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Supporting Information

Enantioselective Kinetic Resolution/Desymmetrization of *Para*-Quinols: A Case Study in Boronic-Acid-Directed Phosphoric Acid Catalysis

Banruo Huang,[+] Ying He,[+] Mark D. Levin, Jaime A. S. Coelho, Robert G. Bergman, and F. Dean Toste*

Enantioselective Kinetic Resolution/Desymmetrization of *para*-Quinols: A Case Study in Boronic-Acid-Directed Phosphoric Acid Catalysis

Banruo Huang[§], Ying He[§], Mark D. Levin, Jaime A. S. Coelho, Robert G. Bergman and F. Dean Toste*

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General Information

Unless otherwise noted, reagents were obtained from commercial sources and used without further purification.

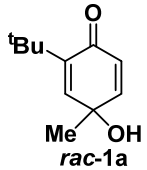
Dichloromethane, toluene, and THF were purified by passage through an activated alumina column under argon. The reactions were run in vials fitted with a screw cap and stirred using an 8 mm magenetic stir bars. Thin-layer chromatography (TLC) analysis of reaction mixtures was performed using Merck silica gel 60 F254 TLC plates, and visualized under UV. Flash column chromatography was carried out on Merck Silica Gel 60 Å, 230 X 400 mesh. The preparative TLC was carried out on Merck silica gel 60 F254 TLC plates. Nuclear magnetic resonance (NMR) spectra were recorded using Bruker AV-600, DRX-500, AV-500, AVB-400, or AVQ-400 spectrometers. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad resonance. Abbreviations are reported as follows: EtOAc = ethyl acetate, DCM = dichloromethane, MeOH = methanol, THF = tetrahydrofuran, DMF = N,N-dimethylformamide. Mass spectral data were obtained from the PerkinElmer AxION 2 Facility operated by the College of Chemistry, University of California, Berkeley. Enantiomeric excesses were determined on a Shimadzu VP Series Chiral HPLC using AD or IA columns. X-Ray crystallographic analysis was carried out by X-Ray Crystallographic Facility (CHEXRAY, University of California, Berkeley). The syntheses of phosphoric acids (*R*)-TRIP, (*R*)-H_8-TRIP, (*R*)-C_8-TRIP, (*R*)-TCYP and (*R*)-H_8-TCYP have been previously described. Dimethyl fumarate was selected to be an internal standard. Racemic products were synthesized by carrying out the reactions using diphenyl phosphate as catalyst. Selectivity factor (***s***) was calculated by the equation $\boldsymbol{s} = \ln(1-c)(1-ee_1)/\ln(1-c)(1+ee_1)$, c: conversion by ^{1}H-NMR using internal standard; ee_1: enantiomeric excess of recovered starting material.

Synthesis of the phenol substrates

The uncommercial 2,4-disubstituted phenols were synthesized by Friedel-Crafts reaction of corresponding phenols according literature[1]. A mixture of *para*-substituted phenol (0.05 mol) and cyclopentanol (isopropyl alcohol or *tert*-butanol) (0.10 mol) in H_3PO_4 (25 mL) was stirred at 100^{o}C overnight. The reaction mixture was then cooled to room temperature, diluted with water, and extracted with EtOAc. The organic layer was washed with brine, dried over Na_2SO_4 and concentrated under vaccuo. The residue was purified by column chromatography using EtOAc/hexane as eluent to give the desired product.

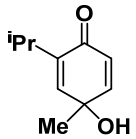
Synthesis of the *para*-quinols

The *para*-quinols (except for **1k**) were synthesized by oxidation of corresponding phenols according literature[2]. To a mixture of corresponding phenol (1.0 eq) in MeCN/H_2O (0.1 M) was added $PhI(OAc)_2$ (1.1 eq) at 0^{o}C. The reaction was then stirred at the same temperature for 0.5-1.0 h. The reaction mixture was diluted with DCM, and washed with $NaHCO_3$ and brine. The organic phase was separated, dried with Na_2SO_4 and filtered. The filtrate was evaporated to the crude mixture, which was purified by column affording the desired product.



