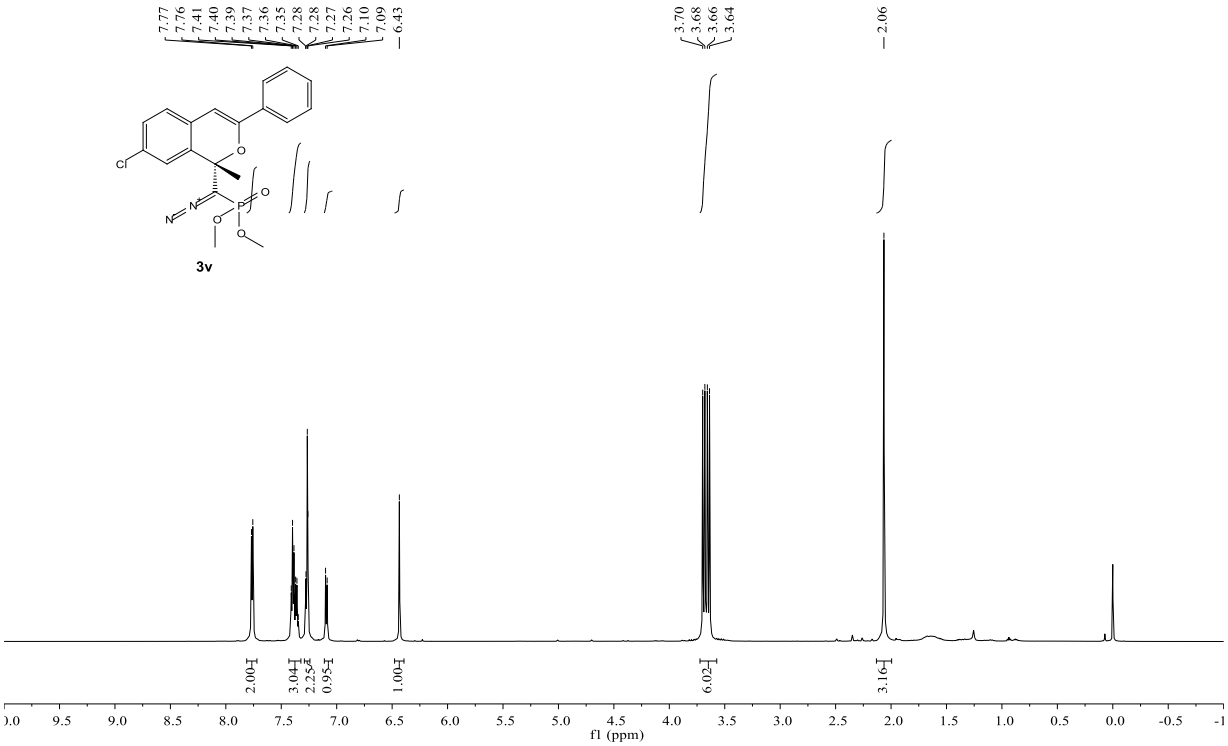

159.20
149.12
134.42
132.67
132.63
128.54
128.29
126.00
124.77
124.07
113.87
110.56
100.59
80.75
80.69
55.49
52.96
52.92
52.91
52.87
50.89
49.39
25.36
3s
f1 (ppm)

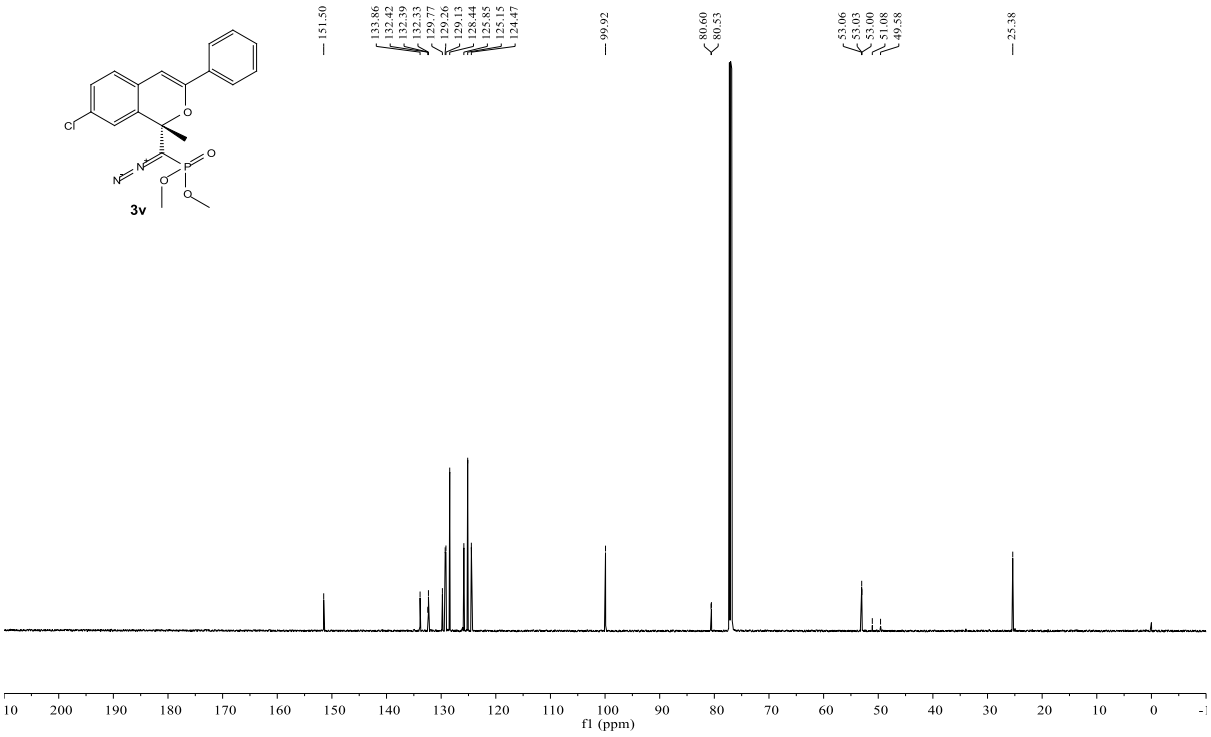

7.78
7.77
7.41
7.40
7.38
7.37
7.36
7.26
7.25
7.25
7.24
6.93
6.93
6.92
6.91
6.90
6.90
6.86
6.85
6.84
6.84
6.41
3.67
3.65
3.63
2.08
F
O
N
N
P
O
O
O
3t
1.97
3.05
1.11
1.00
0.98
1.00
6.07
3.03
f1 (ppm)

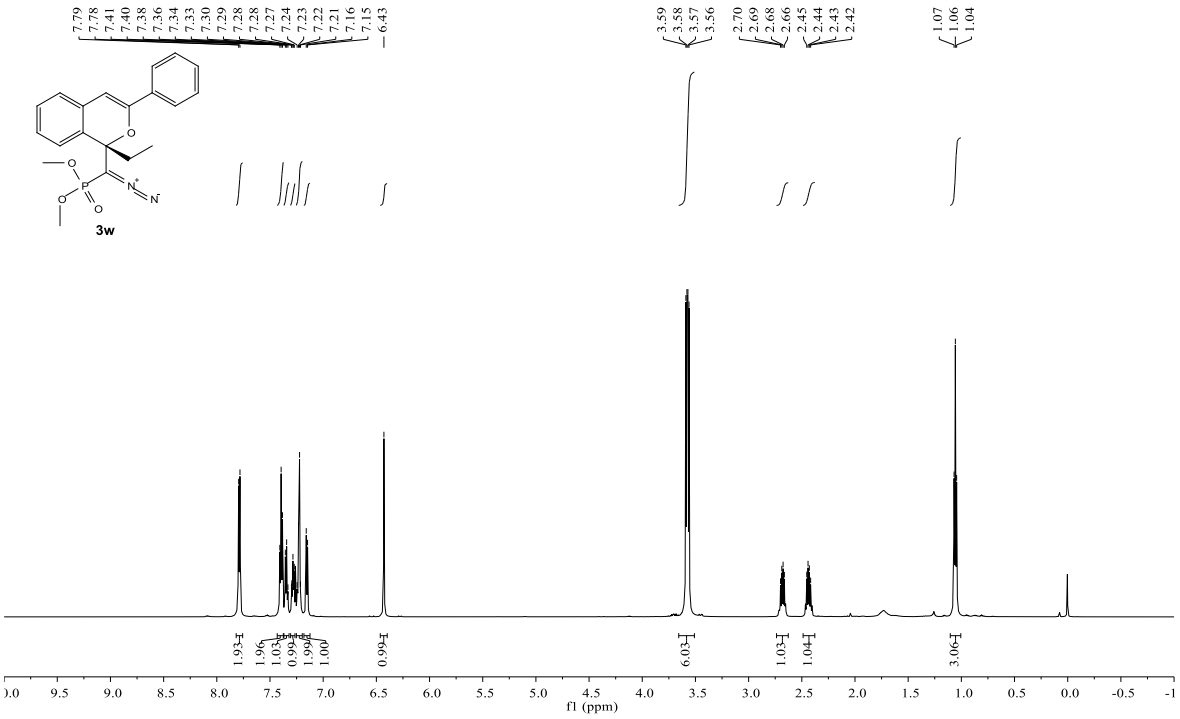

163.89
162.26
152.33
133.75
133.56
133.50
129.37
128.40
126.61
126.59
126.58
126.56
126.04
125.98
125.26
113.66
113.51
111.10
110.95
100.10
100.08
80.86
80.79
52.97
52.94
52.90
51.22
49.71
25.63
F
O
N
N
P
O
O
O
3t
f1 (ppm)

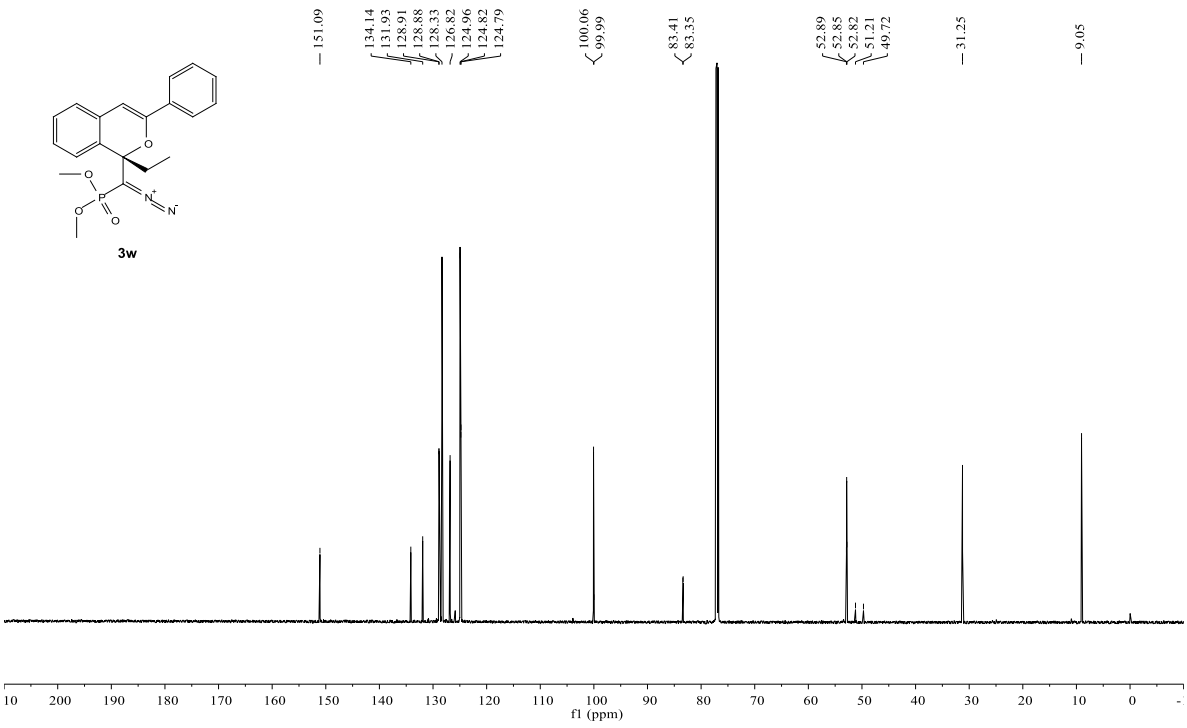

7.77
7.76
7.41
7.40
7.39
7.38
7.37
7.35
7.22
7.20
7.19
7.19
7.14
7.14
6.39
3.68
3.66
3.66
3.64
2.06
Cl
O
N
N
P
O
O
O
3u
2.07
3.13
2.09
1.02
1.00
6.35
3.23
f1 (ppm)

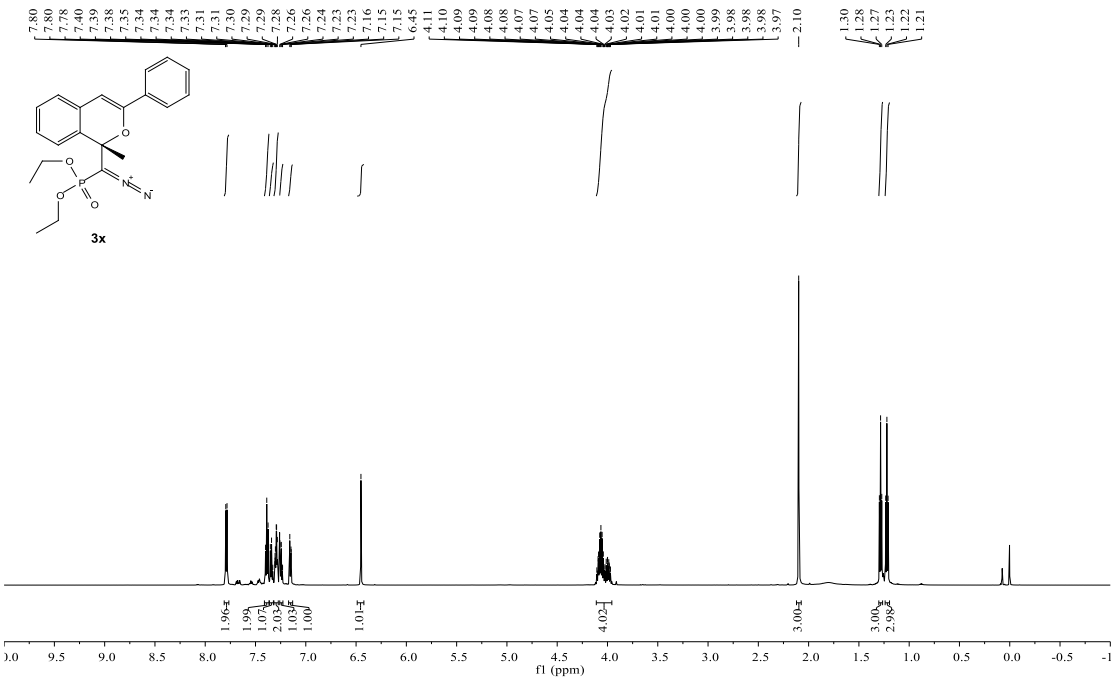

152.37
134.88
133.74
132.99
129.41
129.17
129.14
128.43
126.84
125.58
125.25
124.30
99.68
80.85
80.78
53.01
52.98
52.94
51.15
49.65
25.48
Cl
O
N
N
P
O
O
O
3u
f1 (ppm)

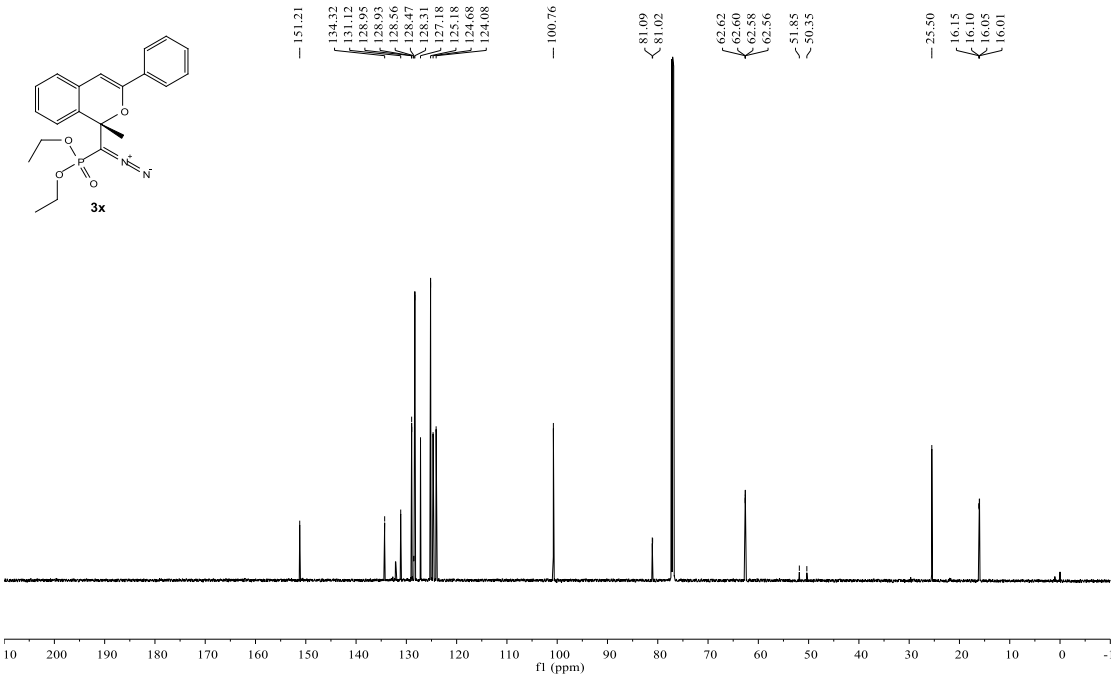

7.77
7.76
7.41
7.40
7.39
7.37
7.36
7.35
7.28
7.28
7.27
7.26
7.10
7.09
6.43
3.70
3.68
3.66
3.64
2.06
Cl
O
N
N
P
O
O
O
3v
2.00
3.04
2.25
0.95
1.00
6.02
3.16
f1 (ppm)

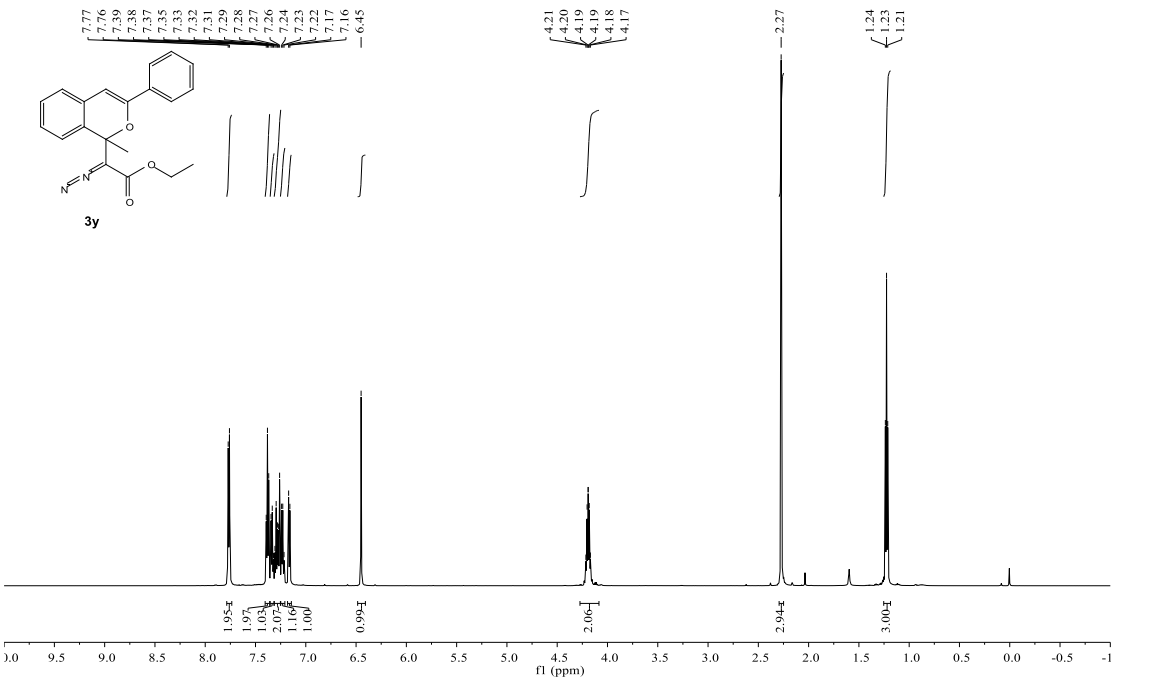

151.50
133.86
132.42
132.39
132.33
129.77
129.26
129.13
128.44
125.85
125.15
124.47
99.92
80.60
80.53
53.06
53.03
53.00
51.08
49.58
25.38
Cl
O
N
N
P
O
O
O
3v
f1 (ppm)