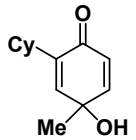
***rac*-1a**

Pale yellow solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.78 – 6.75 (m, 1H), 6.63 (d, *J* = 2.8 Hz, 1H), 6.03 (dd, *J* = 9.8, 1.1 Hz, 1H), 1.90 (br, 1H), 1.45 (d, *J* = 1.0 Hz, 3H), 1.22 (d, *J* = 1.1 Hz, 10H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 185.35, 149.36, 145.33, 144.33, 128.94, 67.68, 34.28, 29.06, 27.25. HRMS (ESI) m/z: calculated for $[C_{11}H_{16}O_2 + Na]^+$ 203.1048, found 203.1041.



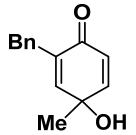
***rac*-1c**

Pale yellow solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.82 (dd, *J* = 9.9, 3.0 Hz, 1H), 6.56 (dd, *J* = 2.9, 1.2 Hz, 1H), 6.09 (d, *J* = 9.9 Hz, 1H), 2.94 – 2.87 (m, 1H), 2.18 (br, 1H), 1.45 (s, 3H), 1.05 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 185.13, 151.04, 144.34, 143.20, 127.53, 67.48, 27.05, 25.94, 21.64, 21.44. HRMS (ESI) m/z: calculated for $[C_{10}H_{14}O_2 + Na]^+$ 189.0892, found 189.0894.



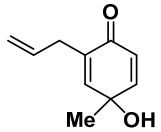
***rac*-1d**

Pale yellow solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.81 (dd, *J* = 9.9, 3.0 Hz, 1H), 6.53 (dd, *J* = 3.1, 1.2 Hz, 1H), 6.09 (d, *J* = 9.9 Hz, 1H), 2.59 – 2.55 (m, 1H), 2.02 (br, 1H), 1.78 – 1.68 (m, 5H), 1.44 (s, 3H), 1.37 (dddd, *J* = 16.0, 12.5, 7.8, 6.2 Hz, 2H), 1.21 – 1.05 (m, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 184.96, 150.86, 144.79, 142.49, 127.59, 67.51, 35.51, 32.39, 32.19, 27.08, 26.54, 26.52, 26.22. HRMS (ESI) m/z: calculated for $[C_{13}H_{18}O_2 + Na]^+$ 229.1205, found 229.1204.



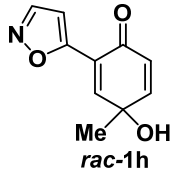
***rac*-1e**

Yellow oil.^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.30 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.16 (m, 3H), 6.83 (dd, *J* = 10.0, 3.1 Hz, 1H), 6.44 (dd, *J* = 3.0, 1.4 Hz, 1H), 6.13 (d, *J* = 9.9 Hz, 1H), 3.60 (q, *J* = 15.7 Hz, 2H), 1.81 (br, 1H), 1.42 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 184.97, 151.38, 147.66, 138.42, 137.38, 129.19, 128.50, 127.20, 126.35, 67.63, 34.90, 26.87. HRMS (ESI) m/z: calculated for $[C_{14}H_{14}O_2 + Na]^+$ 237.0892, found 237.0895.



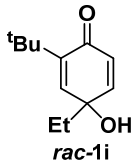
***rac*-1f**

Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.85 (ddd, *J* = 10.0, 3.1, 1.0 Hz, 1H), 6.61 (dt, *J* = 2.9, 1.4 Hz, 1H), 6.11 (dd, *J* = 10.0, 1.2 Hz, 1H), 5.81 (ddt, *J* = 17.2, 10.4, 6.8 Hz, 1H), 5.11 – 5.07 (m, 2H), 3.02 – 3.01 (m, 2H), 2.08 (br, 1H), 1.45 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 185.09, 151.66, 147.35, 135.94, 134.61, 127.09, 117.29, 67.54, 32.78, 26.90. HRMS (ESI) m/z: calculated for $[C_{10}H_{12}O_2 + Na]^+$ 187.0735, found 187.0737.