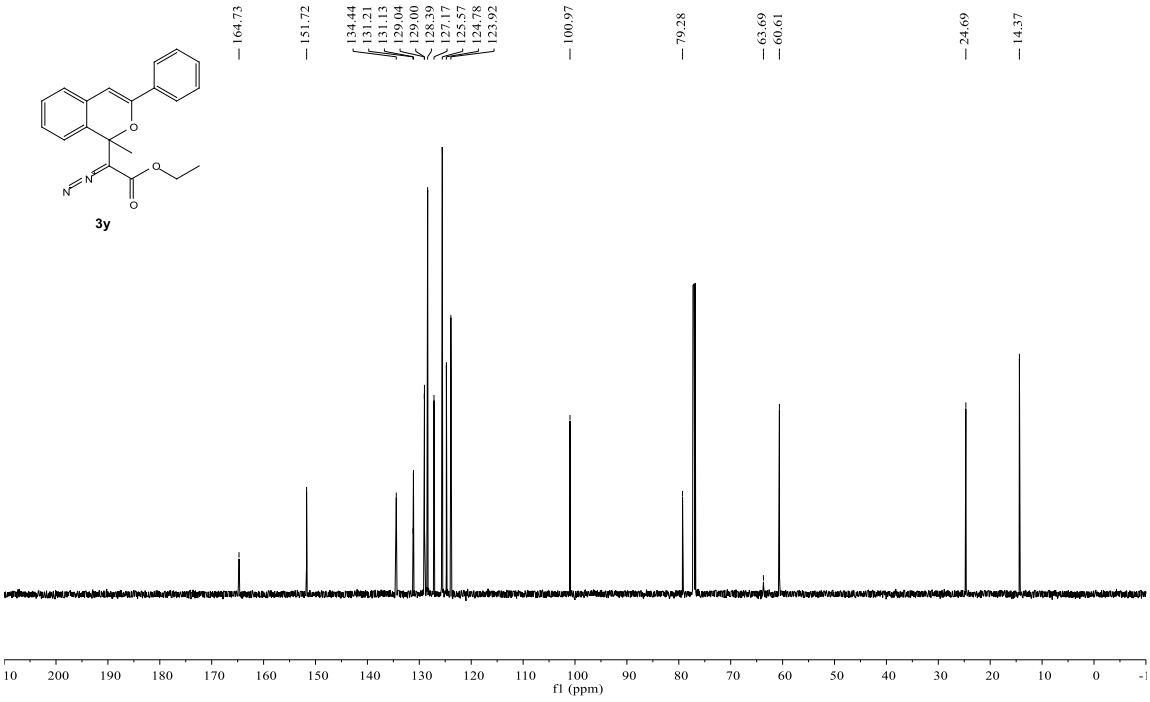

7.79
7.78
7.41
7.40
7.38
7.36
7.34
7.33
7.30
7.29
7.28
7.28
7.27
7.24
7.23
7.22
7.21
7.16
7.15
6.43
3.59
3.58
3.57
3.56
2.70
2.69
2.68
2.66
2.45
2.44
2.43
2.42
1.07
1.06
1.04
3w
1.93
1.96
1.03
0.99
1.99
1.00
0.99
6.03
1.03
1.04
3.06
f1 (ppm)

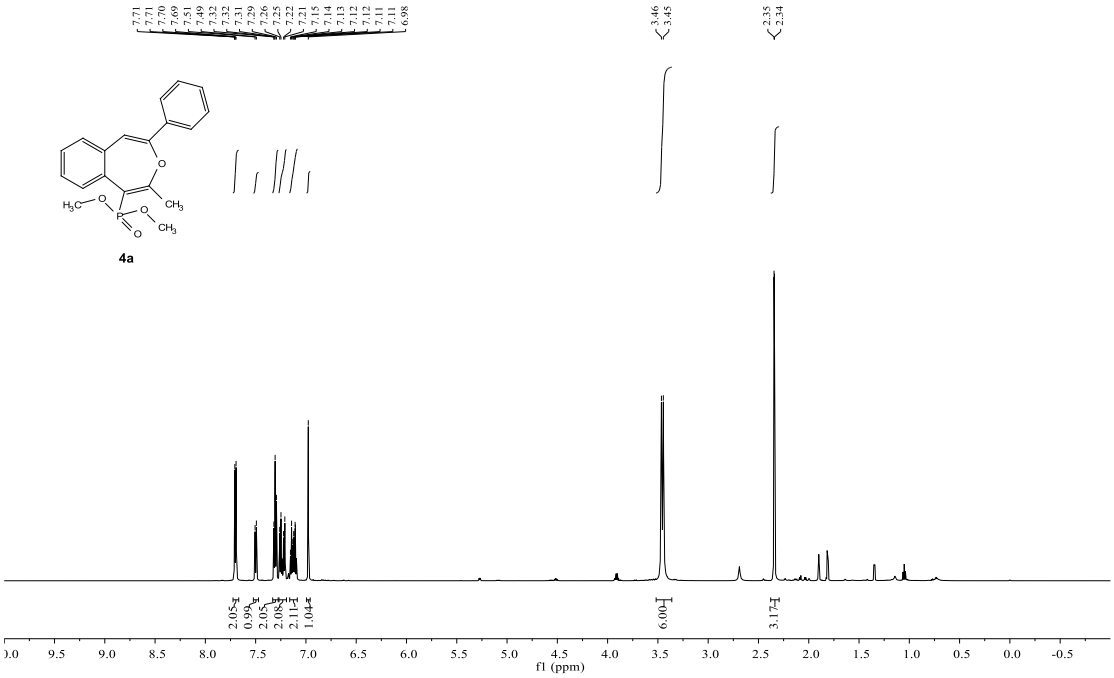

151.09
134.14
131.93
128.91
128.88
128.33
126.82
124.96
124.82
124.79
100.06
99.99
83.41
83.35
52.89
52.85
52.82
51.21
49.72
31.25
9.05
3w
f1 (ppm)

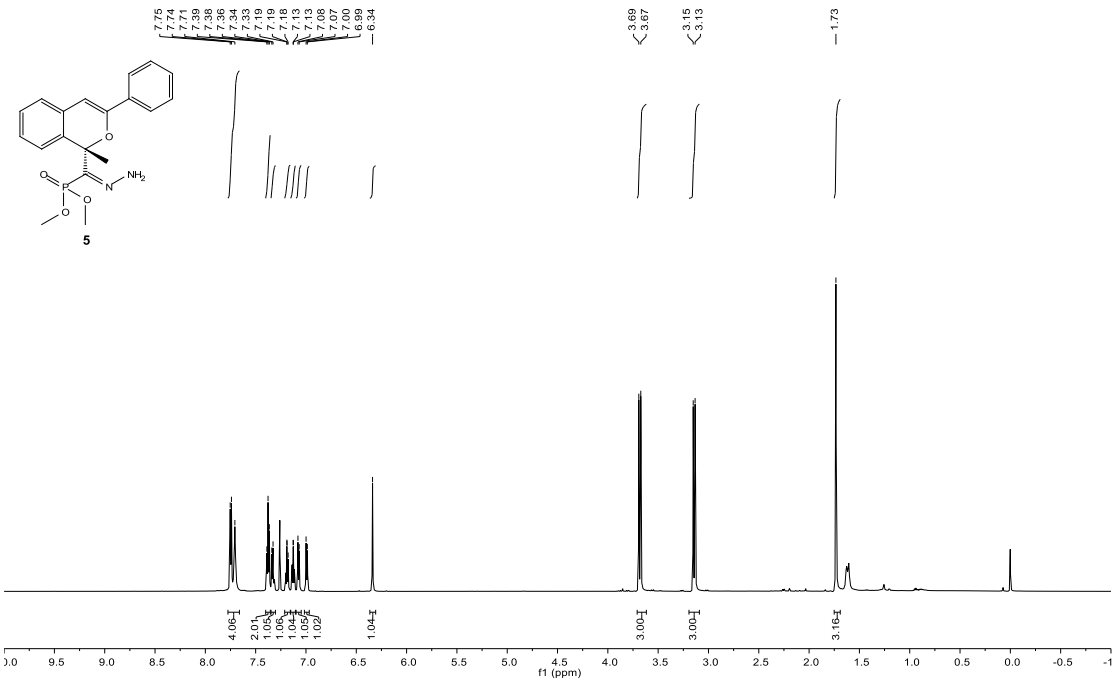

3x
f1 (ppm)

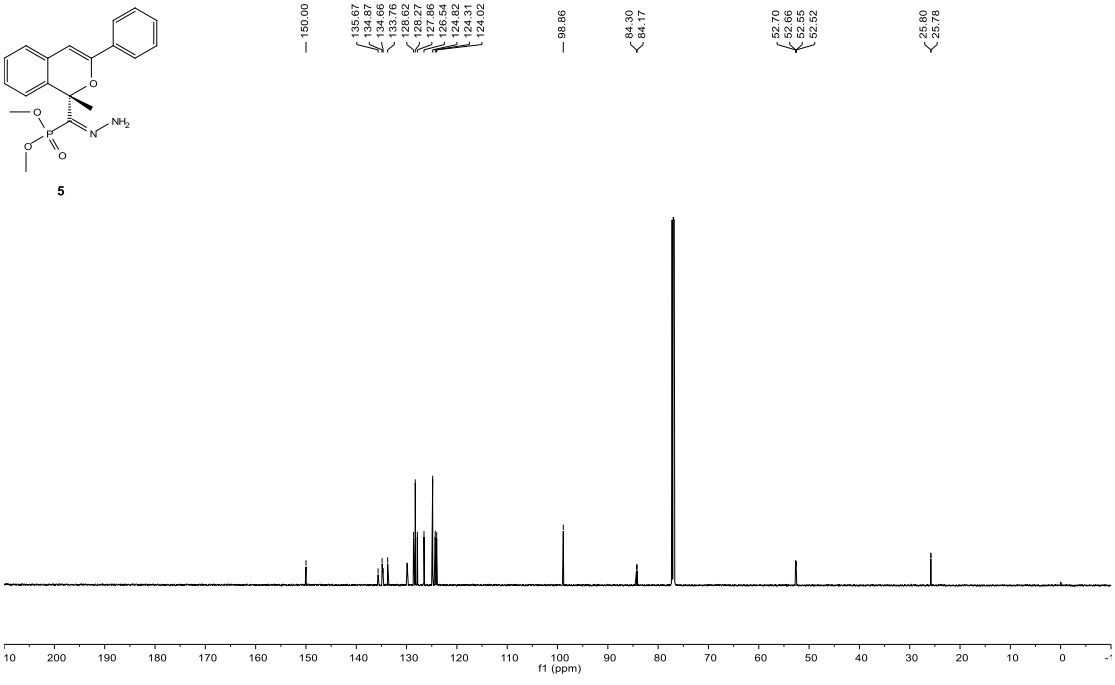

3x
f1 (ppm)

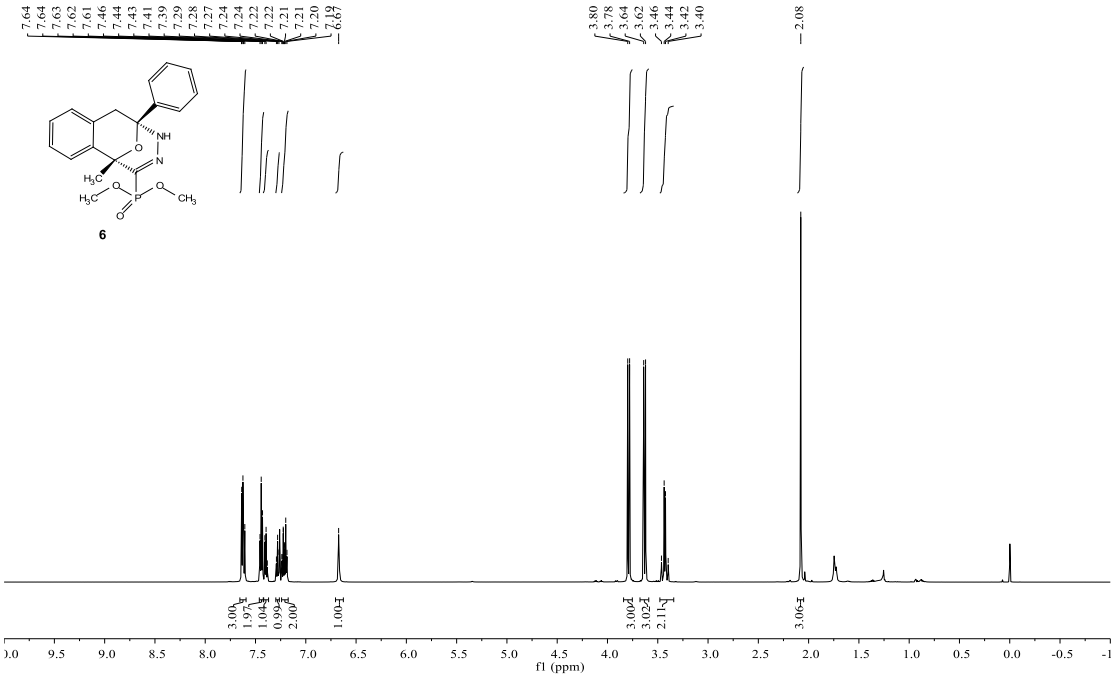

7.77
7.76
7.39
7.38
7.37
7.35
7.33
7.32
7.31
7.29
7.28
7.27
7.26
7.24
7.23
7.22
7.17
7.16
6.45
4.21
4.20
4.19
4.19
4.18
4.17
2.27
1.24
1.23
1.21
1.95
1.97
1.03
2.07
1.16
1.00
0.99
2.06
2.94
3.00
f1 (ppm)
3y

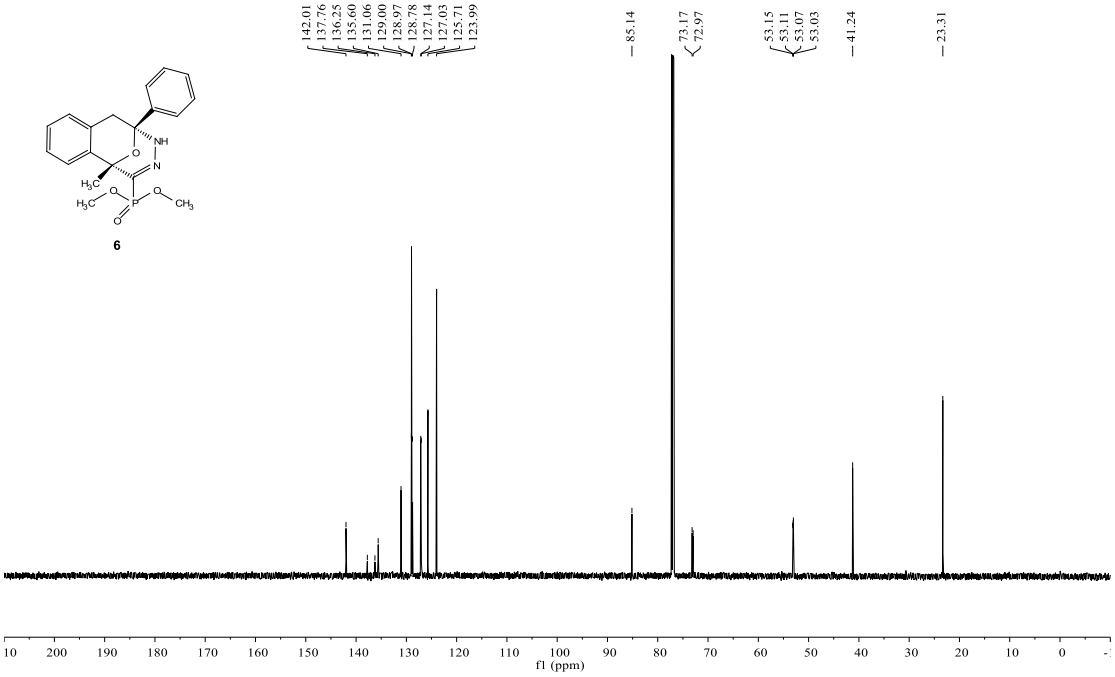

164.73
151.72
134.44
131.21
131.13
129.04
129.00
128.39
127.17
125.57
124.78
123.92
100.97
79.28
63.69
60.61
24.69
14.37
f1 (ppm)
3y

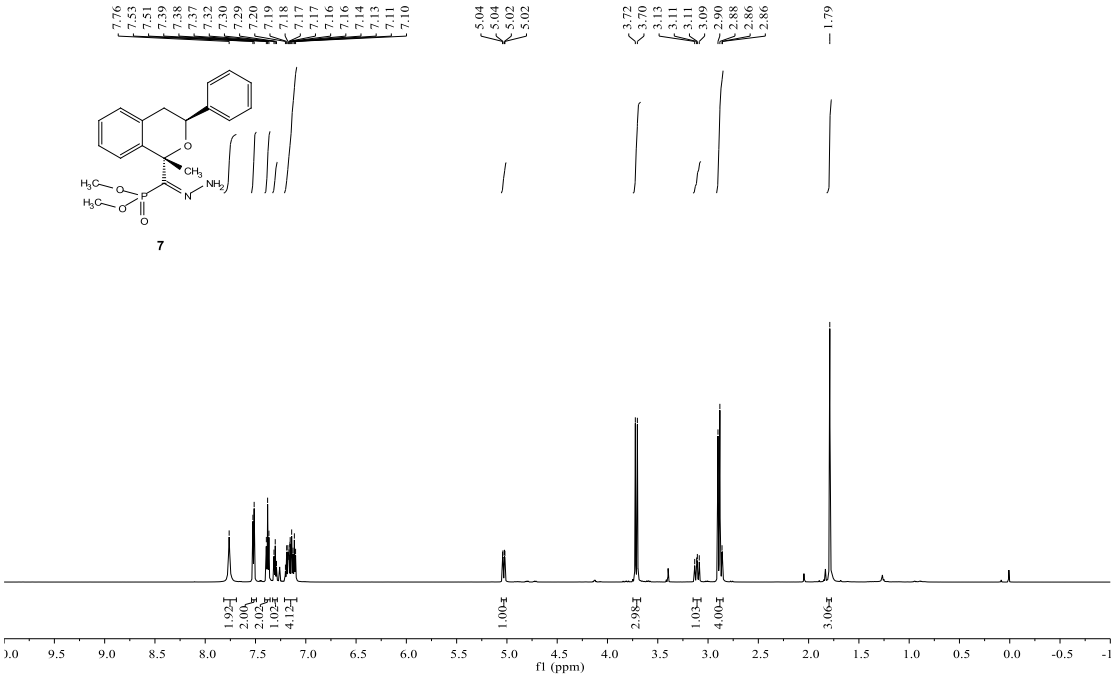

7.71
7.71
7.70
7.69
7.51
7.49
7.32
7.32
7.31
7.29
7.26
7.25
7.22
7.21
7.15
7.14
7.13
7.12
7.12
7.11
7.11
6.98
3.46
3.45
2.35
2.34
4a
2.05
0.99
2.05
2.08
2.11
1.04
6.00
3.17
f1 (ppm)


7.75
7.74
7.71
7.39
7.38
7.36
7.34
7.33
7.19
7.19
7.18
7.13
7.13
7.08
7.07
7.00
6.99
6.34
3.69
3.67
3.15
3.13
1.73
NH2
5
4.06
2.01
1.05
1.06
1.04
1.05
1.02
1.04
3.00
3.00
3.16
f1 (ppm)

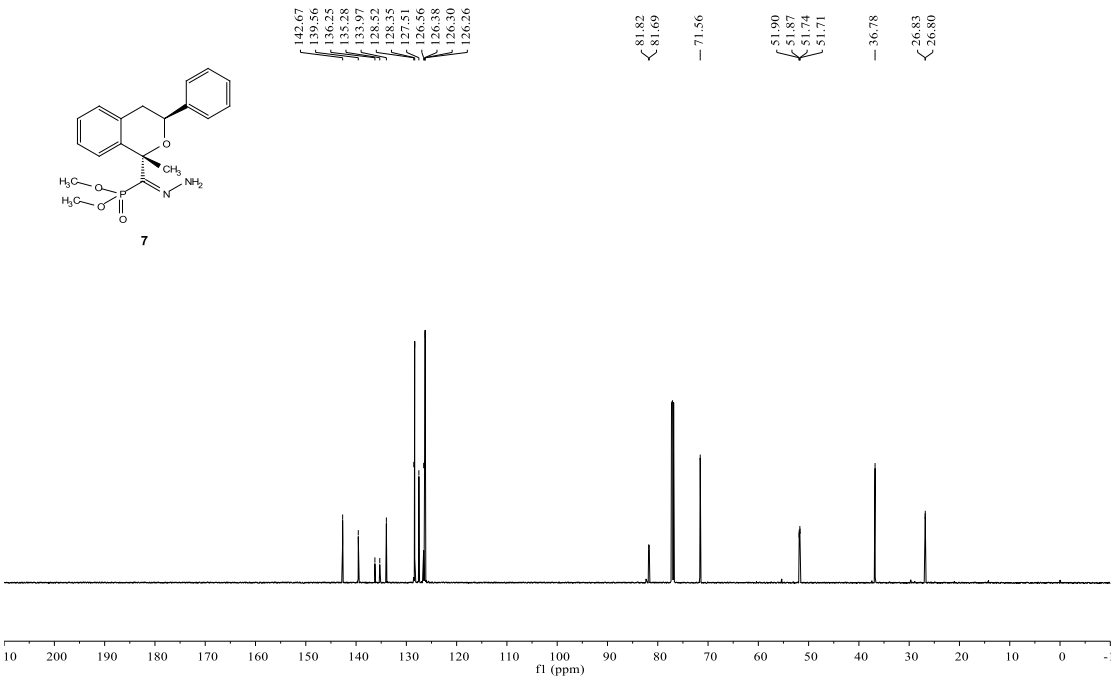

150.00
135.67
134.87
134.66
133.76
128.62
128.27
127.86
126.54
124.82
124.31
124.02
98.86
84.30
84.17
52.70
52.66
52.55
52.52
25.80
25.78
NH2
5
f1 (ppm)

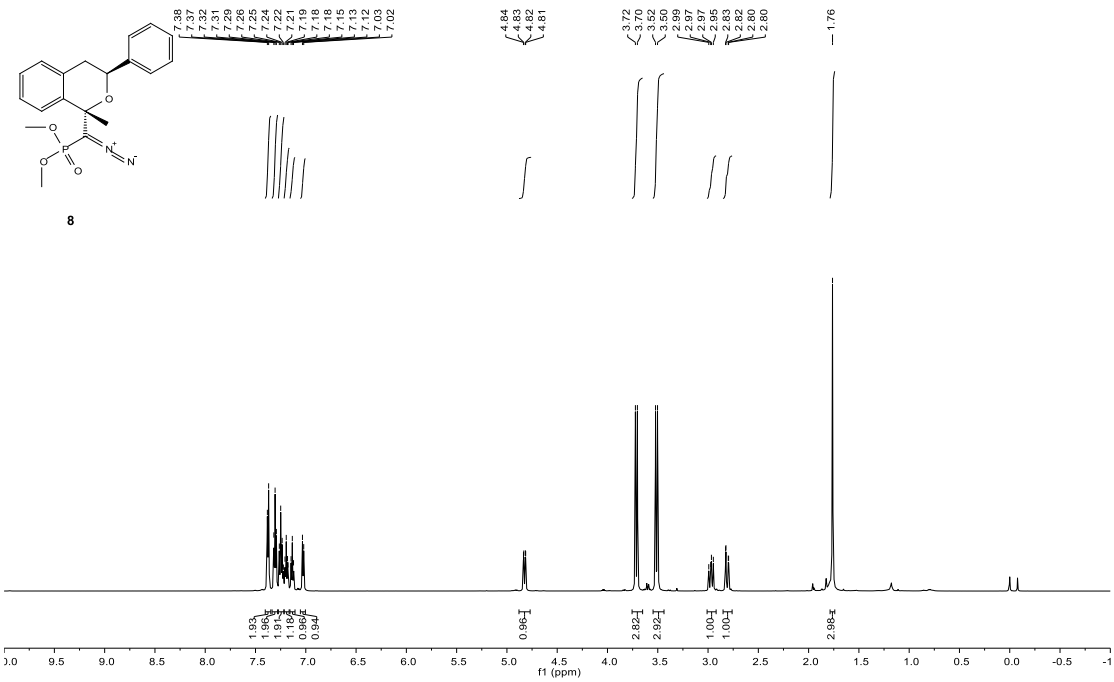

7.64
7.64
7.63
7.62
7.61
7.46
7.44
7.43
7.41
7.39
7.29
7.28
7.27
7.24
7.24
7.22
7.22
7.21
7.21
7.20
7.19
6.67
3.80
3.78
3.64
3.62
3.46
3.44
3.42
3.40
2.08
NH
O
N
H3C
O
O
P
O
CH3
O
6
3.00
1.97
1.04
0.99
2.00
1.00
3.00
3.02
2.11
3.06
f1 (ppm)