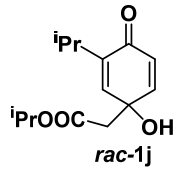
***rac*-1h**

Pale yellow solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 1.8 Hz, 1H), 7.65 (d, *J* = 3.0 Hz, 1H), 7.01 (d, *J* = 1.8 Hz, 1H), 6.97 (dd, *J* = 10.1, 3.0 Hz, 1H), 6.22 (d, *J* = 10.1 Hz, 1H), 3.00 (br, 1H), 1.59 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 181.14, 162.01, 151.66, 150.90, 150.19, 127.07, 123.88, 104.51, 67.18, 26.91. HRMS (ESI) m/z: calculated for $[C_{10}H_9NO_3 + Na]^+$ 214.0480, found 214.0476.



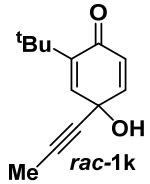
rac-1i

Pale yellow solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.67 (ddd, *J* = 9.9, 3.1, 1.3 Hz, 1H), 6.54 (dd, *J* = 3.1, 1.3 Hz, 1H), 6.10 (dd, *J* = 9.9, 1.3 Hz, 1H), 1.99 (br, 1H), 1.78 (q, *J* = 7.5 Hz, 2H), 1.22 (d, *J* = 1.4 Hz, 9H), 0.80 (td, *J* = 7.5, 1.3 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 185.75, 148.36, 145.93, 144.39, 130.31, 70.99, 34.44, 33.10, 29.15, 8.05. HRMS (ESI) m/z: calculated for $[C_{12}H_{18}O_2 + Na]^+$ 217.1205, found 217.1206.



rac-1j

Pale yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.90 (ddd, *J* = 10.0, 3.1, 0.7 Hz, 1H), 6.59 (dd, *J* = 3.1, 1.1 Hz, 1H), 6.17 (dd, *J* = 10.0, 0.7 Hz, 1H), 5.10 – 5.06 (m, 1H), 2.93 (pd, *J* = 6.9, 1.1 Hz, 1H), 2.66 – 2.59 (m, 2H), 1.25 (d, *J* = 6.3 Hz, 6H), 1.05 (dd, *J* = 6.9, 3.6 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 184.81, 170.69, 147.93, 144.40, 141.34, 128.64, 69.20, 67.85, 44.22, 26.10, 21.71, 21.69, 21.56, 21.41. HRMS (ESI) m/z: calculated for $[C_{14}H_{20}O_4 + Na]^+$ 275.1260, found 275.1265.



rac-1k

Prepared as follows: To a flask was dissolved 2-(tert-butyl)cyclohexa-2,5-diene-1,4-dione (10 mmol) in anhydrous THF. The solution was then cooled to -78^{o}C under N_2 atmosphere. The 1-propynylmagnesium bromide solution (11 mmol, 0.5M) was then added dropwise at the same temperature. The reaction was stirred for 0.5-1.0 h and then quenched by saturated NH4Cl aq. The EtOAc was then added and the mixture was washed with H_2O and brine. The organic phase was separated, dried with Na_2SO_4 and filtered. The filtrate was evaporated to the crude mixture, which was purified by column affording the desired product.

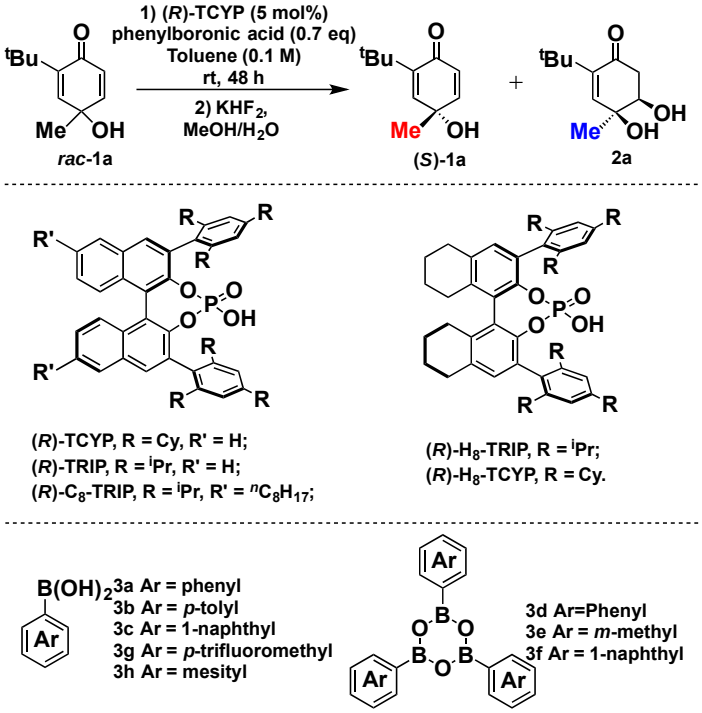
Yellow oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.73 (ddd, *J* = 9.8, 3.0, 1.3 Hz, 1H), 6.62 (dd, *J* = 3.0, 1.4 Hz, 1H), 6.07 – 6.05 (m, 1H), 2.36 (br, 1H), 1.87 – 1.87 (m, 3H), 1.24 – 1.23 (m, 9H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 184.96, 144.54, 143.87, 140.83, 128.51, 82.45, 76.63, 63.09, 34.42, 28.95, 3.77. HRMS (ESI) m/z: calculated for $[C_{13}H_{16}O_2 + Na]^+$ 227.1048, found 227.1065.

General procedure of kinetic resolution of *para*-quinols

The ***rac*-1** (0.20 mmol), 1-naphthylboroxine (0.04 mmol) and (*R*)-TCYP (2.0 mol%) were added to a vial containing a stir bar. The vial was twined with Teflon tape, toluene (2.0 ml) was added using a syringe, and the vial was fitted with a cap. The reaction mixture was stirred at room temperature for the indicated time. To the mixture was added MeOH/H_2O (1/1, 2.0 ml), and then KHF_2 (10 eq) was added and the mixture was stirred vigorously for 5-30 min until the boronic ester was removed as evident from TLC analysis. The aqueous phase was separated and collected, and the organic phase was evaporated and then re-dissolved in *n*-hexanes. The mixture was then washed MeOH/H_2O (1/1) twice and the aqueous phase was combined. The combined aqueous layers were then evaporated and purified by column chromatography carefully over silica gel affording the desired chiral *p*-quinols and diols. The products were further purified by preparative TLC as necessary.

Optimized conditions of kinetic resolution of *para*-quinols

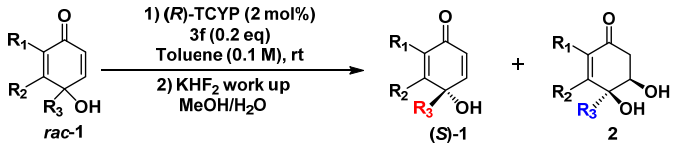
Table S1. Optimization of the reaction conditions[a].

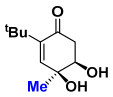
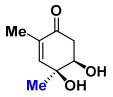
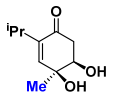
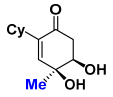
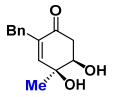
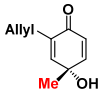
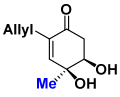
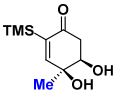
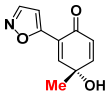
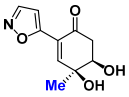
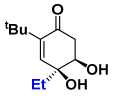
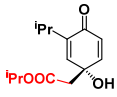
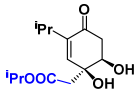
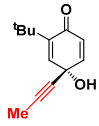
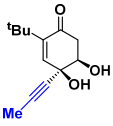
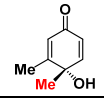
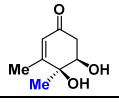


Entry	Variation from "indicated conditions"	Conv. (%)[b]	(*S*)-**1a** ee_1 (%)[c]	**2a** ee_2 (%)[c]	*s*[d]
1	None	58	71	54	6
2	**3b**, instead of **3a**	64	86	54	7
3	**3c**, instead of **3a**	54	90	78	23
4	**3g**, instead of **3a**	60	73	47	6
5	**3h**, instead of **3a**	49	65	70	10
6[e]	**3d**, instead of **3a**	51	70	73	10
7[e]	**3e**, instead of **3a**	45	62	78	14
8[e]	**3f**, instead of **3a**	53	90	84	27
9	**3f**, instead of **3a** (*R*)-TRIP, instead of (*R*)-TCYP	38	52	82	21
10	**3f**, instead of **3a** (*R*)-C_8-TRIP, instead of (*R*)-TCYP	34	44	86	20
11	**3f**, instead of **3a** (*R*)-H_8-TRIP, instead of (*R*)-TCYP	31	37	86	15
12	**3f**, instead of **3a** (*R*)-H_8-TCYP, instead of (*R*)-TCYP	41	56	80	16
13	**3f**, instead of **3a** DCM, instead of toluene	46	66	73	15
14	**3f**, instead of **3a** Hexane, instead of toluene	38	48	77	13