142.01
137.76
136.25
135.60
131.06
129.00
128.97
128.78
127.14
127.03
125.71
123.99
85.14
73.17
72.97
53.15
53.11
53.07
53.03
41.24
23.31
NH
O
N
H3C
O
O
P
O
CH3
O
6
f1 (ppm)

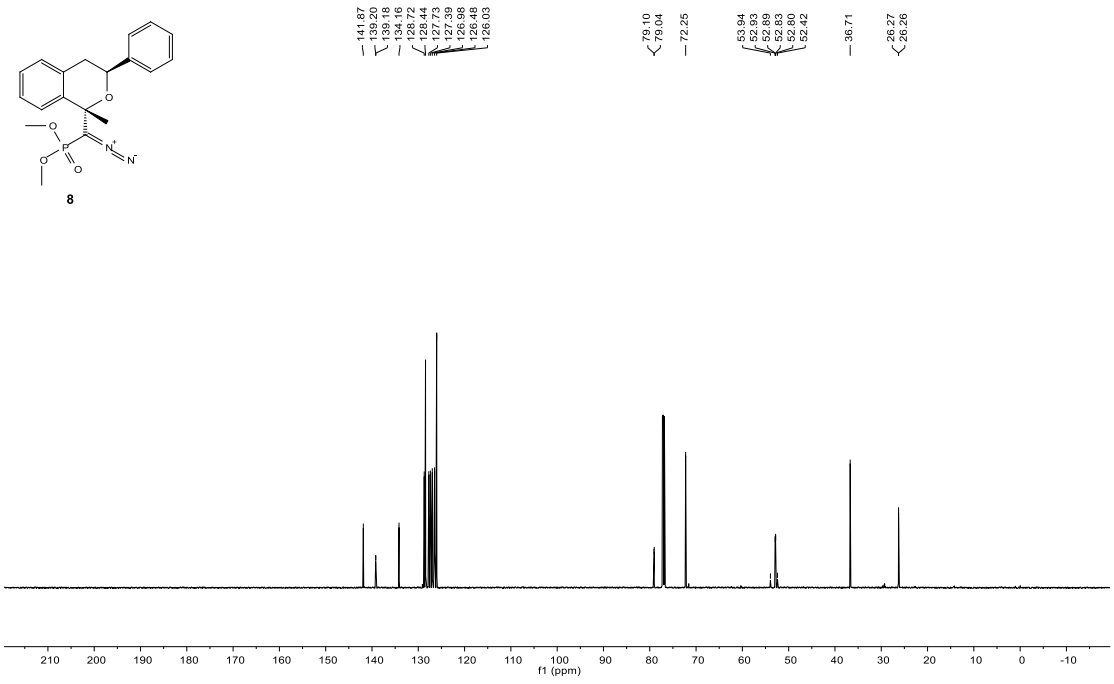

7.76
7.53
7.51
7.39
7.38
7.37
7.32
7.30
7.29
7.20
7.19
7.18
7.17
7.17
7.17
7.16
7.16
7.14
7.13
7.11
7.10
5.04
5.04
5.02
5.02
3.72
3.70
3.13
3.11
3.11
3.09
2.90
2.88
2.86
2.86
1.79
1.92
2.00
2.02
1.02
4.12
1.00
2.98
1.03
4.00
3.06
f1 (ppm)

7

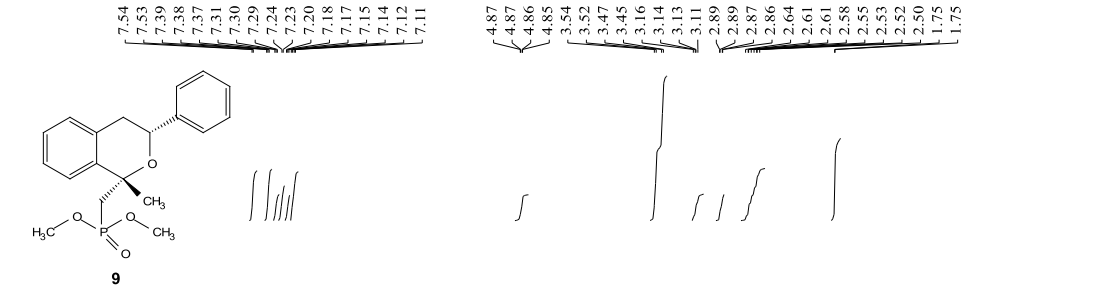

142.67
139.56
136.25
135.28
133.97
128.52
128.35
127.51
126.56
126.38
126.30
126.26
81.82
81.69
71.56
51.90
51.87
51.74
51.71
36.78
26.83
26.80
f1 (ppm)


7.38
7.37
7.32
7.31
7.29
7.26
7.25
7.24
7.22
7.21
7.19
7.18
7.18
7.15
7.13
7.12
7.03
7.02
4.84
4.83
4.82
4.81
3.72
3.70
3.52
3.50
2.99
2.97
2.97
2.95
2.83
2.82
2.80
2.80
1.76
1.93
1.96
1.91
1.18
0.96
0.94
0.96
2.82
2.92
1.00
1.00
2.98
f1 (ppm)

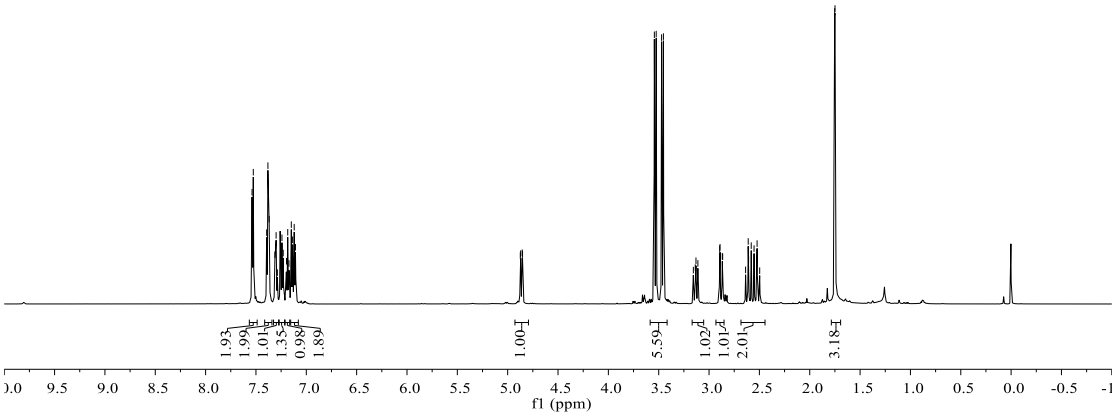
8

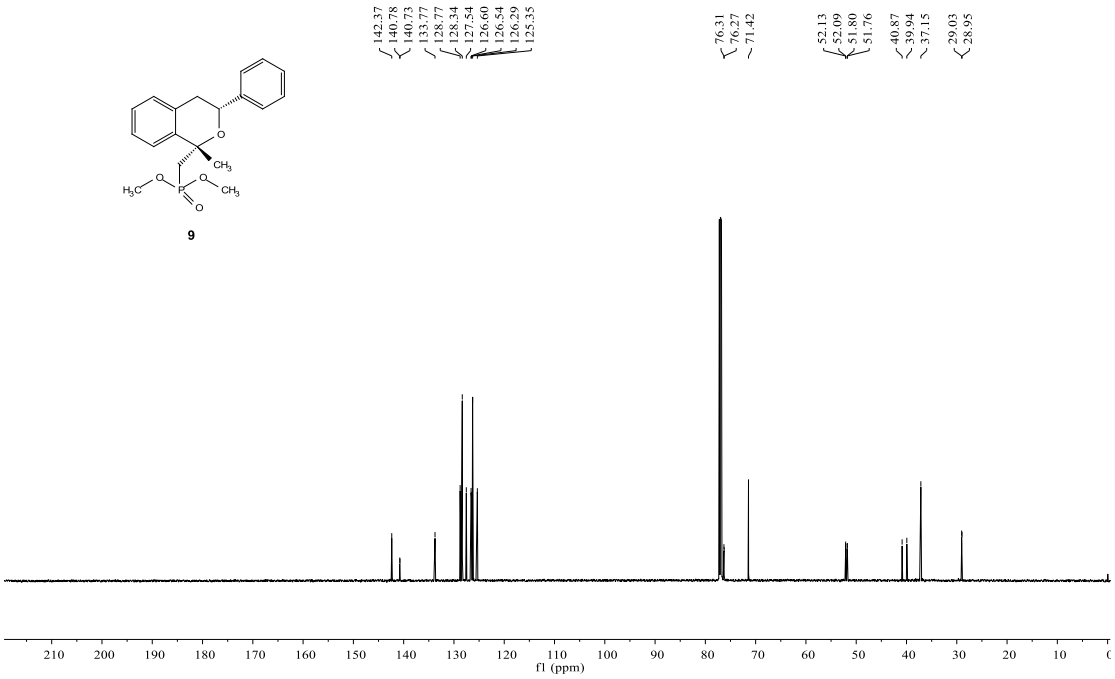

141.87
139.20
139.18
134.16
128.72
128.44
127.73
127.39
126.98
126.48
126.03
79.10
79.04
72.25
53.94
52.93
52.89
52.83
52.80
52.42
36.71
26.27
26.26
f1 (ppm)

8

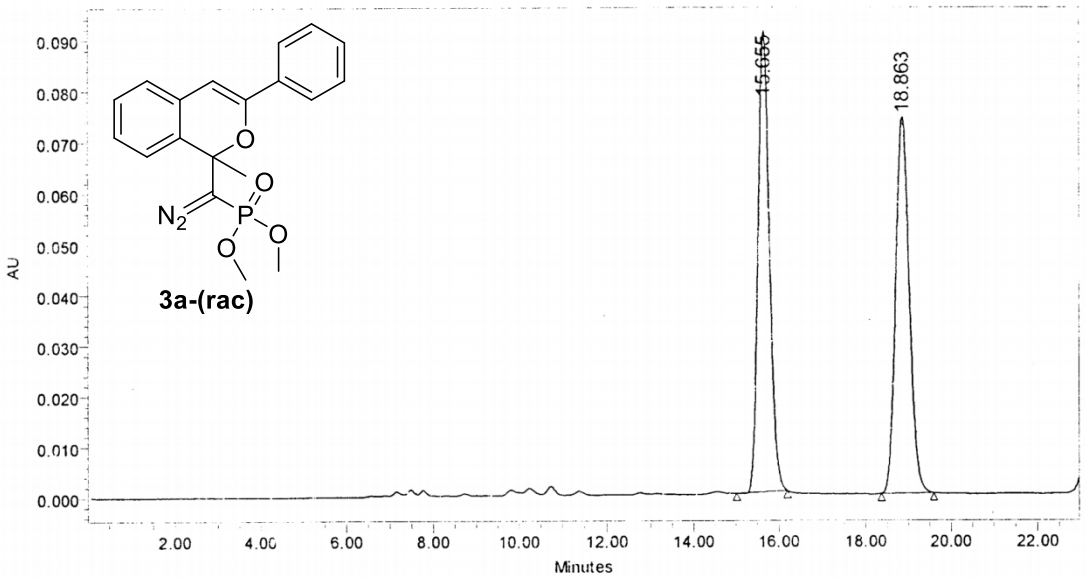

7.54
7.53
7.39
7.38
7.37
7.31
7.30
7.29
7.24
7.23
7.20
7.18
7.17
7.15
7.14
7.12
7.11
4.87
4.87
4.86
4.85
3.54
3.52
3.47
3.45
3.16
3.14
3.13
3.11
2.89
2.89
2.87
2.86
2.64
2.61
2.61
2.58
2.55
2.53
2.52
2.50
1.75
1.75

9

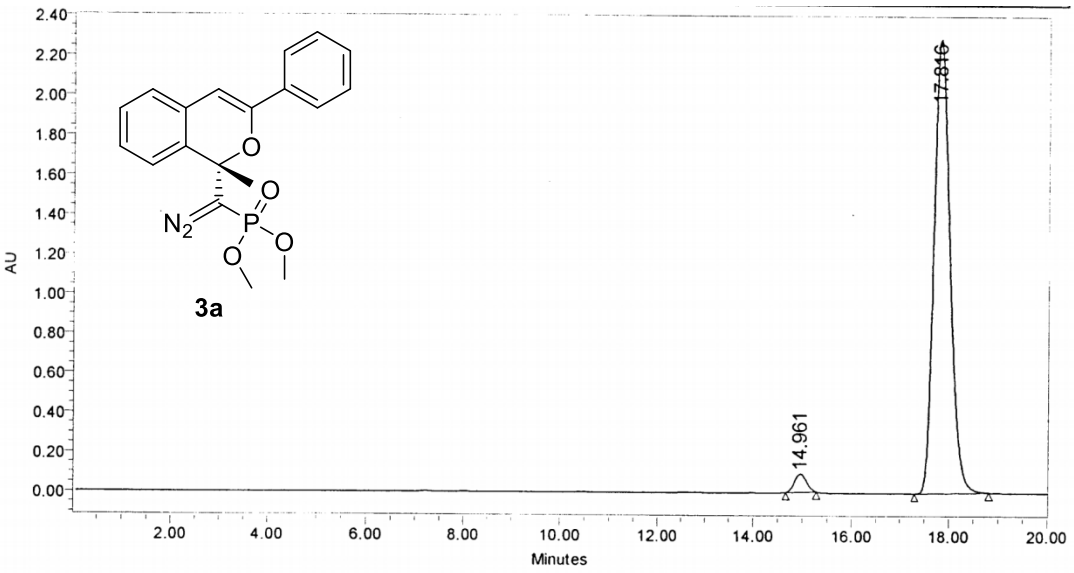

1.93
1.99
1.01
1.35
0.98
1.89
1.00
5.59
1.02
1.01
2.01
3.18
f1 (ppm)


142.37
140.78
140.73
133.77
128.77
128.34
127.54
126.60
126.54
126.29
125.35
76.31
76.27
71.42
52.13
52.09
51.80
51.76
40.87
39.94
37.15
29.03
28.95
f1 (ppm)

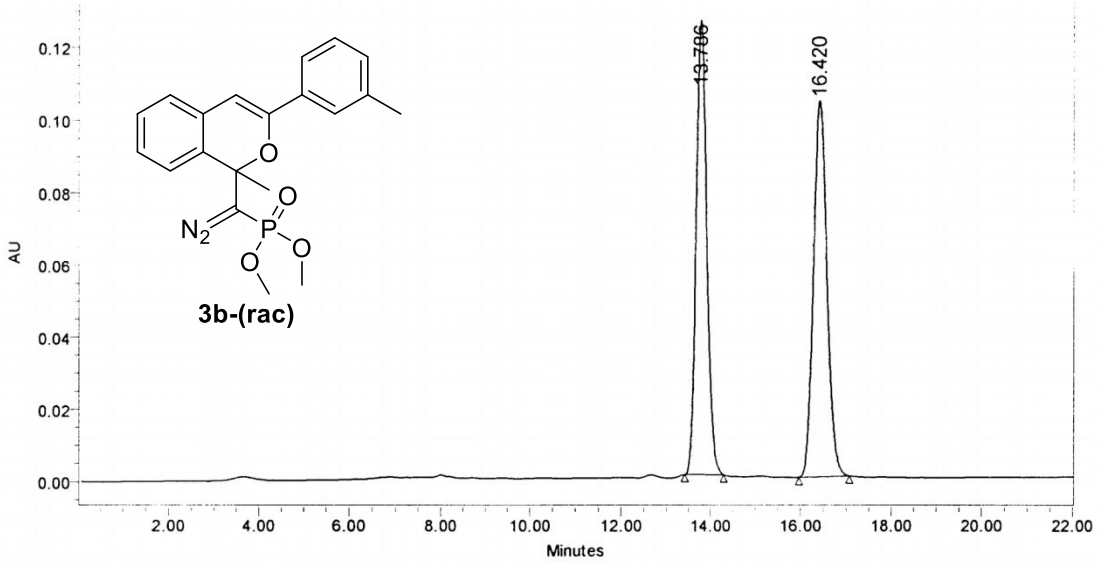
9



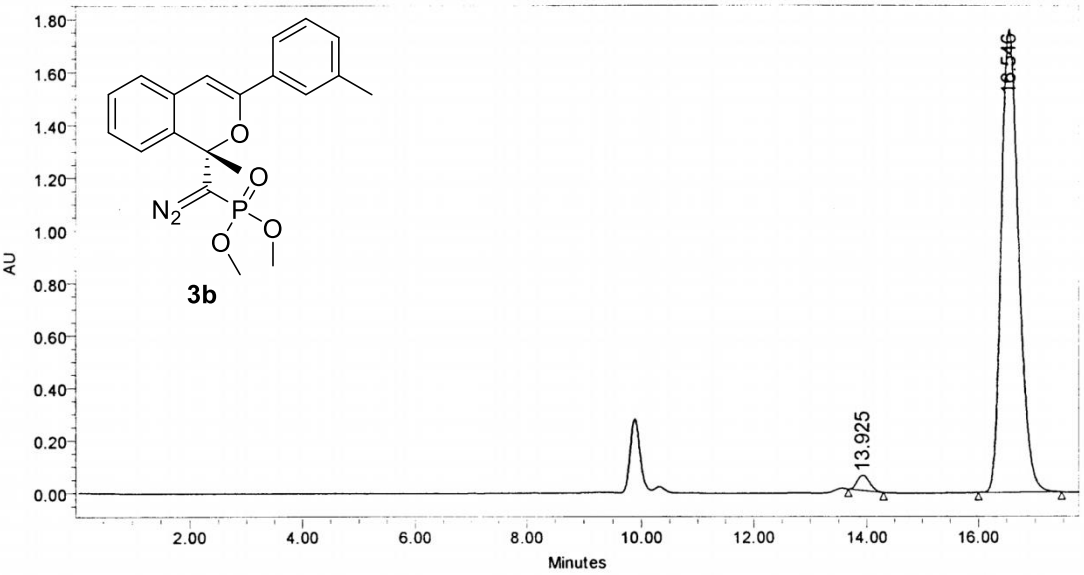
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	15.655	1685893	50.37	90784	55.03
2	18.863	1661387	49.63	74173	44.97



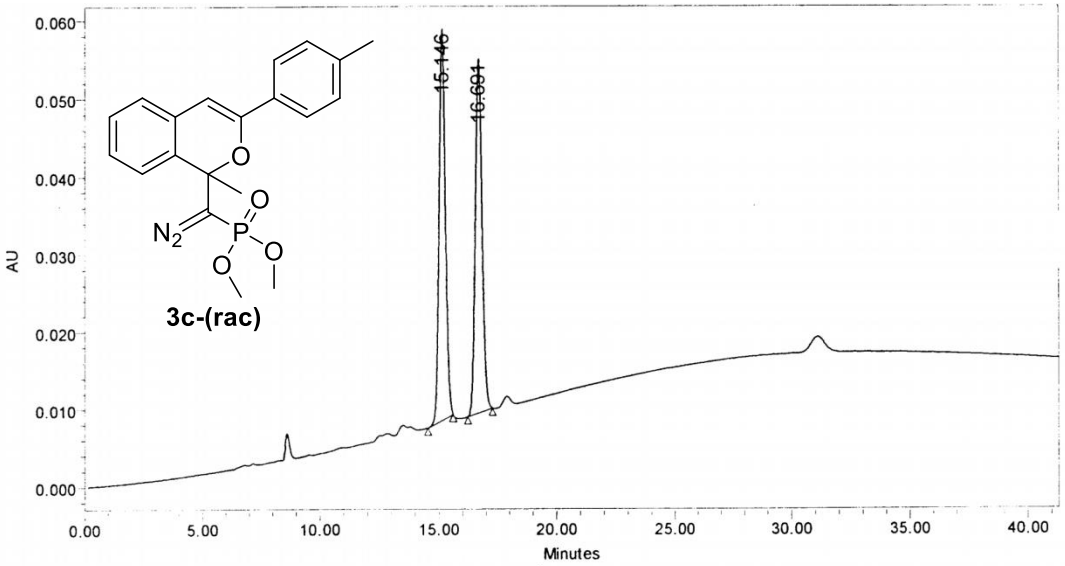
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.961	1551647	2.87	92789	3.89
2	17.816	52530356	97.13	2290401	96.11