[a] Reaction conditions: ***rac*-1a** (0.2 mmol), Cat. (5.0 mol%), Boronic acid (0.7 eq), solvent (2.0 ml), rt for 48 h; [b] Determined by ^{1}H NMR yield using internal standard; [c] Determined by chiral phase HPLC; [d] Selectivity factor (***s***) was calculated according to the reported method (see SI); [e] **3d/e/f** (0.2 eq), Cat. (2.0 mol%), rt for 24 h.

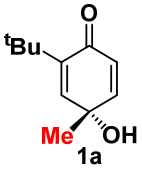
Table S2. Detailed Scope of substrates[a].



Entry	Time	Conv.[b]	(*S*)-1	yield / ee[c]	2	yield / ee[c]	*s*[d]
1	24 h	53%		**1a**, 34% / 90%		**2a**, 45% / 84%	27
2	24 h	58%		**1b**, 40% / 87%		**2b**, 44% / 65%	12
3	24 h	58%		**1c**, 39% / 94%		**2c**, 52% / 70%	18
4	24 h	60%		**1d**, 34% / 88%		**2d**, 51% / 65%	11
5	24 h	56%		**1e**, 41% / 86%		**2e**, 56% / 73%	14
6	20 h	54%		**1f**, 43% / 80%		**2f**, 52% / 73%	13
7	12 h	57 %		**1g**, 34% / 96%		**2g**, 47% / 74%	24
8[e]	24 h	24%		**1h**, 76% / 21%		**2h**, 20% / 77%	6
9	24 h	47 %		**1i**, 48% / 78%		**2i**, 45% / 89%	37
10[e]	24 h	40 %		**1j**, 55% / 37%		**2j**, 26% / 76%	5
11[e]	24 h	35 %		**1k**, 61% / 42%		**1k**, 30% / 86%	12
12	18 h	60 %		**1l**, 40% / 80%		**2l**, 45% / 69%	8

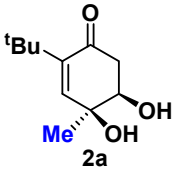
[a] Reaction conditions: ***rac*-1** (0.2 mmol), Cat. (2.0 mol%), **3f** (0.2 eq), toluene (2.0 ml), rt, isolated yield. Absolute configuration assigned by analogy to that of **1g**, which was determined to be (***S***) by single-crystal X-ray diffraction (See SI

for details). [b] Determined by ^{1}H NMR yield using internal standard; [c] Determined by chiral phase HPLC; [d] Selectivity factor (**s**) was calculated according to the reported method (see General information); [e] 5.0 mol% of catalyst was used.



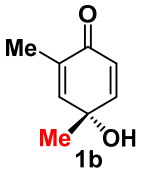
1a

White solid. HPLC (Chiralpak AD column, 98:2 hexanes/isopropanol, 1 ml/min), tr = 13.9 min (minor), 23.9 min (major); ee = 90%.



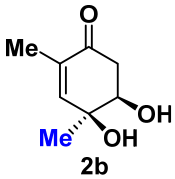
2a

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.41 (d, *J* = 1.6 Hz, 1H), 3.98 – 3.96 (m, 1H), 2.72 – 2.64 (m, 2H), 2.39 (br, 2H), 1.45 (s, 3H), 1.17 (s, 10H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.18, 146.09, 144.37, 73.15, 70.44, 44.81, 34.24, 29.09, 25.63. HRMS (ESI) m/z: calculated for $[C_{11}H_{18}O_3 + Na]^+$ 221.1154, found 221.1145. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 6.7 min (major), 18.0 min (minor); ee = 84%.