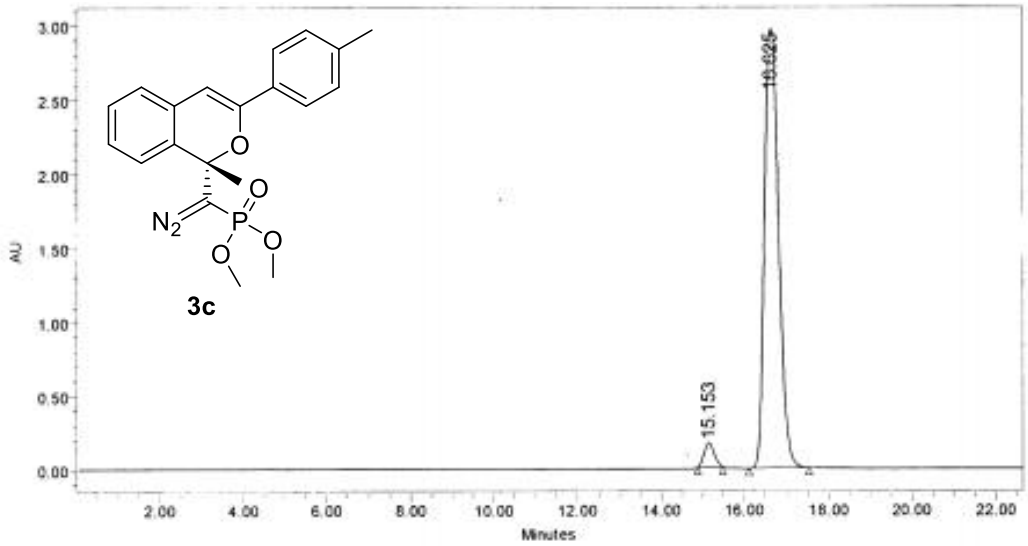
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	13.786	2095122	49.65	125515	54.66
2	16.420	2124993	50.35	104130	45.34



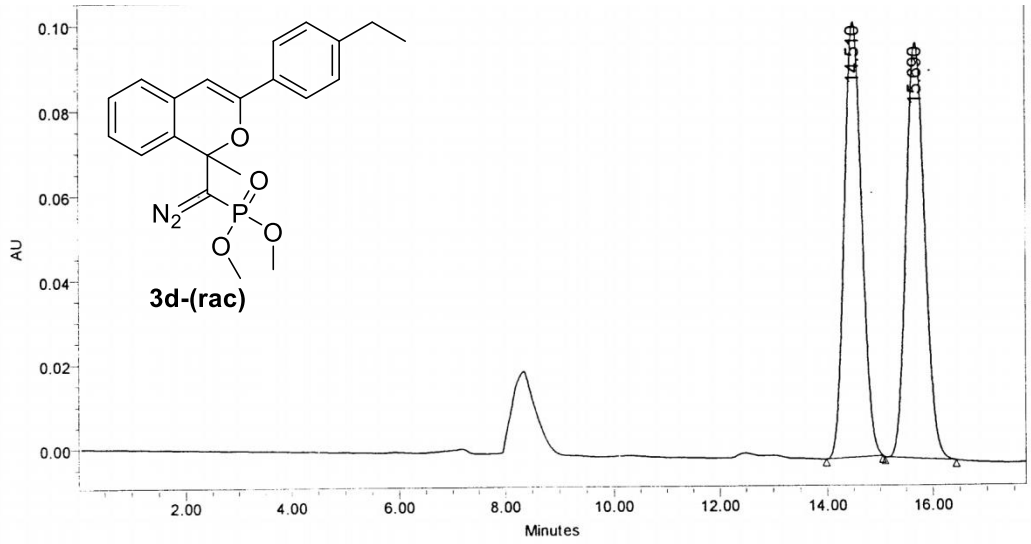
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	13.925	902503	2.36	58562	3.21
2	16.546	37406590	97.64	1763624	96.79



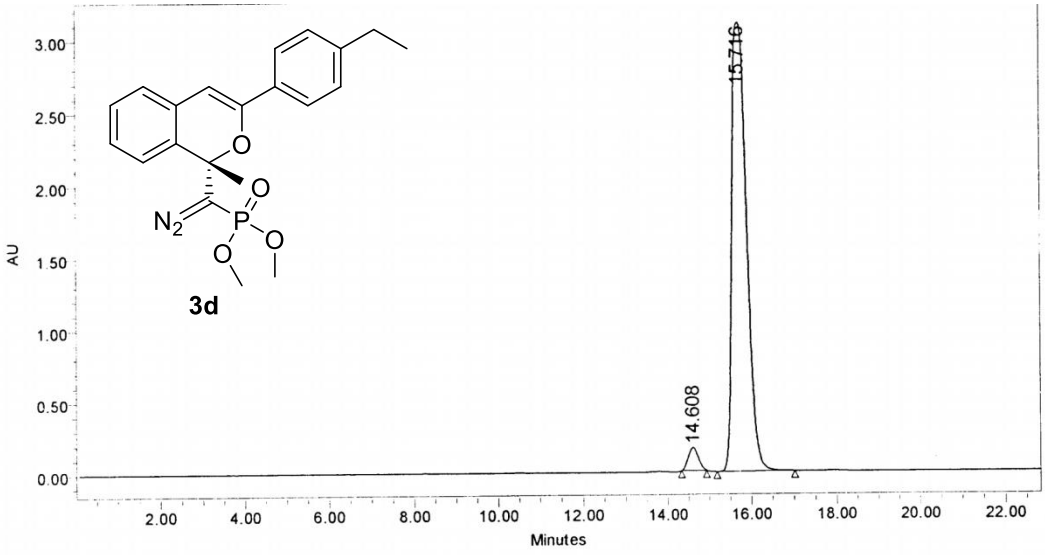
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	15.146	926586	49.92	50321	52.46
2	16.691	929427	50.08	45596	47.54



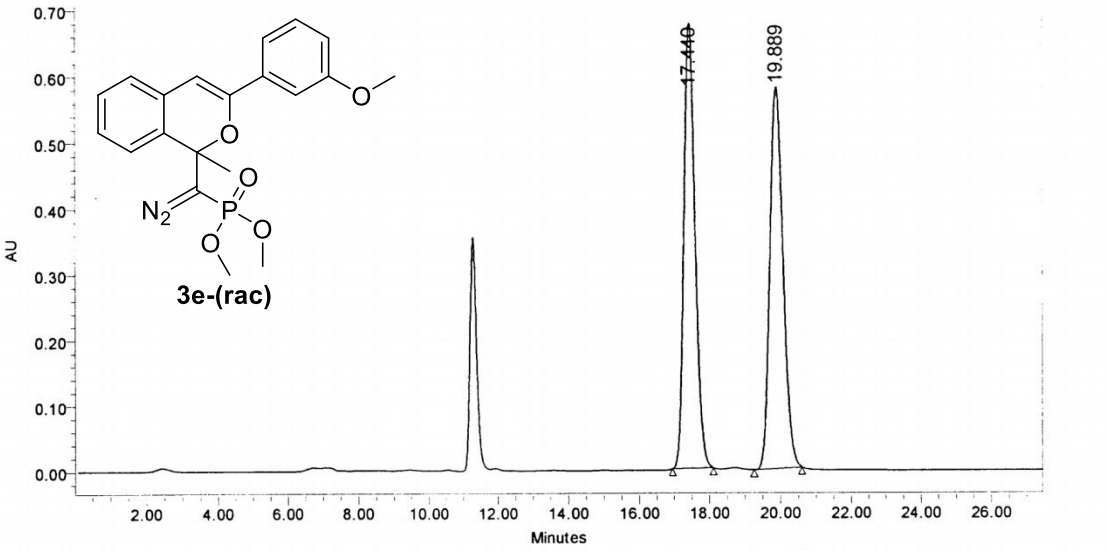
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	15.153	2761881	3.85	164174	5.24
2	16.625	68990787	96.15	2969075	94.76



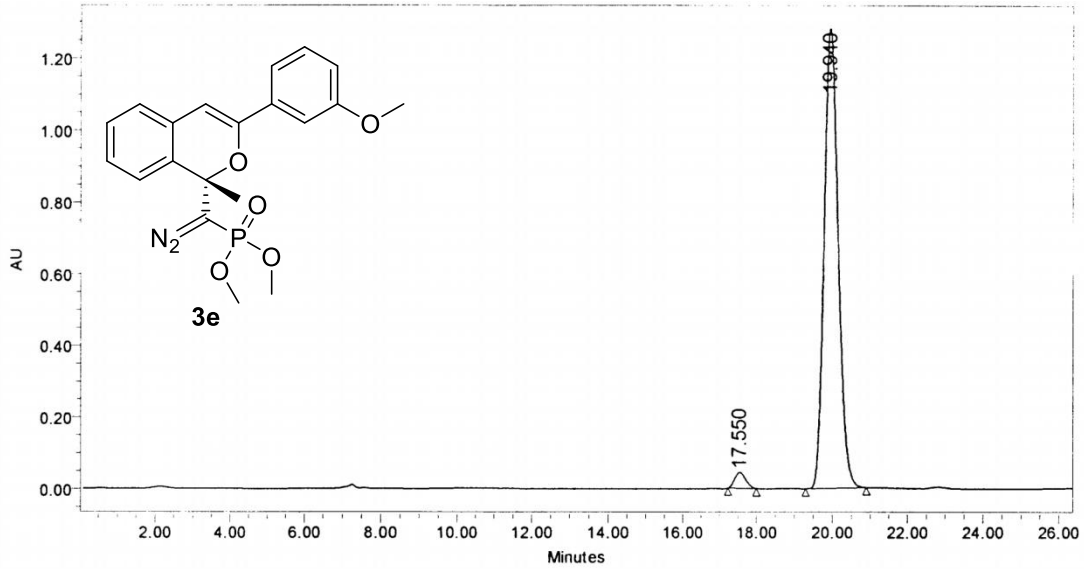
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.510	2376394	49.75	102926	51.16
2	15.690	2400646	50.25	98272	48.84



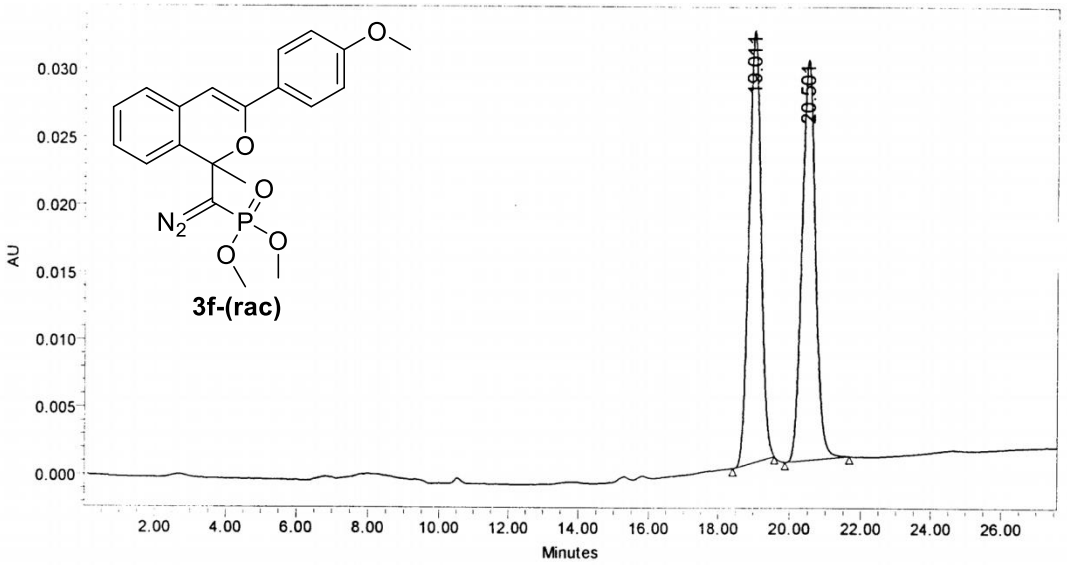
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.608	2679020	3.42	159944	4.90
2	15.716	75613318	96.58	3101645	95.10



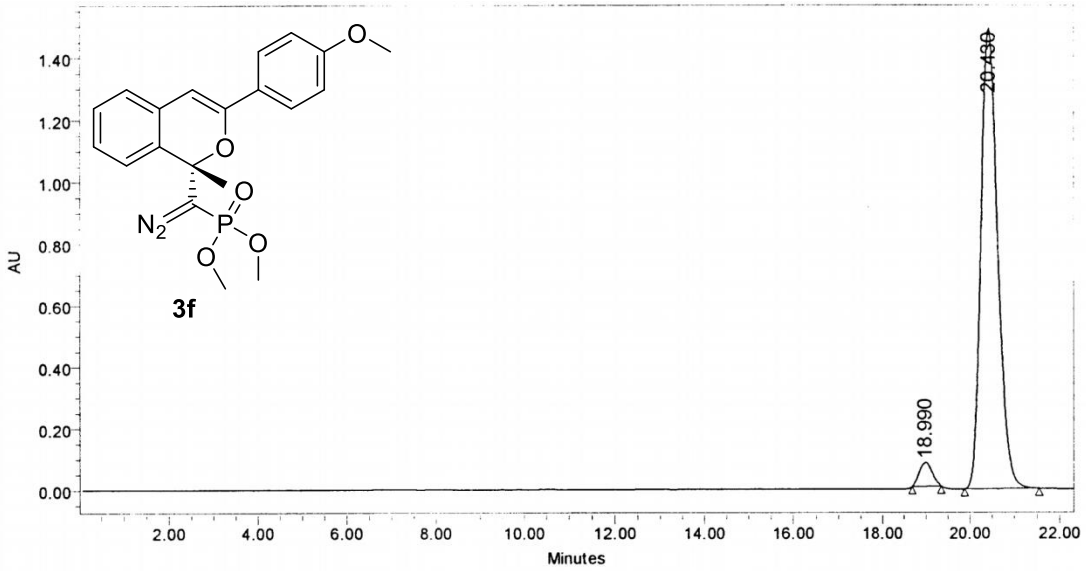
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.440	14864808	50.00	676900	53.82
2	19.889	14862768	50.00	580738	46.18



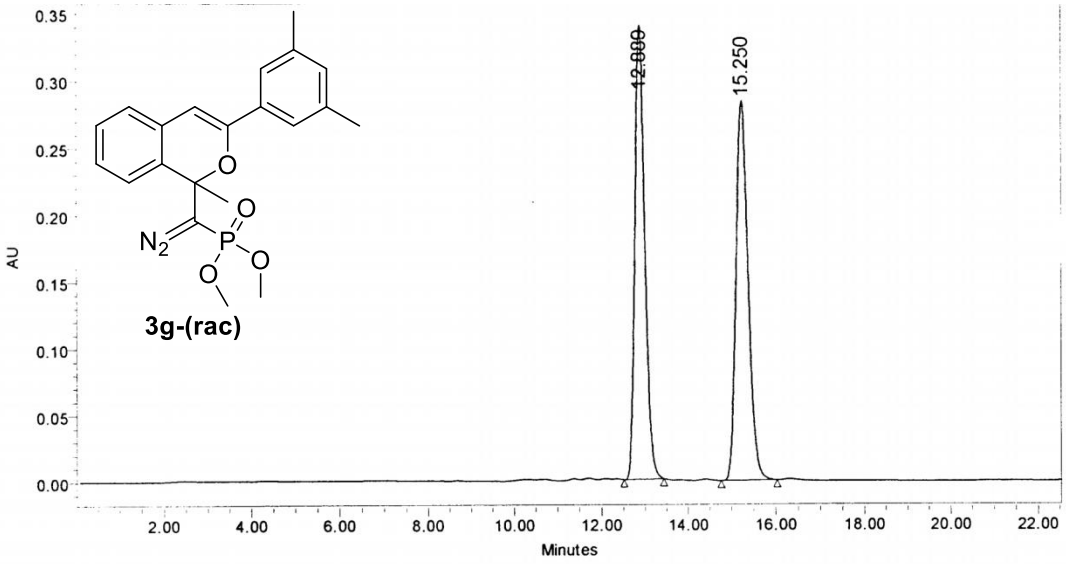
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.550	904482	2.68	44542	3.36
2	19.940	32855706	97.32	1282122	96.64



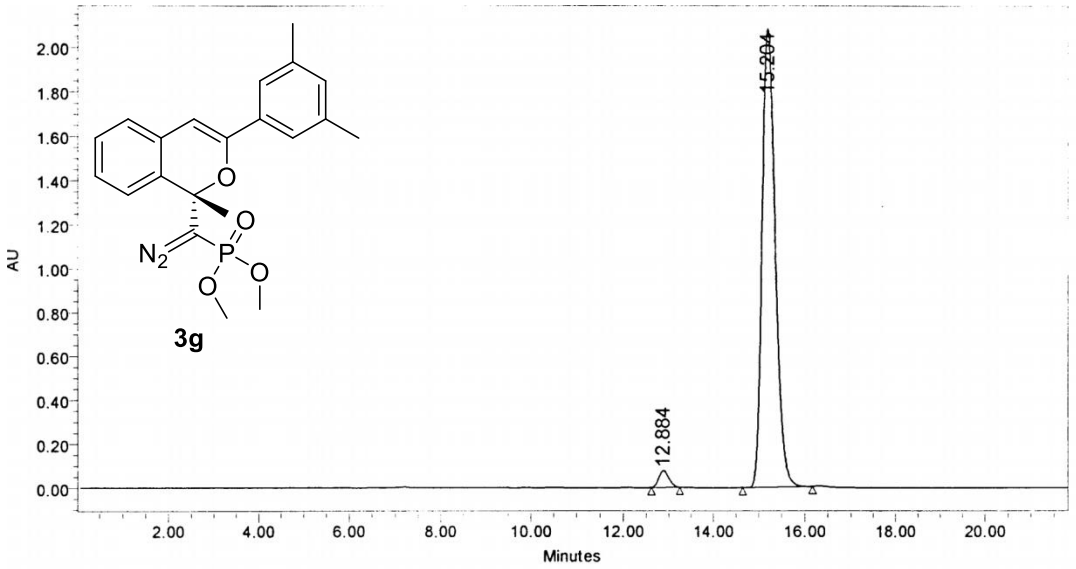
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	19.011	748914	49.33	32000	51.89
2	20.501	769298	50.67	29670	48.11



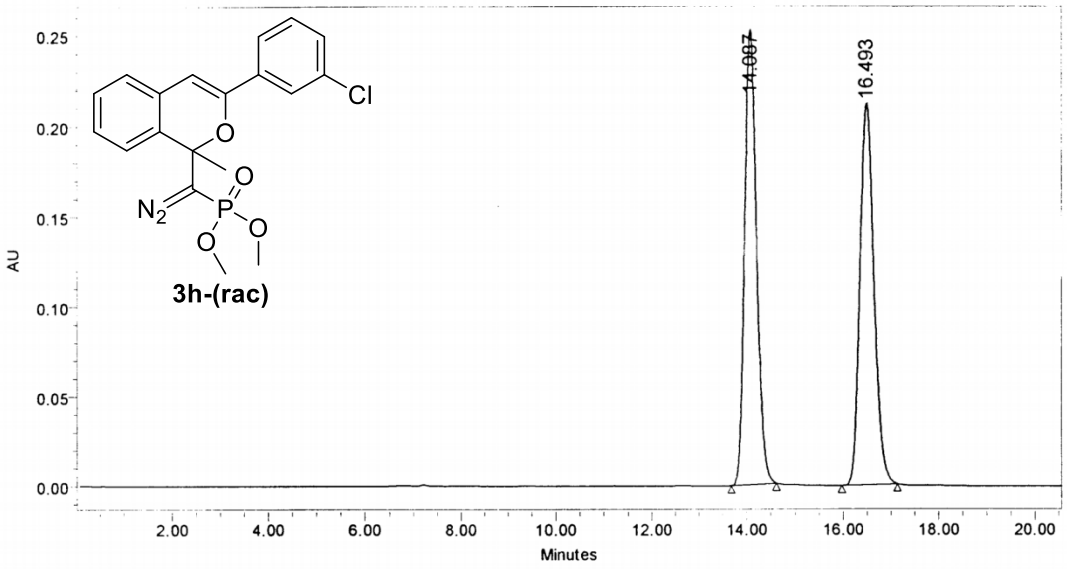
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	18.990	1586014	3.91	77838	4.96
2	20.430	38933760	96.09	1491031	95.04



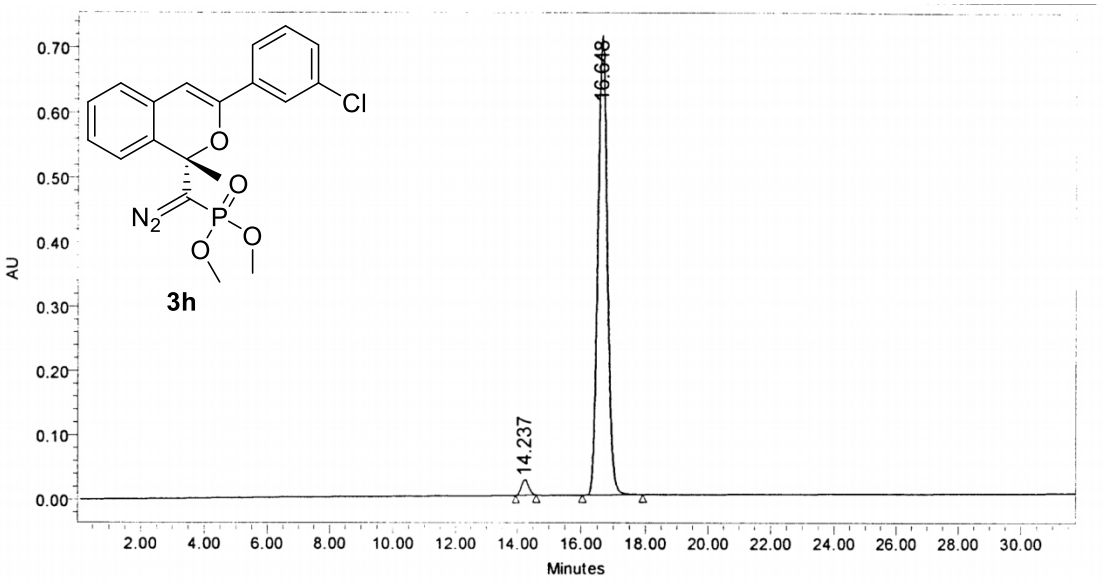
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	12.889	5380467	49.71	339489	54.48
2	15.250	5443089	50.29	283652	45.52