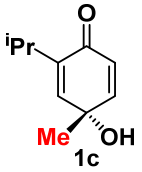
1b

White wax solid. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 10.2 min (minor), 11.5 min (major); ee = 87%.



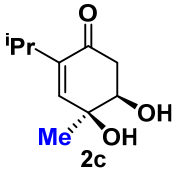
2b

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.45 – 6.45 (m, 1H), 4.01 (ddd, *J* = 5.7, 3.9, 1.4 Hz, 1H), 2.76 – 2.68 (m, 2H), 2.46 (br, 2H), 1.79 (s, 3H), 1.46 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.68, 146.63, 135.32, 73.56, 70.29, 42.74, 25.42, 15.43. HRMS (ESI) m/z: calculated for $[C_8H_{12}O_3 + Na]^+$ 179.0684, found 179.0695. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 8.9 min (major), 12.6 min (minor); ee = 65%.



1c

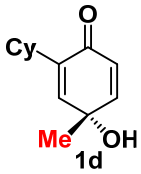
Colorless oil. HPLC (Chiralpak AD column, 98:2 hexanes/isopropanol, 1 ml/min), tr = 17.2 min (minor), 21.3 min (major); ee = 94%.



2c

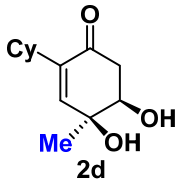
Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.34 (d, *J* = 1.3 Hz, 1H), 4.00 (t, *J* = 4.9 Hz, 1H), 2.87 – 2.80 (m, 1H), 2.71 (qd, *J* = 16.6, 4.9 Hz, 2H), 2.41 (br, 2H), 1.46 (s, 3H), 1.02 (dd, *J* = 13.5, 6.9 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.97, 144.95, 143.49, 73.31, 70.28, 43.33, 26.03, 25.57, 21.69, 21.46. HRMS (ESI) m/z: calculated for

$[C_{10}H_{16}O_3 + Na]^+$ 207.0997, found 207.0982. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 6.7 min (major), 13.8 min (minor); ee = 70%.



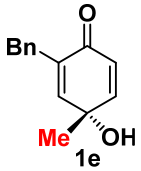
1d

White solid. HPLC (Chiralpak AD column, 97:3 hexanes/isopropanol, 1 ml/min), tr = 15.8 min (major), 21.9 min (minor); ee = 88%.



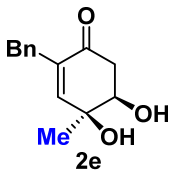
2d

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.31 (s, 1H), 3.98 – 3.97 (m, 1H), 2.74 – 2.65 (m, 2H), 2.64 (br, 2H), 2.48 (tt, *J* = 12.0, 3.1 Hz, 1H), 1.77 – 1.65 (m, 5H), 1.44 (s, 3H), 1.37 – 1.30 (m, 2H), 1.19 – 1.00 (m, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.17, 144.21, 144.10, 73.24, 70.32, 43.29, 35.65, 32.47, 32.16, 26.53, 26.49, 26.18, 25.54. HRMS (ESI) m/z: calculated for $[C_{13}H_{20}O_3 + Na]^+$ 247.1310, found 247.1295. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 7.5 min (major), 10.9 min (minor); ee = 65%.



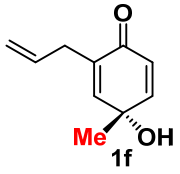
1e

Colorless oil. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 10.2 min (minor), 12.7 min (major); ee = 86%.



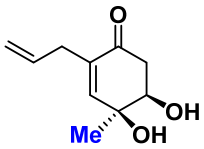
2e

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28 (q, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.16 – 7.15 (m, 2H), 6.24 (q, *J* = 1.6 Hz, 1H), 4.00 (ddd, *J* = 5.7, 3.7, 1.6 Hz, 1H), 3.52 (s, 2H), 2.72 (qd, *J* = 16.8, 4.7 Hz, 2H), 2.48 (br, 2H), 1.41 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.15, 147.62, 138.54, 138.47, 129.08, 128.48, 126.30, 73.50, 70.47, 42.94, 34.89, 25.26. HRMS (ESI) m/z: calculated for $[C_{14}H_{16}O_3 + Na]^+$ 255.0997, found 255.0983. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 10.6 min (major), 13.2 min (minor); ee = 73%.