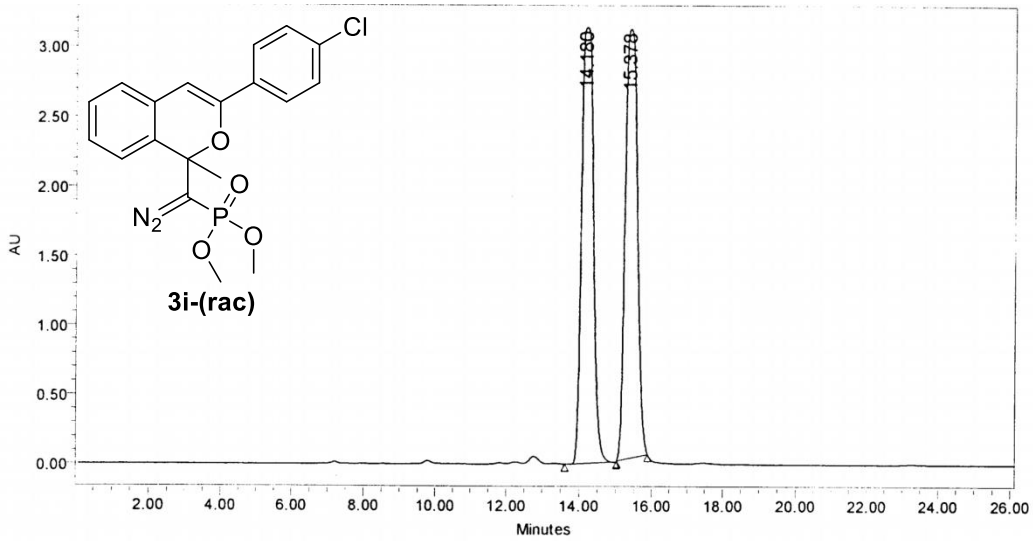
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	12.884	1173189	2.76	76119	3.52
2	15.204	41367046	97.24	2083718	96.48



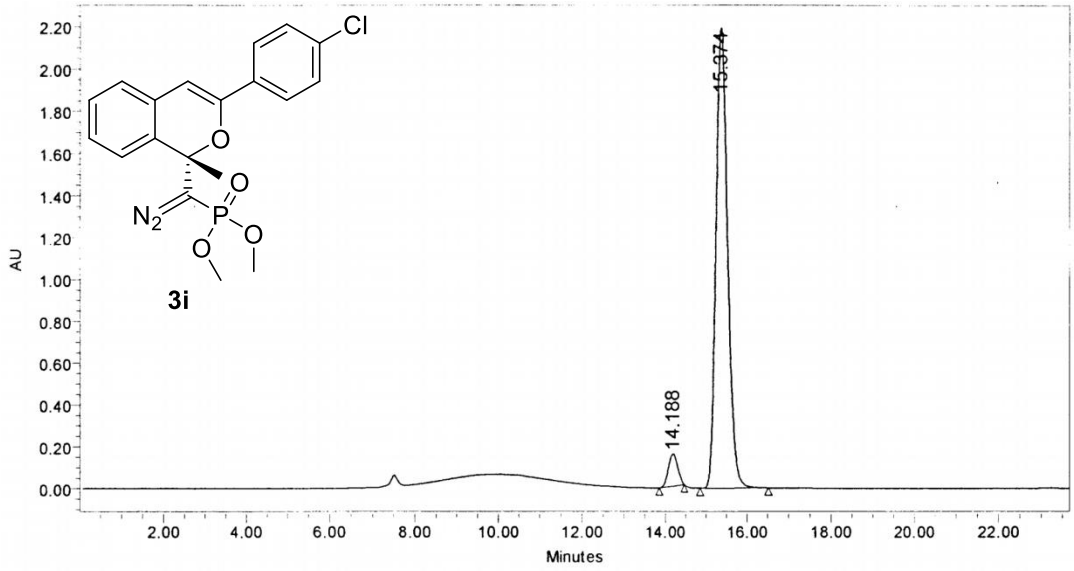
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.087	4341206	49.88	252773	54.31
2	16.493	4362445	50.12	212615	45.69



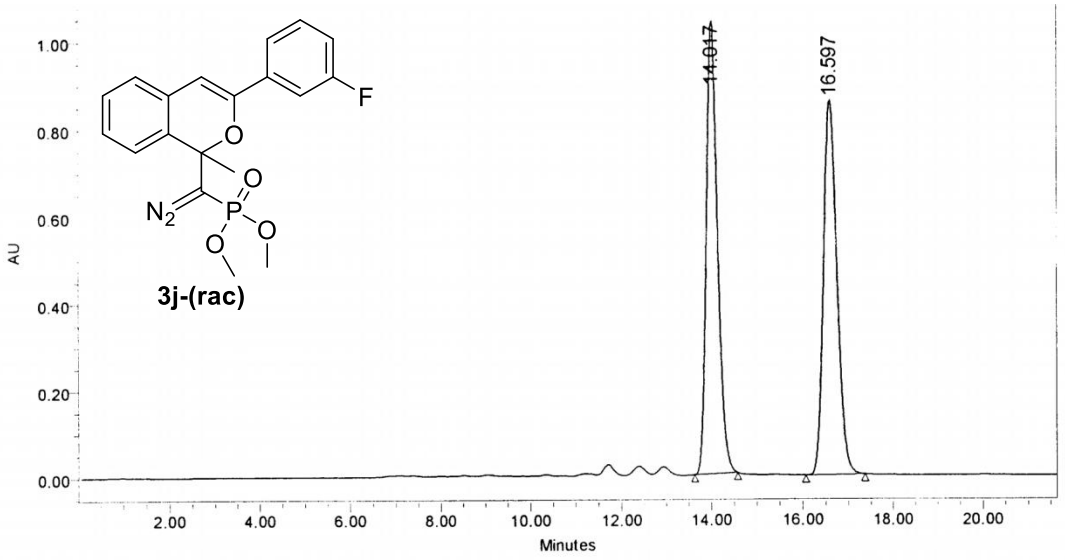
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.237	388151	2.61	23905	3.25
2	16.648	14475566	97.39	711036	96.75



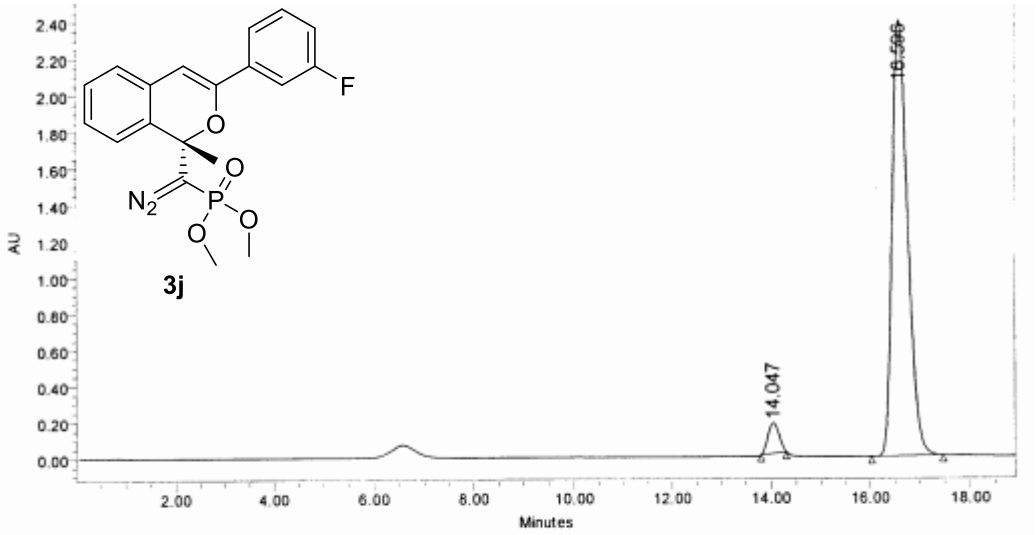
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.180	70083384	49.36	3135106	50.38
2	15.378	71908648	50.64	3087357	49.62



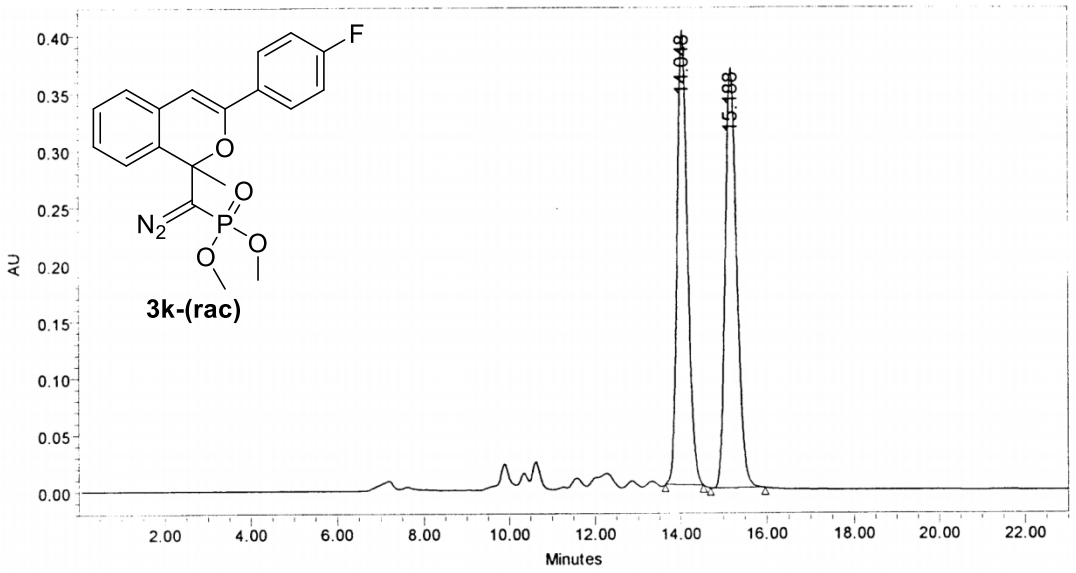
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.188	2460826	5.36	155003	6.59
2	15.374	43444445	94.64	2195329	93.41



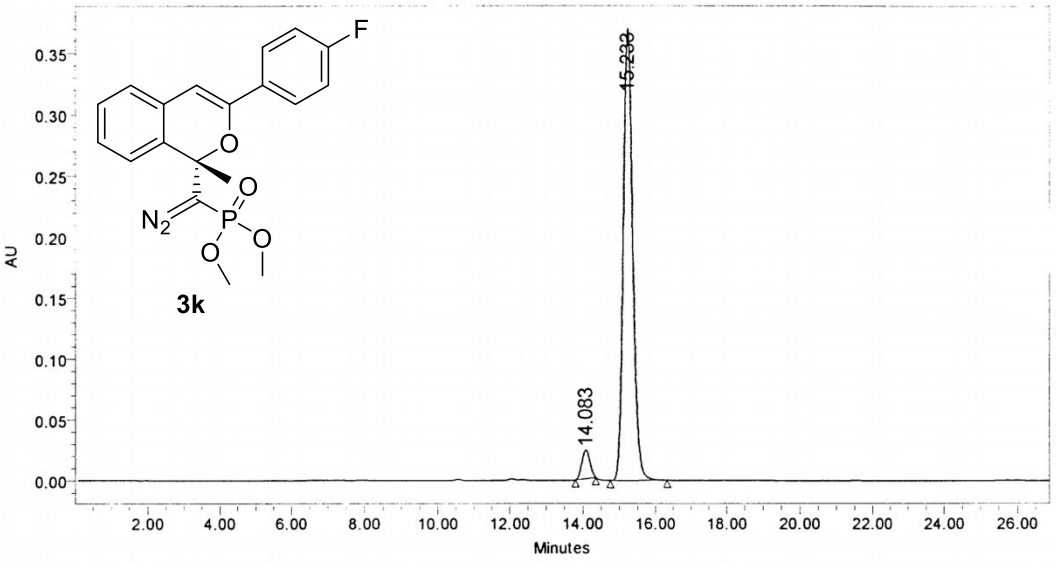
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.017	17971718	50.36	1038491	54.64
2	16.597	17713015	49.64	862123	45.36



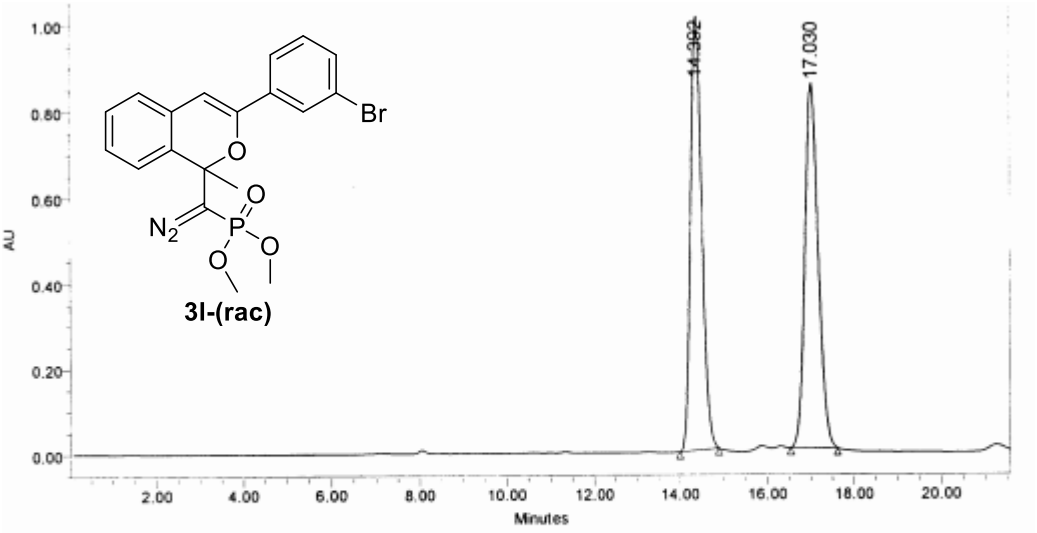
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.047	2531090	4.65	168461	6.55
2	16.596	51869510	95.35	2402491	93.45



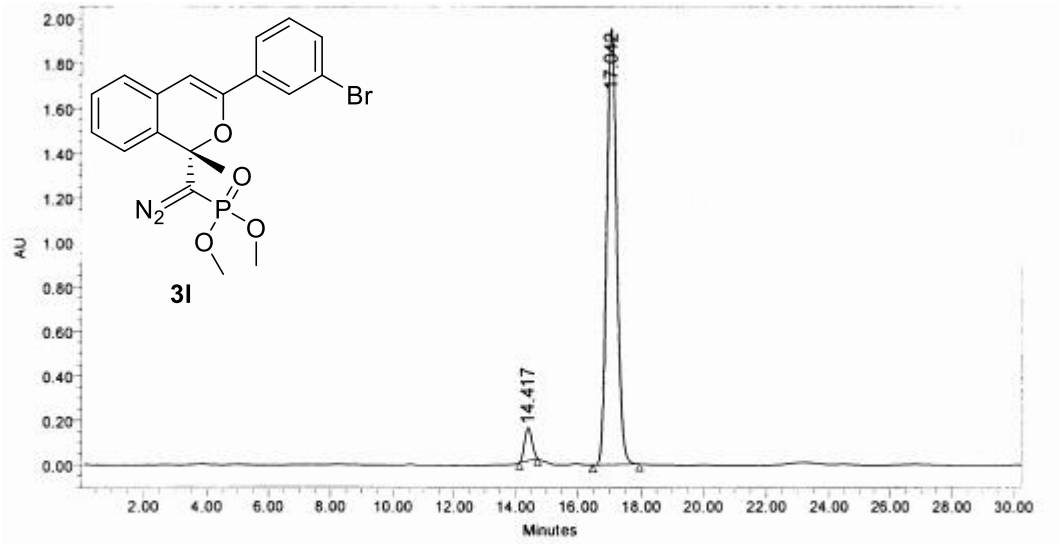
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.048	6803776	49.70	398659	51.92
2	15.188	6884682	50.30	369238	48.08



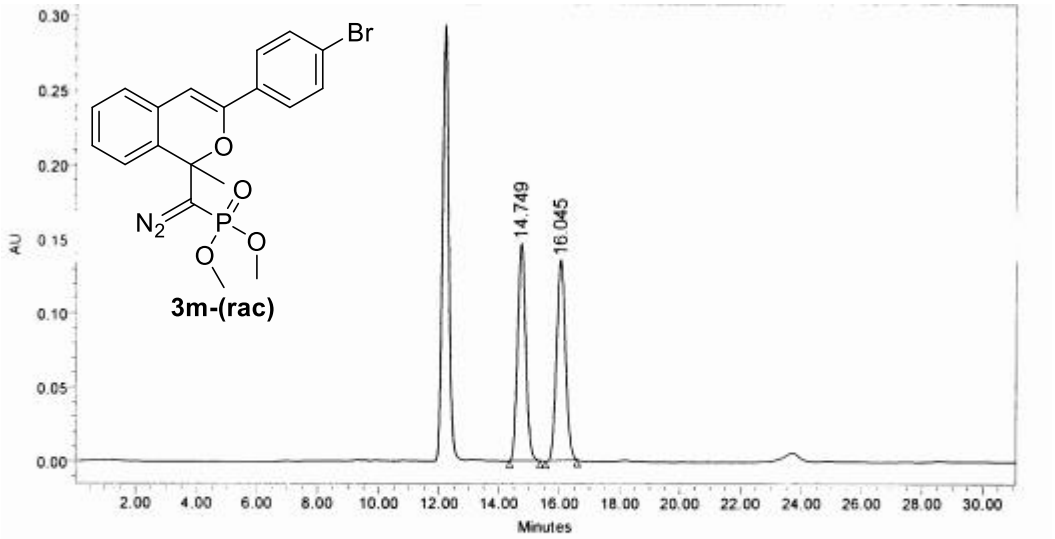
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.083	356143	5.00	23513	5.97
2	15.233	6767427	95.00	370107	94.03



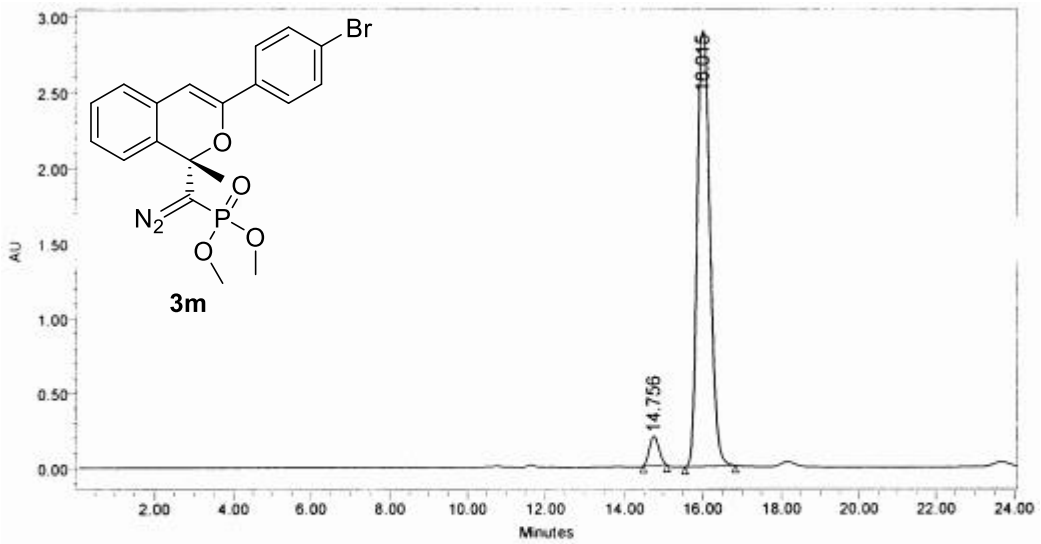
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.392	18139359	49.69	1012675	54.30
2	17.030	18363007	50.31	852216	45.70



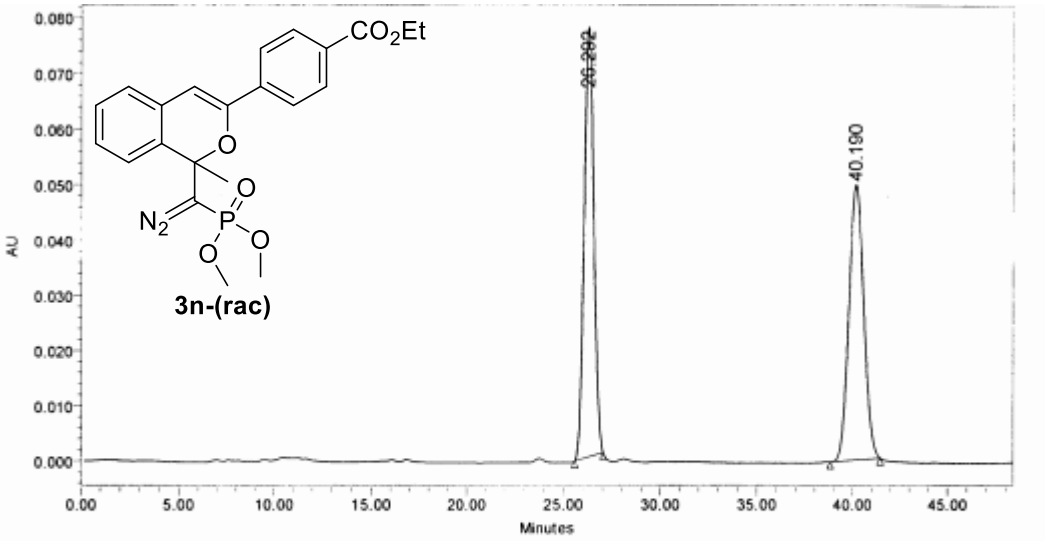
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.417	2466259	5.36	149498	7.10
2	17.042	43562032	94.64	1956548	92.90



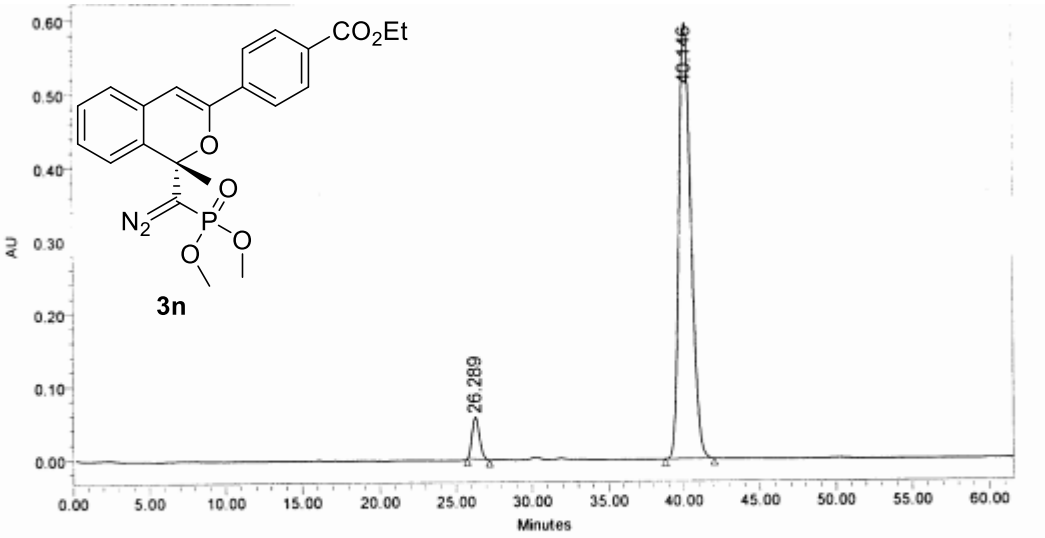
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.749	2733744	49.90	147459	52.00
2	16.045	2744873	50.10	136119	48.00



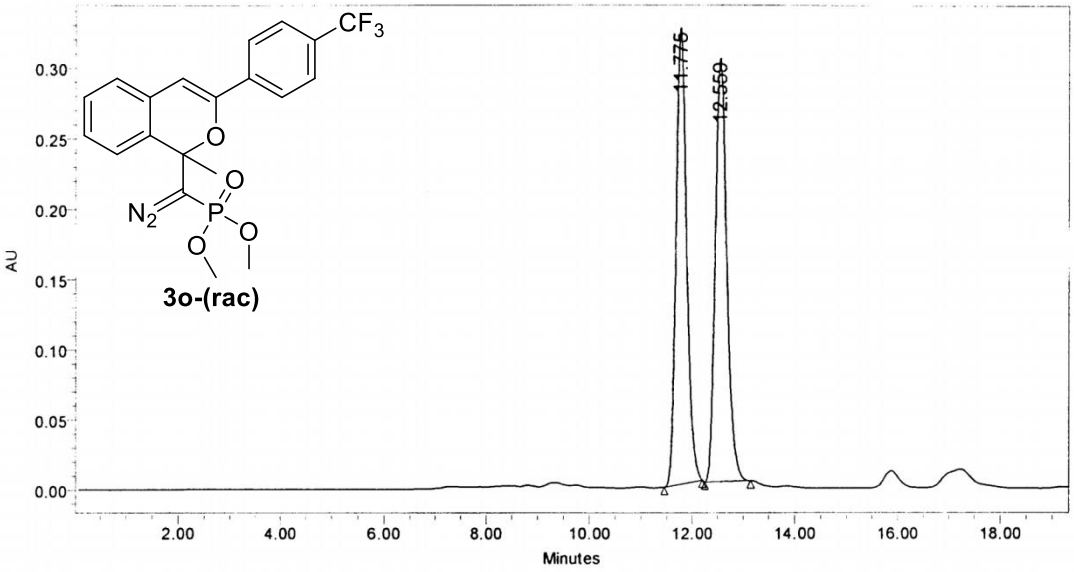
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.756	3320158	4.86	195611	6.32
2	16.015	64947656	95.14	2897125	93.68



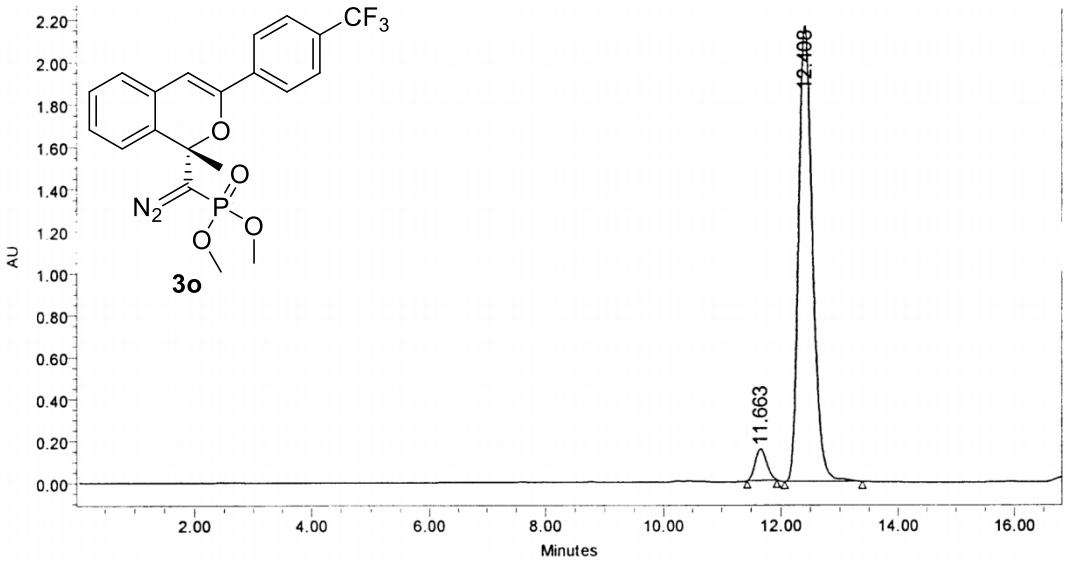
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	26.292	2652823	49.38	77675	60.85
2	40.190	2719826	50.62	49972	39.15



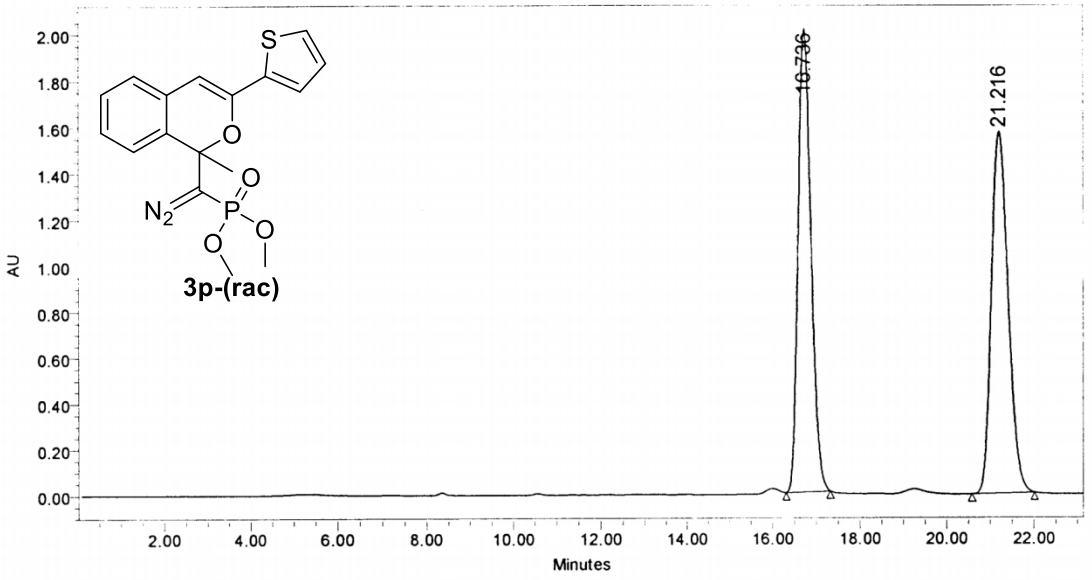
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	26.289	1925533	5.53	57498	8.81
2	40.146	32913207	94.47	594977	91.19



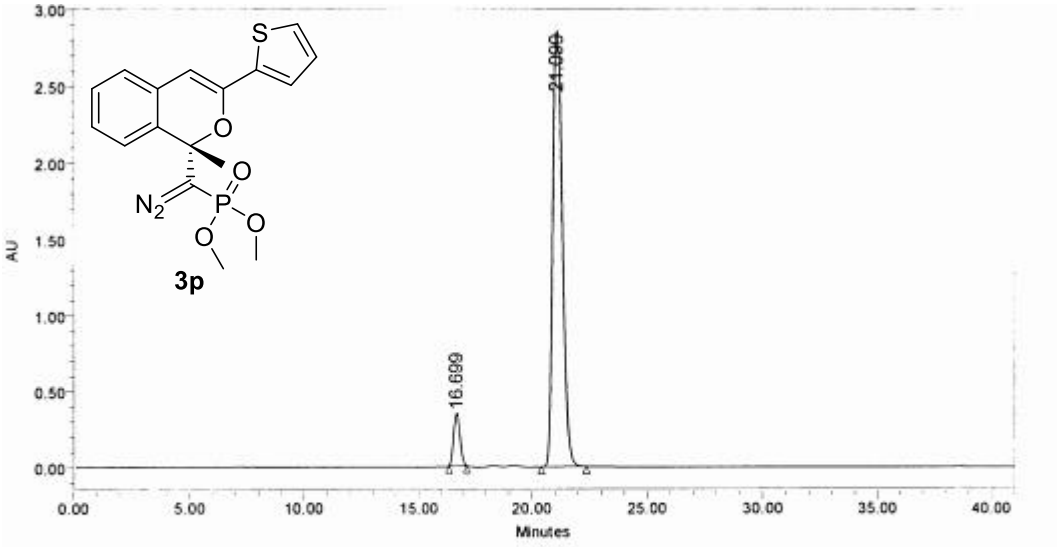
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.775	4716105	50.06	325120	51.89
2	12.559	4704767	49.94	301486	48.11



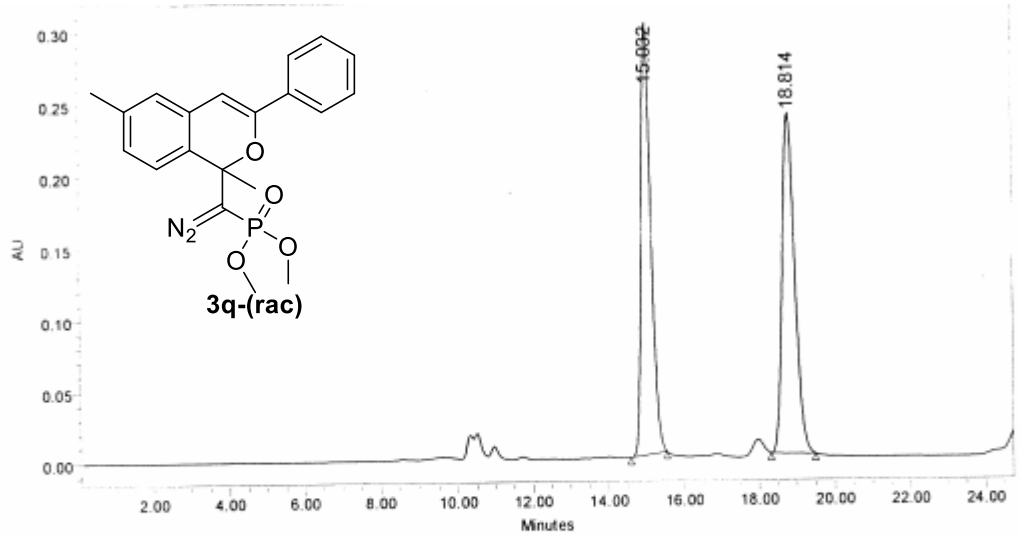
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.663	2028776	5.44	149736	6.45
2	12.408	35274619	94.56	2171319	93.55



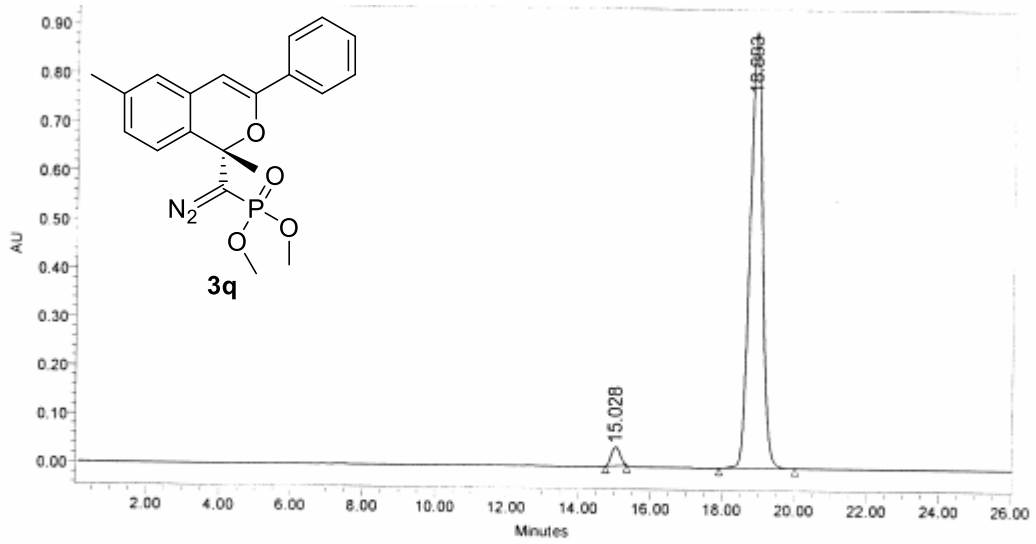
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	16.736	41141649	49.59	2010394	56.08
2	21.216	41816666	50.41	1574229	43.92



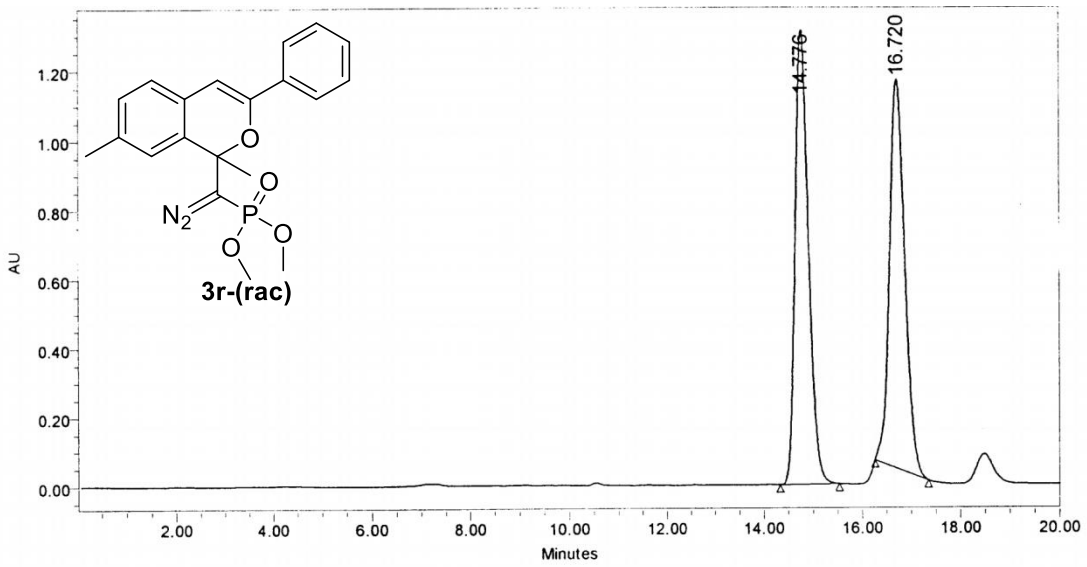
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	16.699	6871469	7.74	348013	10.86
2	21.099	81937830	92.26	2857297	89.14



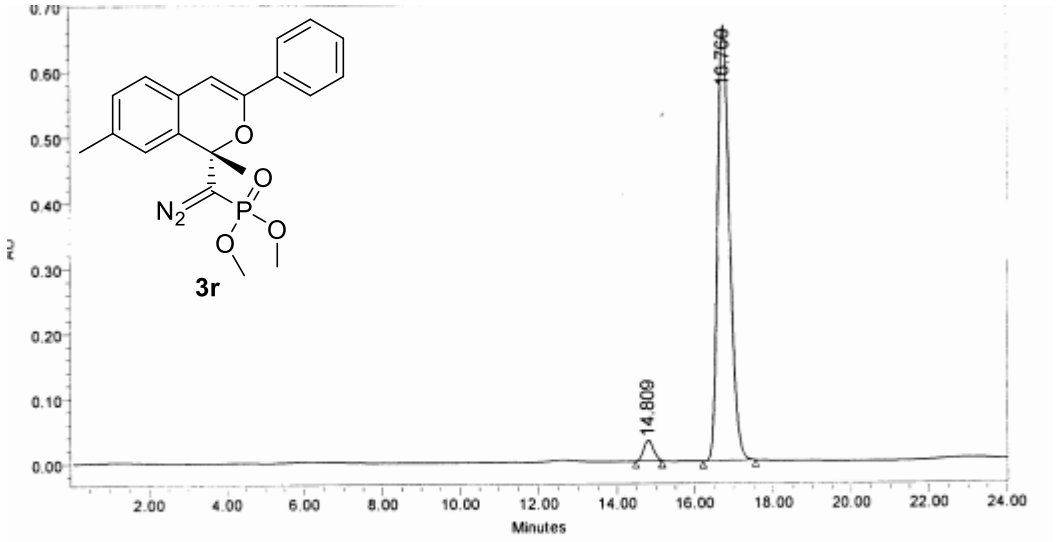
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	15.032	5404396	49.85	300945	55.90
2	18.814	5435992	50.15	237384	44.10



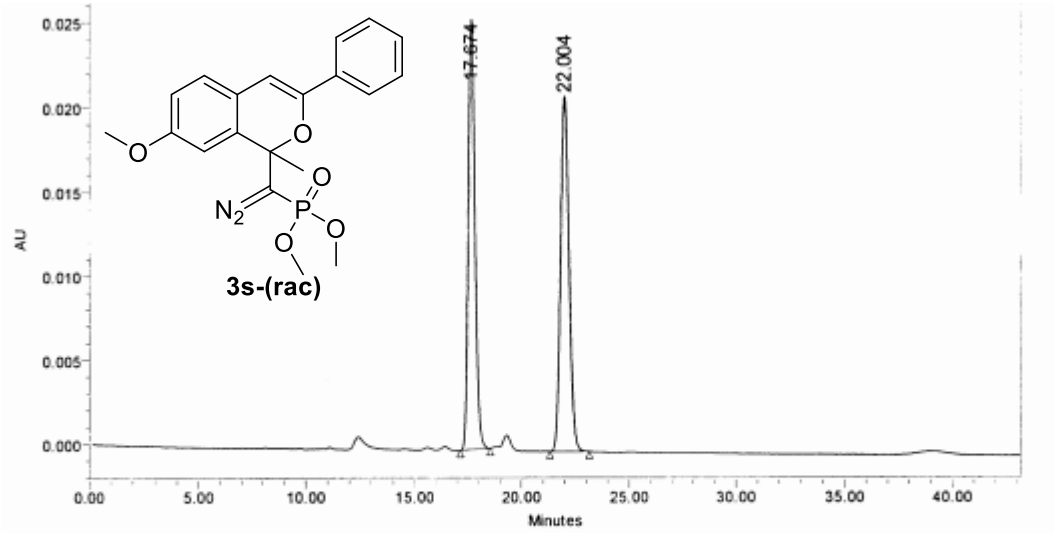
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	15.028	653058	2.93	39062	4.17
2	18.883	21666946	97.07	896967	95.83



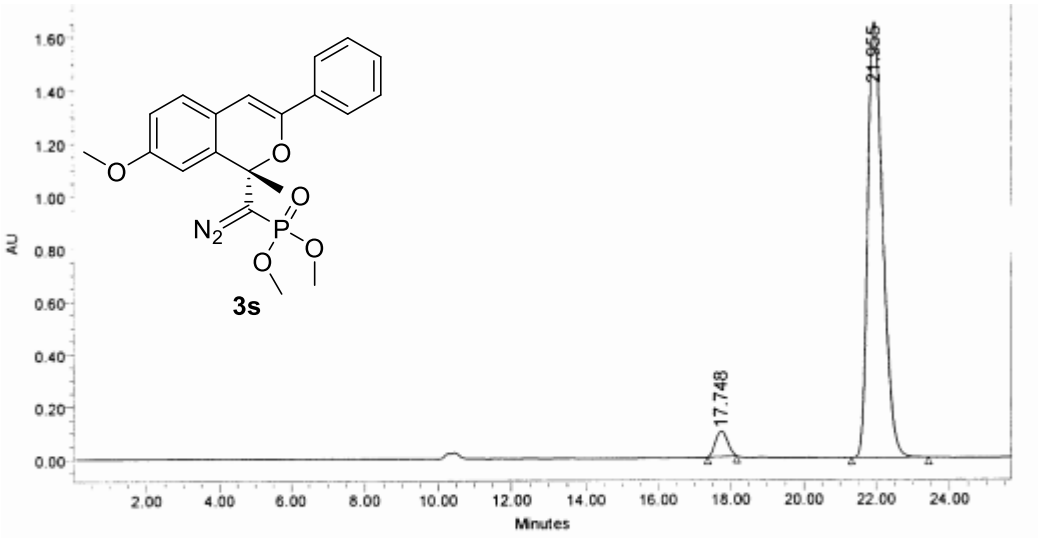
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.776	24573285	50.33	1313269	53.84
2	16.720	24250184	49.67	1125718	46.16



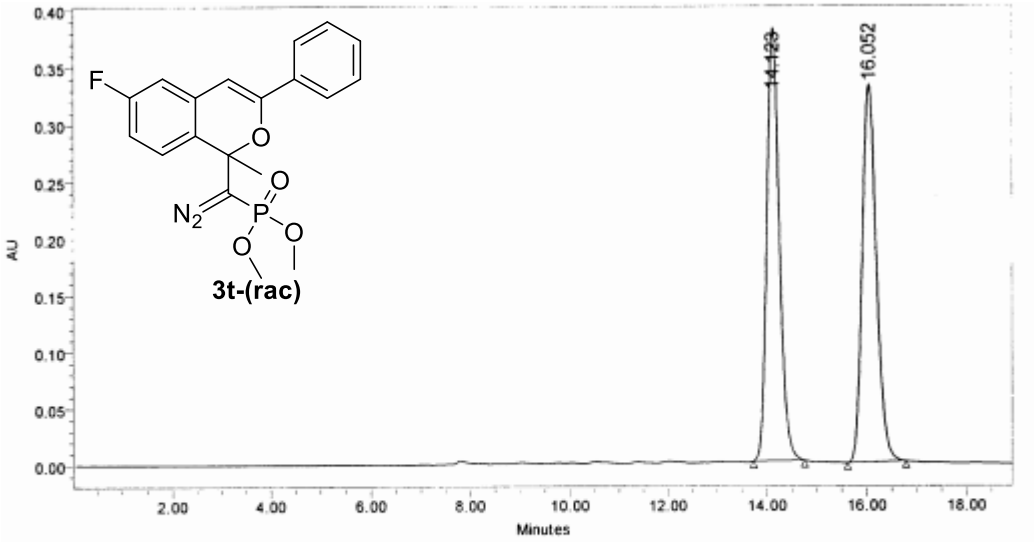
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.809	554675	3.78	31499	4.51
2	16.760	14102318	96.22	666554	95.49