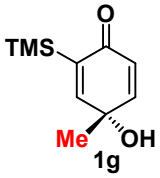
1f

Colorless oil. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 9.7 min (minor), 13.3 min (major); ee = 80%.



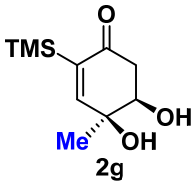
2f

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.41 – 6.41 (m, 1H), 5.79 (dddd, *J* = 16.2, 10.3, 7.3, 6.2 Hz, 1H), 5.10 – 5.05 (m, 2H), 4.03 – 4.01 (m, 1H), 2.96 – 2.94 (m, 2H), 2.77 – 2.68 (m, 2H), 2.54 (br, 2H), 1.46 (s, 3H).^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.83, 146.76, 137.45, 134.65, 117.17, 73.51, 70.39, 42.90, 32.71, 25.40. HRMS (ESI) m/z: calculated for $[C_{10}H_{14}O_3 + Na]^+$ 205.0841, found 205.0838. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 8.7 min (major), 17.7 min (minor); ee = 73%.



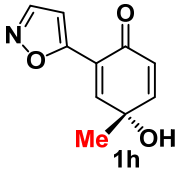
1g

White solid. HPLC (Chiralpak AD column, 98:2 hexanes/isopropanol, 1 ml/min), tr = 12.6 min (minor), 15.9 min (major); ee = 96%.



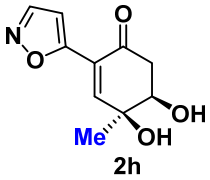
2g

White solid. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.78 (d, *J* = 1.8 Hz, 1H), 4.01 (td, *J* = 4.7, 1.7 Hz, 1H), 2.77 (br, 2H), 2.67 (d, *J* = 4.6 Hz, 2H), 1.44 (s, 3H), 0.14 (s, 9H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 199.77, 158.94, 140.92, 73.61, 70.21, 43.39, 25.03, -1.60. HRMS (ESI) m/z: calculated for $[C_{10}H_{18}O_3Si + Na]^+$ 237.0923, found 237.0920. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 7.9 min (major), 16.4 min (minor); ee = 74%.



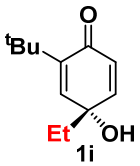
1h

White solid. HPLC (Chiralpak IA column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 34.6 min (major), 45.8 min (minor); ee = 21%.



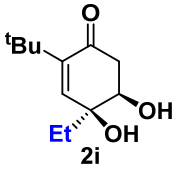
2h

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 1.7 Hz, 1H), 7.48 (d, *J* = 1.7 Hz, 1H), 6.95 (d, *J* = 1.7 Hz, 1H), 4.15 (ddt, *J* = 5.3, 3.4, 1.6 Hz, 1H), 2.94 – 2.83 (m, 2H), 2.50 (br, 2H), 1.59 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.98, 161.90, 150.85, 150.03, 125.26, 104.27, 73.39, 70.47, 43.32, 25.04. HRMS (ESI) m/z: calculated for $[C_{10}H_{11}NO_4 + Na]^+$ 232.0586, found 232.0579. Colorless oil. HPLC (Chiralpak IA column, 85:15 hexanes/isopropanol, 1 ml/min), tr = 14.5 min (major), 20.8 min (minor); ee = 77%.



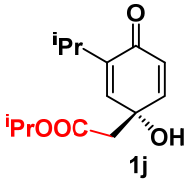
1i

White solid. HPLC (Chiralpak AD column, 98:2 hexanes/isopropanol, 1 ml/min), tr = 13.9 min (minor), 25.0 min (major); ee = 78%.