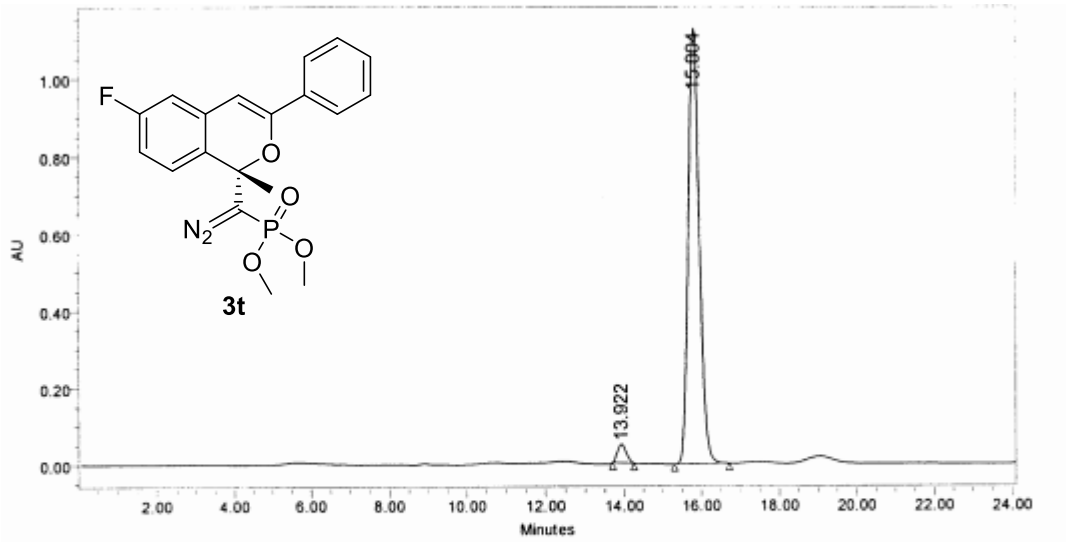
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.674	560370	49.48	25537	54.75
2	22.004	572214	50.52	21102	45.25



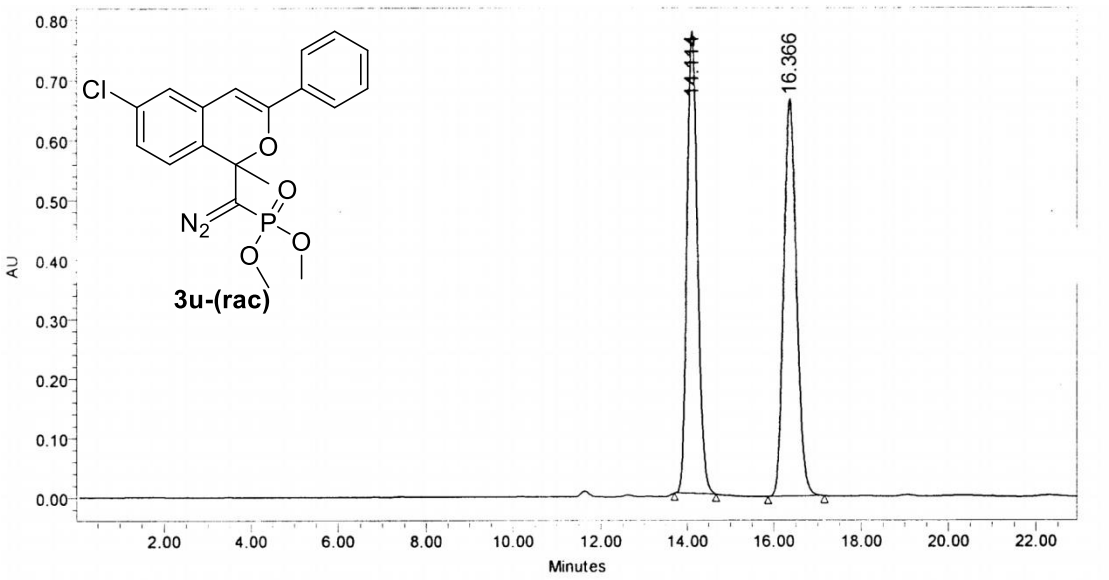
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.748	2231271	4.48	96378	5.51
2	21.955	47592724	95.52	1652992	94.49



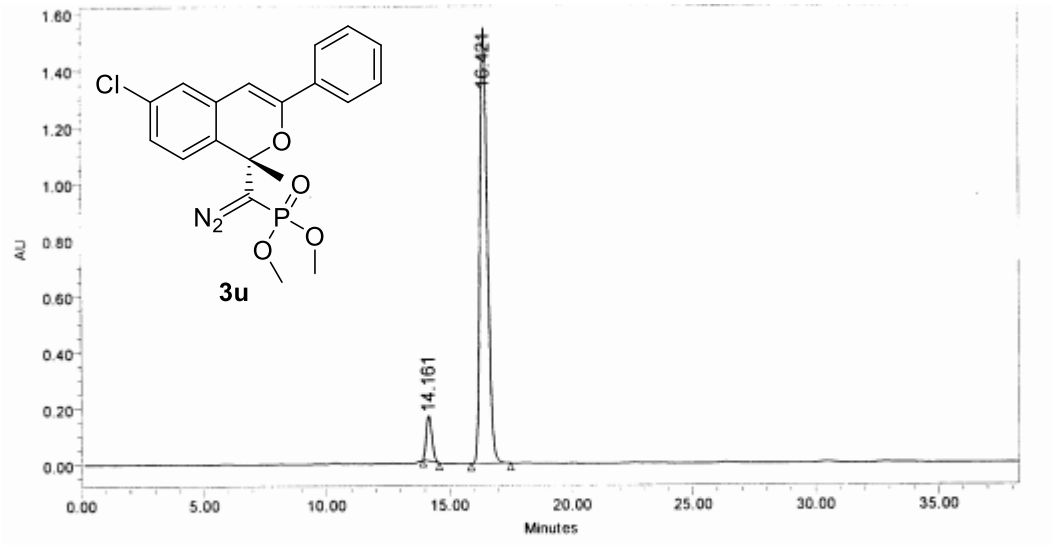
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.123	6561649	50.07	381340	53.41
2	16.052	6542401	49.93	332627	46.59



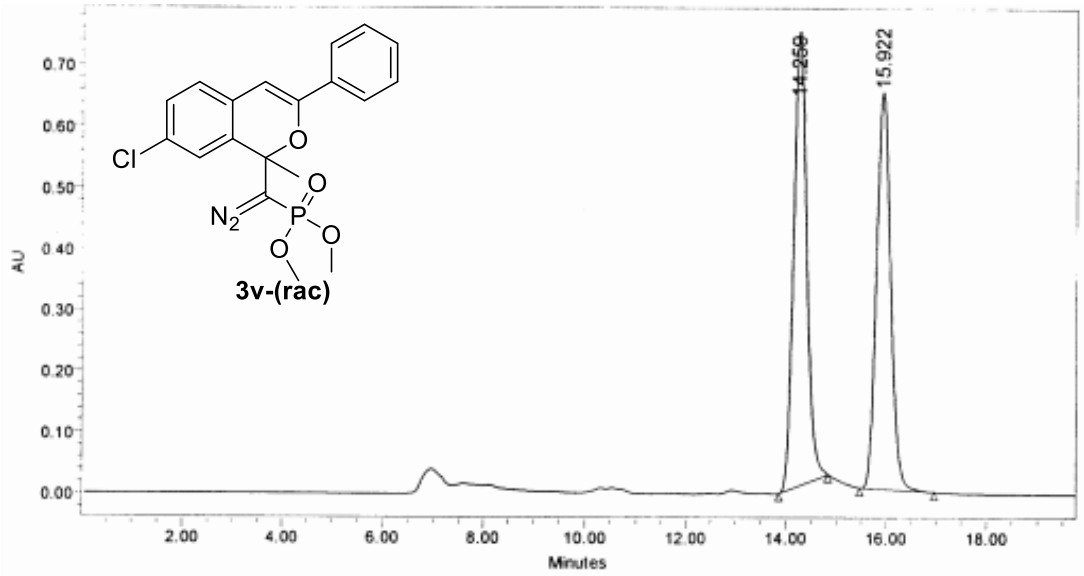
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	13.922	745313	3.24	48118	4.09
2	15.804	22279307	96.76	1128680	95.91



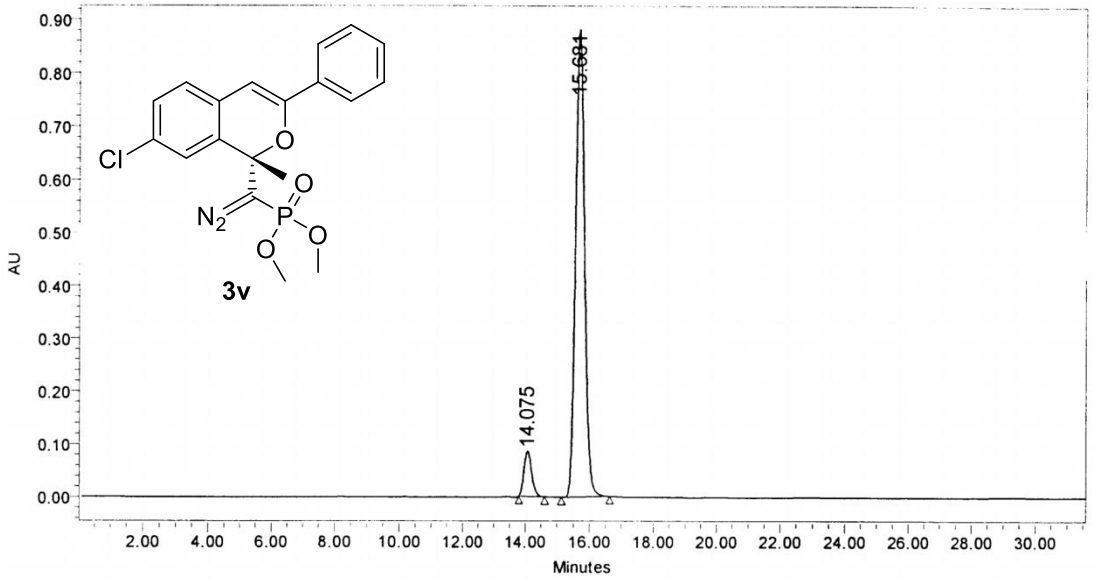
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.114	13253290	49.60	774235	53.74
2	16.366	13464384	50.40	666590	46.26



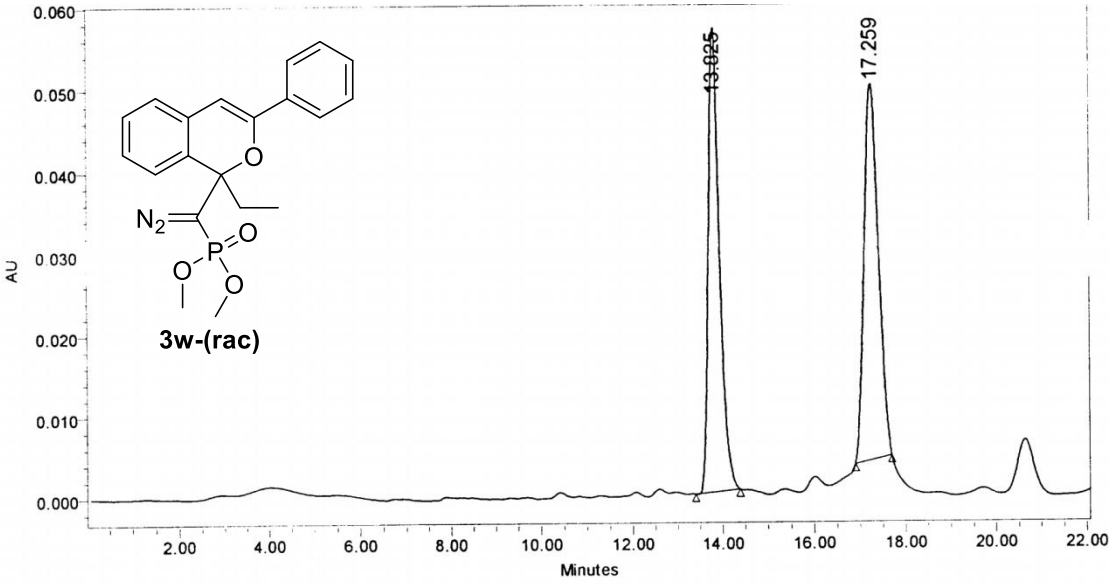
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.161	2610520	7.46	160742	9.42
2	16.421	32364881	92.54	1545219	90.58



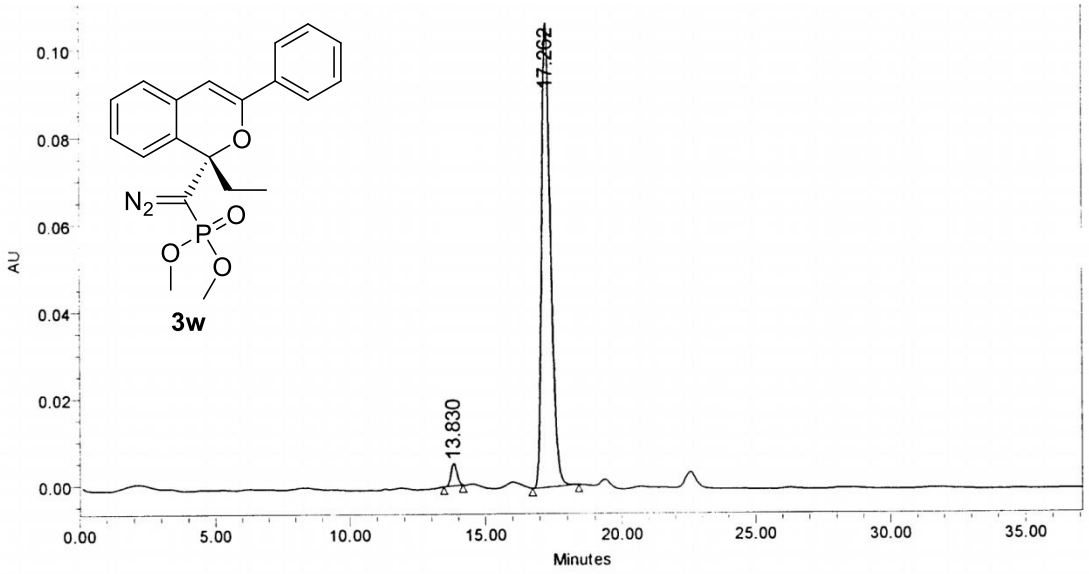
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.259	13277778	50.77	743999	53.35
2	15.922	12874730	49.23	650565	46.65



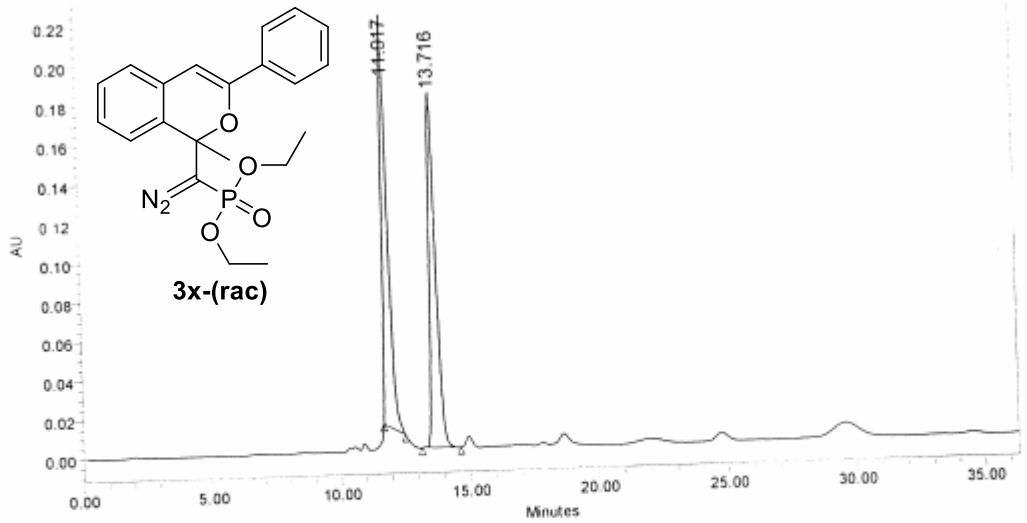
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	14.075	1437613	7.73	85727	8.85
2	15.681	17164429	92.27	882479	91.15



	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	13.825	975775	49.36	56894	55.28
2	17.259	1001108	50.64	46019	44.72

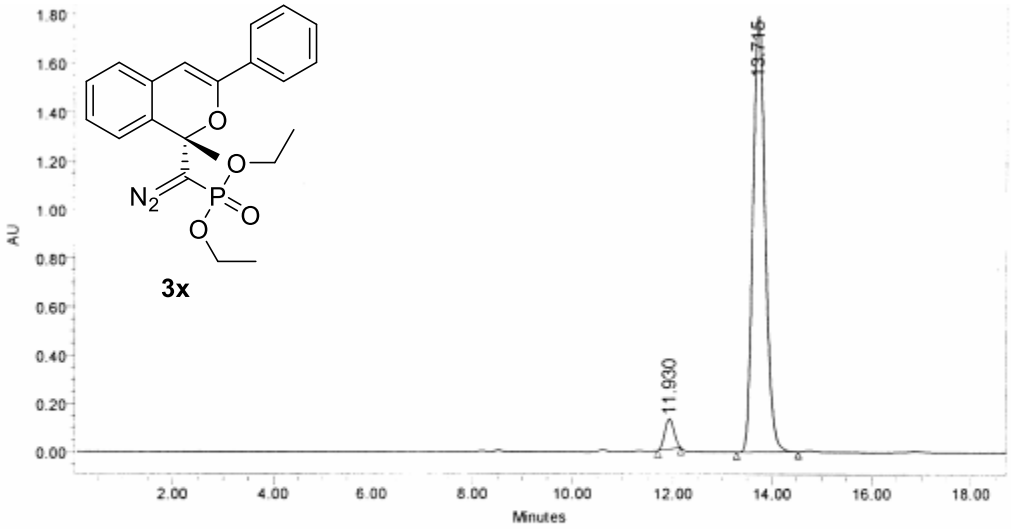


	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	13.830	81179	3.26	5148	4.62
2	17.262	2411218	96.74	106278	95.38



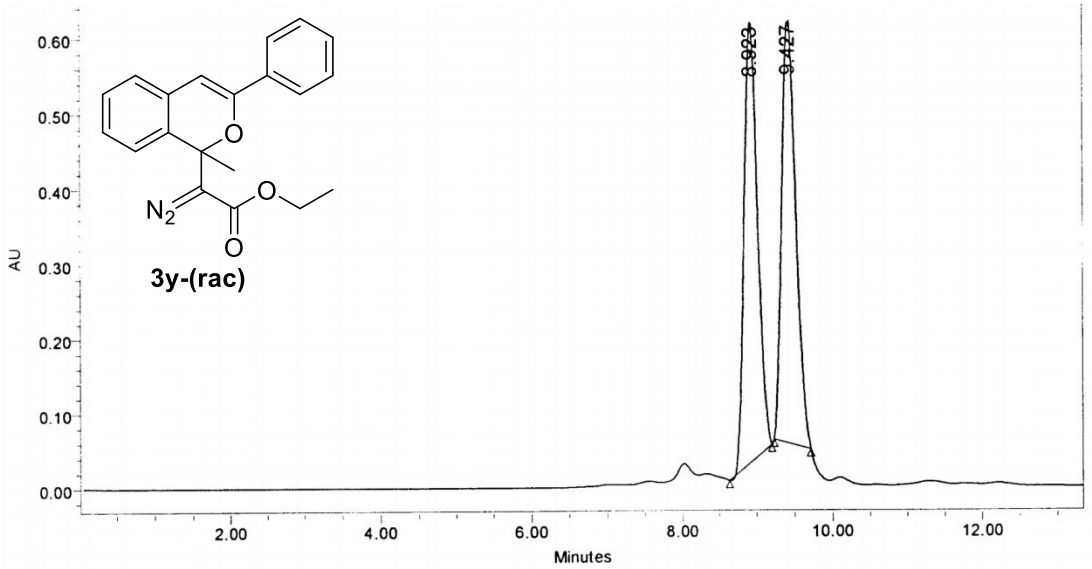
3x-(rac)

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.917	3059858	50.16	209945	53.66
2	13.716	3040373	49.84	181282	46.34

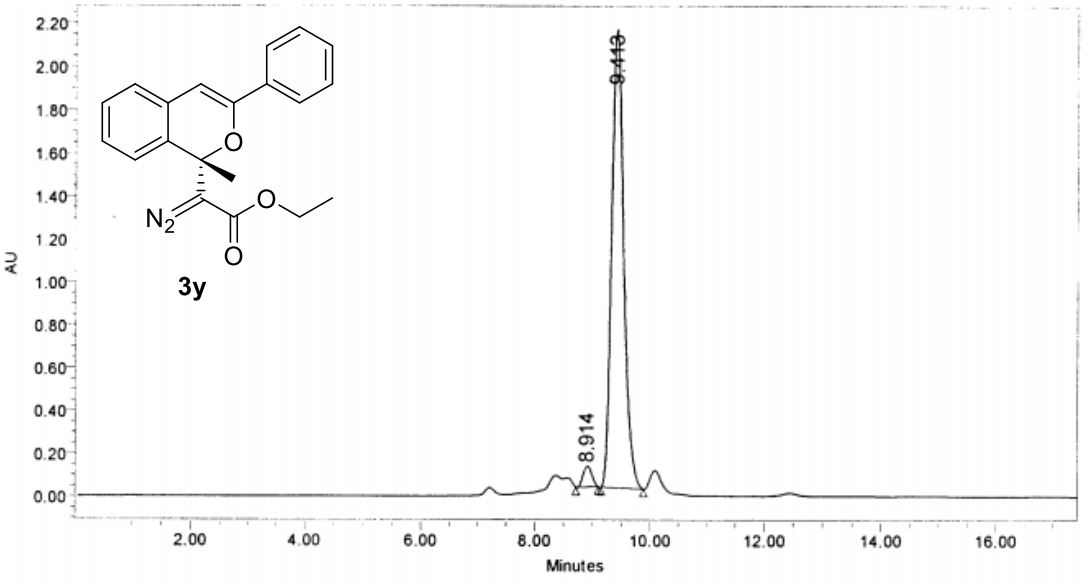


3x

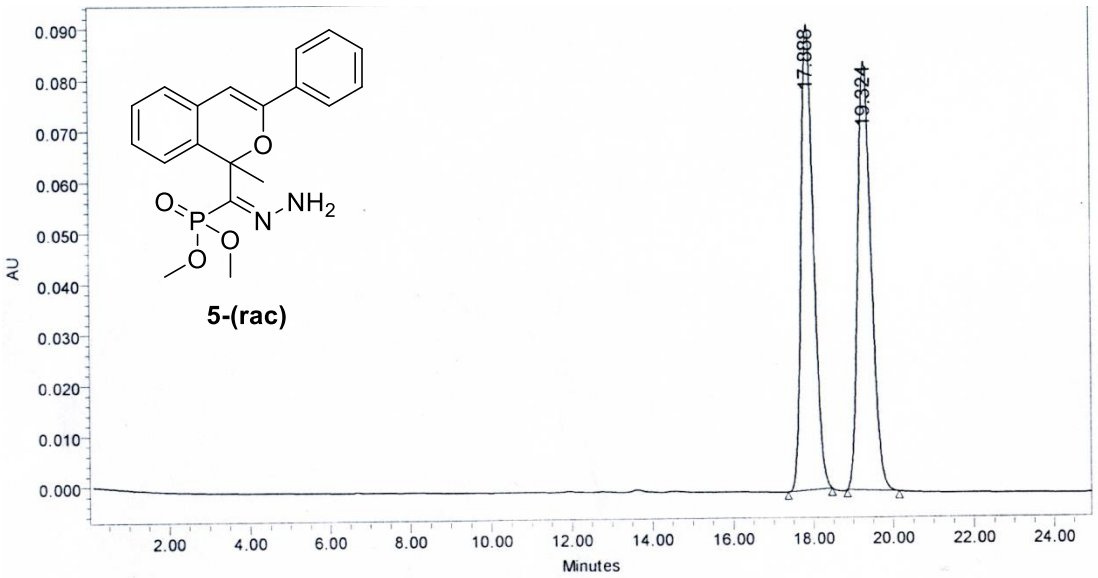
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	11.930	1593084	4.90	125893	6.55
2	13.715	30941865	95.10	1796072	93.45



	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	8.923	7263248	49.90	587010	51.02
2	9.427	7292754	50.10	563568	48.98

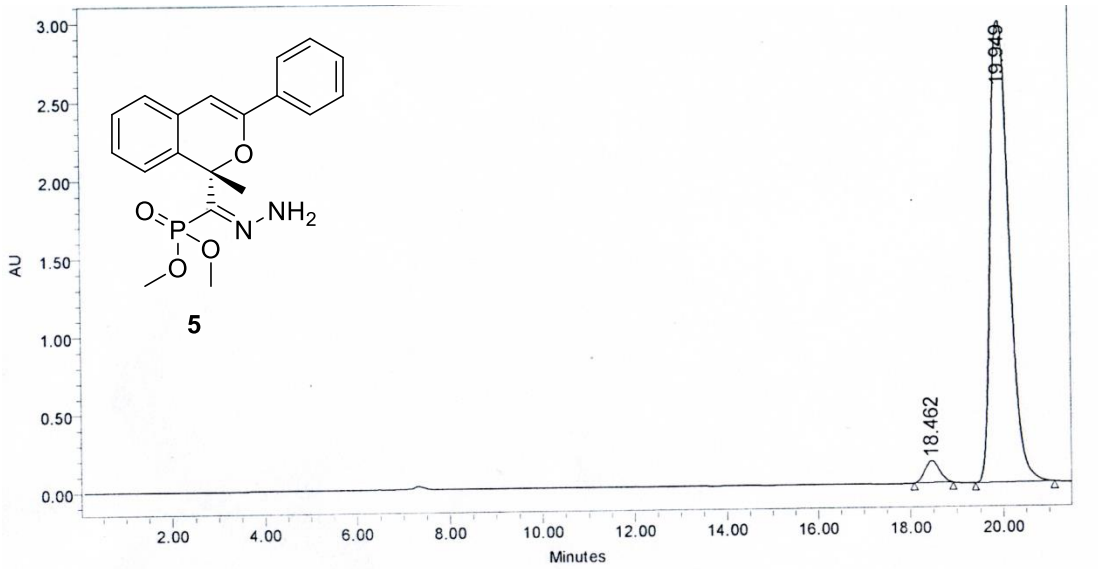


	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	8.914	1022303	3.21	97912	4.39
2	9.413	30821270	96.79	2134090	95.61



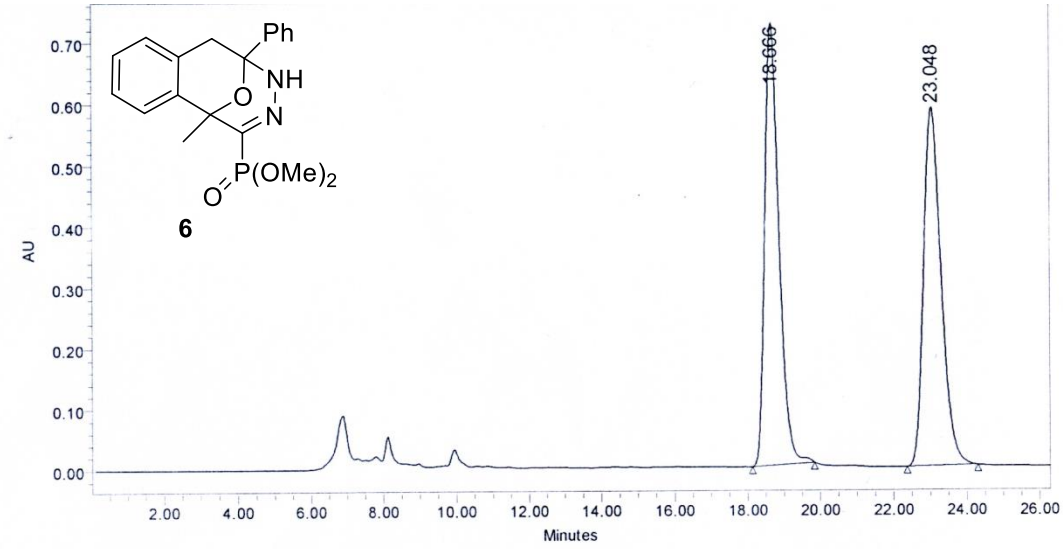
5-(rac)

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	17.888	1986731	49.86	91539	52.07
2	19.324	1997502	50.14	84262	47.93

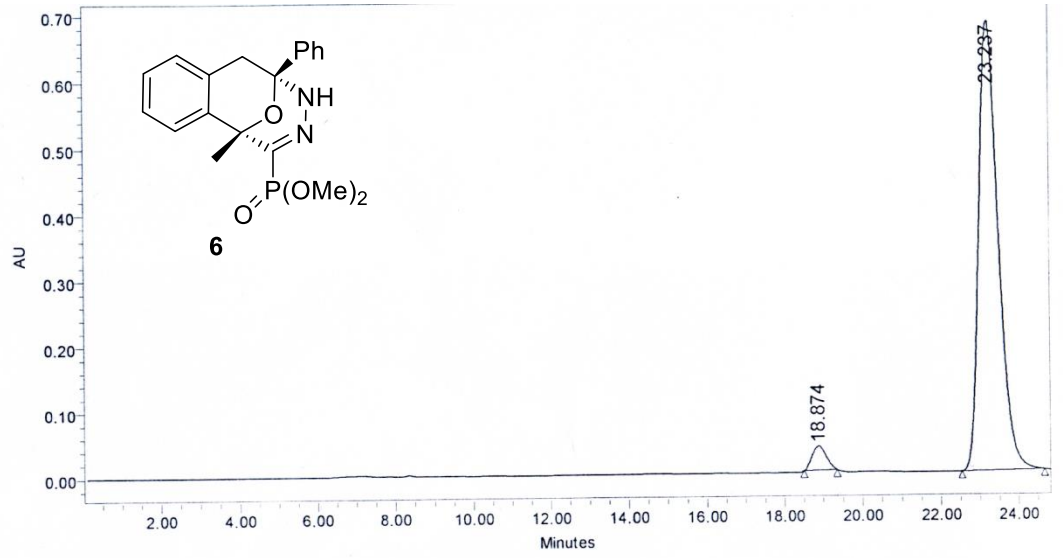


5

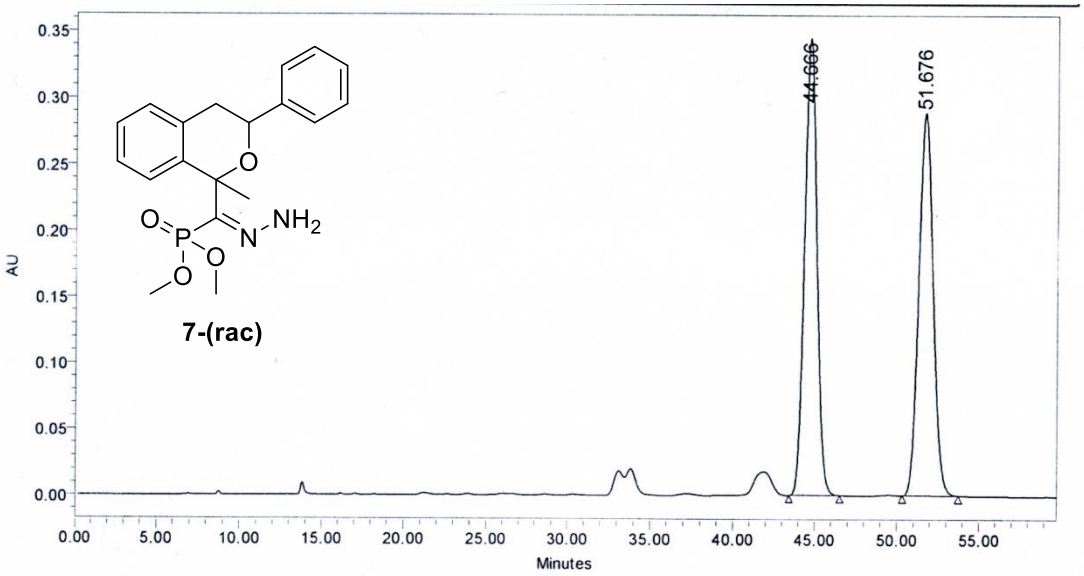
	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	18.462	3059395	3.52	141339	4.57
2	19.949	83783282	96.48	2949693	95.43



	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	18.666	19613625	49.97	724110	55.19
2	23.048	19638568	50.03	587851	44.81

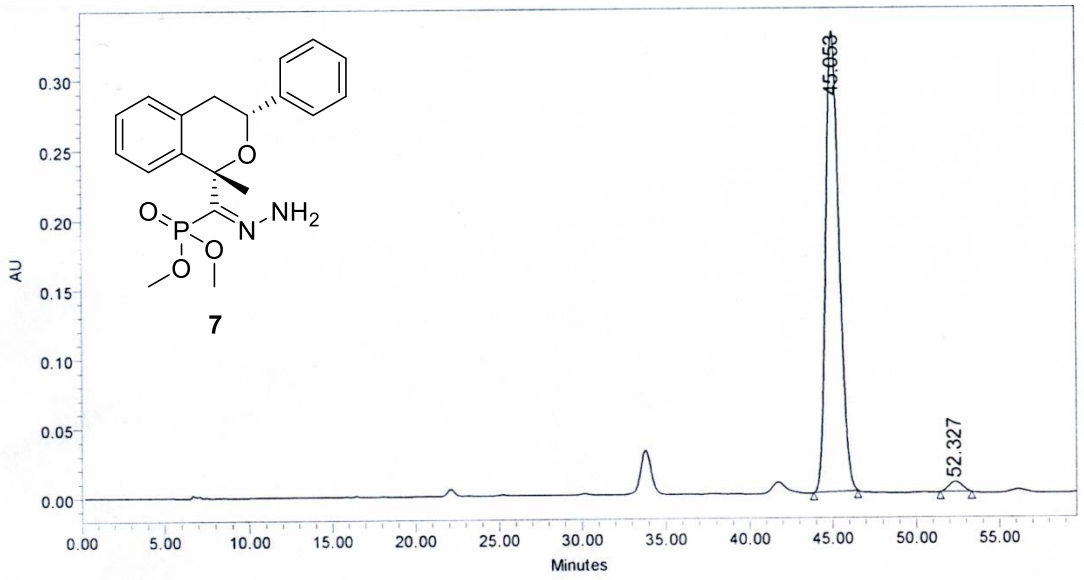


	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	18.874	934733	3.81	36992	5.15
2	23.237	23627983	96.19	681053	94.85



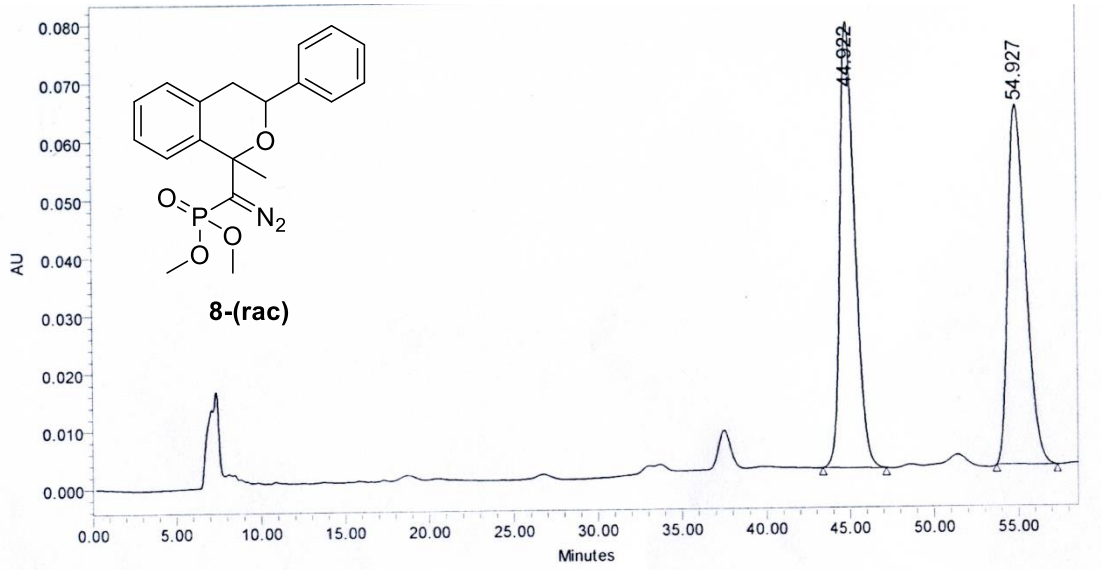
7-(rac)

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	44.666	18150927	50.72	344845	54.39
2	51.676	17636700	49.28	289159	45.61



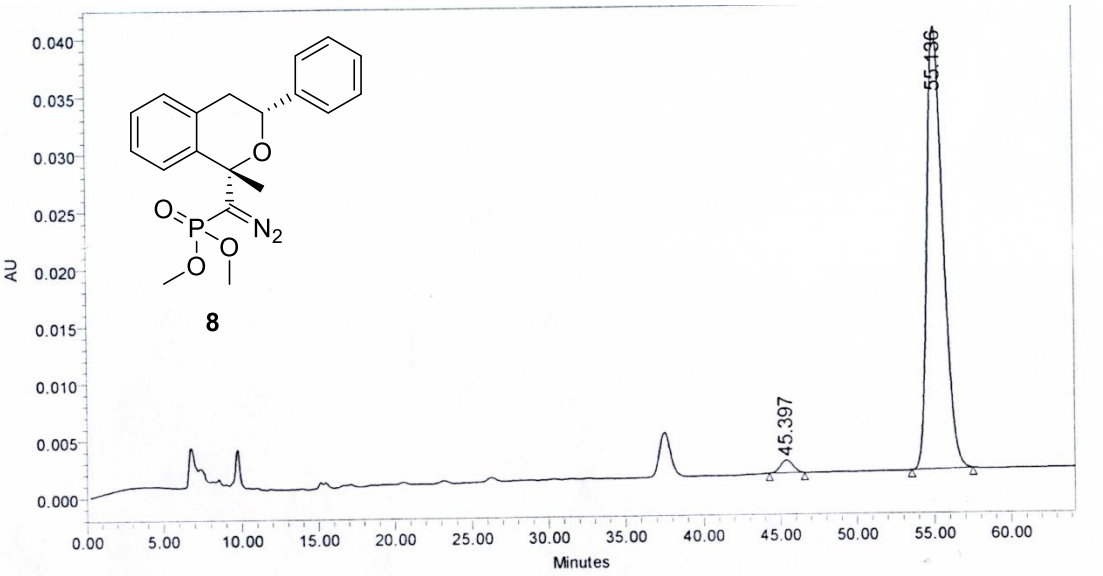
7

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	45.053	18384953	97.80	330508	97.86
2	52.327	413294	2.20	7220	2.14



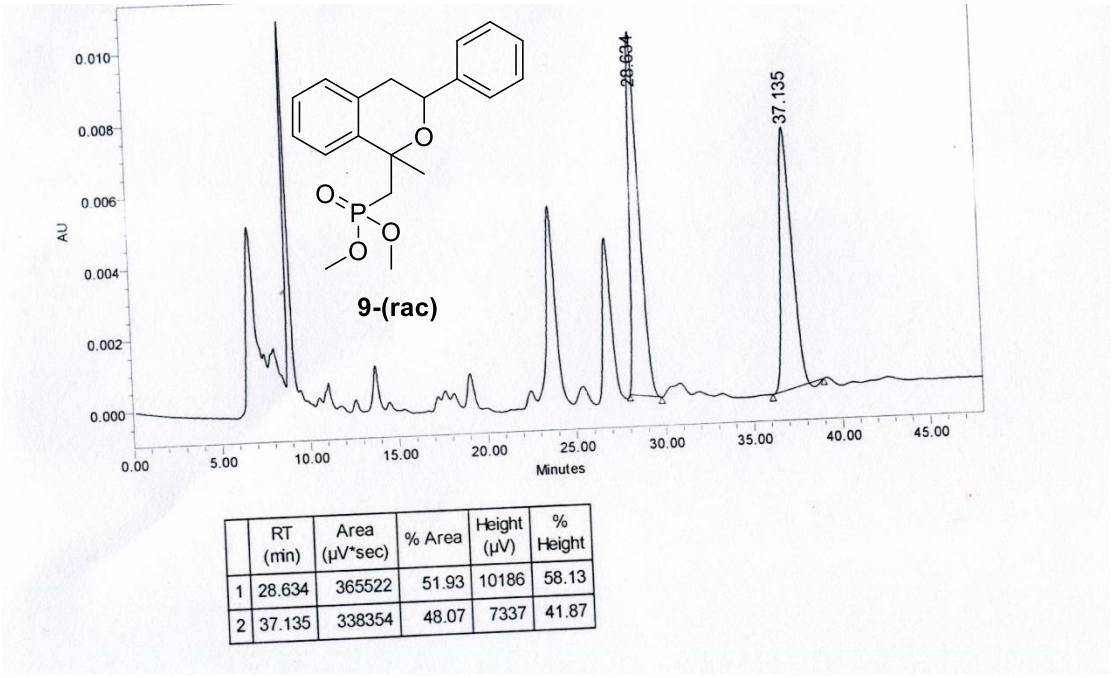
8-(rac)

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	44.922	4781309	50.94	76824	55.27
2	54.927	4604704	49.06	62171	44.73



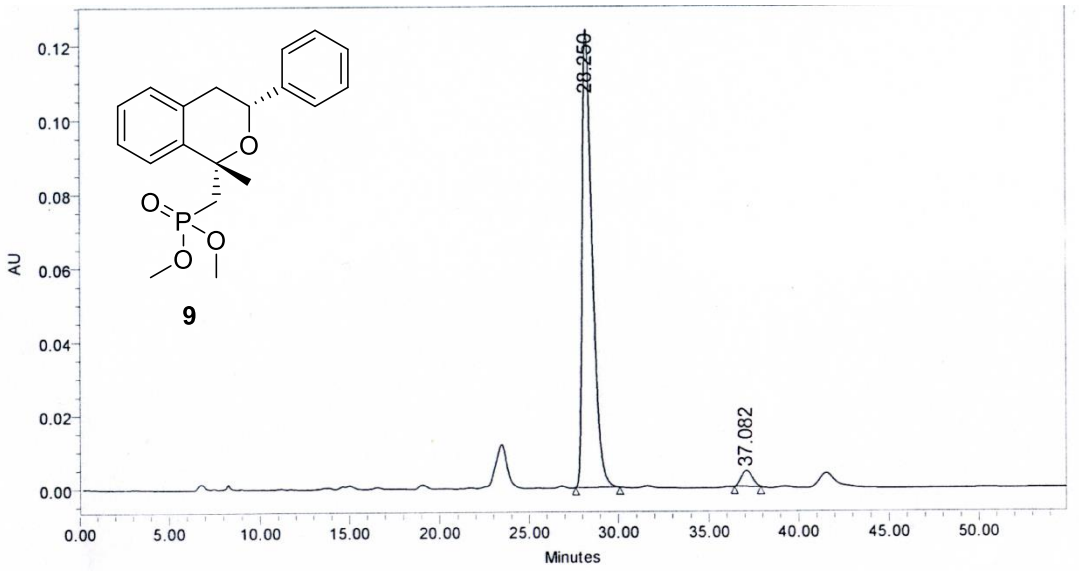
8

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	45.397	63542	2.24	1124	2.83
2	55.136	2769418	97.76	38613	97.17



9-(rac)

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	28.634	365522	51.93	10186	58.13
2	37.135	338354	48.07	7337	41.87



9

	RT (min)	Area (μV*sec)	% Area	Height (μV)	% Height
1	28.250	4776255	96.31	123930	96.62
2	37.082	183131	3.69	4329	3.38