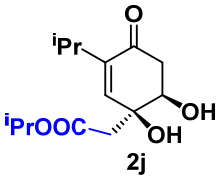
2i

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.42 (d, *J* = 1.3 Hz, 1H), 4.02 (ddd, *J* = 6.8, 3.8, 1.3 Hz, 1H), 2.73 – 2.64 (m, 2H), 2.26 (br, 2H), 1.83 (dq, *J* = 14.9, 7.6 Hz, 1H), 1.69 (dq, *J* = 14.7, 7.5 Hz, 1H), 1.18 (s, 9H), 1.00 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.18, 147.06, 143.47, 72.54, 70.58, 44.62, 34.43, 31.21, 29.15, 7.91. HRMS (ESI) m/z: calculated for $[C_{12}H_{20}O_3 + Na]^+$ 235.1310, found 235.1307. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 5.5 min (major), 17.1 min (minor); ee = 89%.



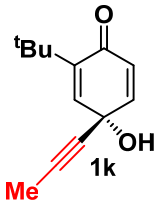
1j

Yellow oil. HPLC (Chiralpak AD column, 98:2 hexanes/isopropanol, 1 ml/min), tr = 20.1 min (minor), 21.9 min (major); ee = 37%.



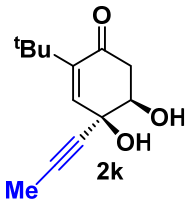
2j

White wax solid.^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.38 (d, *J* = 1.0 Hz, 1H), 5.12 (p, *J* = 6.3 Hz, 1H), 4.50 (br, 1H), 3.94 (ddd, *J* = 8.1, 4.0, 1.0 Hz, 1H), 2.87 – 2.77 (m, 3H), 1.59 (br, 1H), 2.64 – 2.59 (m, 2H), 1.29 (t, *J* = 6.6 Hz, 6H), 1.02 (dd, *J* = 12.0, 6.9 Hz, 6H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.83, 171.95, 146.34, 139.94, 71.29, 70.39, 69.33, 42.47, 41.67, 26.16, 21.78, 21.67, 21.63, 21.45. HRMS (ESI) m/z: calculated for $[C_{14}H_{22}O_5 + Na]^+$ 293.1365, found 293.1351. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 7.5 min (major), 7.9 min (minor); ee = 76%.



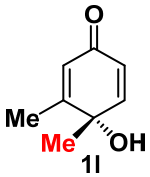
1k

White solid. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 7.9 min (minor), 9.2 min (major); ee = 42%.



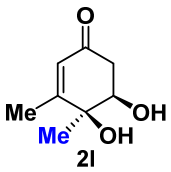
2k

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.42 (d, *J* = 1.5 Hz, 1H), 4.17 (ddd, *J* = 6.9, 3.4, 1.4 Hz, 1H), 2.82 – 2.70 (m, 2H), 2.55 (br, 2H), 1.89 (s, 3H), 1.19 (s, 9H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.75, 146.21, 83.18, 73.07, 67.66, 43.76, 34.40, 28.99, 3.72. HRMS (ESI) m/z: calculated for $[C_{13}H_{18}O_3 + Na]^+$ 245.1154, found 245.1142. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 6.1 min (major), 7.7 min (minor); ee = 86%.



1l

Colorless oil. HPLC (Chiralpak AD column, 95:5 hexanes/isopropanol, 1 ml/min), tr = 12.3 min (minor), 14.3 min (major); ee = 80%.

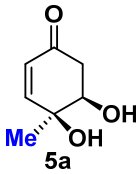


2l

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 5.88 (d, *J* = 1.8 Hz, 1H), 4.10 (t, *J* = 3.6 Hz, 1H), 2.89 (br, 1H), 2.72 (dd, *J* = 3.7, 2.2 Hz, 2H), 2.47 (br, 1H), 2.04 (d, *J* = 1.4 Hz, 3H), 1.46 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 195.31, 163.13, 126.17, 74.82, 72.62, 42.84, 24.00, 18.84. HRMS (ESI) m/z: calculated for $[C_8H_{12}O_3 + Na]^+$ 179.0684, found 179.0689. HPLC (Chiralpak AD column, 90:10 hexanes/isopropanol, 1 ml/min), tr = 9.8 min (minor), 10.6 min (major); ee = 69%.

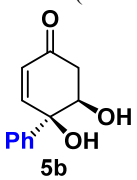
General procedure of desymmetrization of *para*-quinols

The **4** (0.10 mmol), 1-naphthylboroxine (0.04 mmol) and (*R*)-TCYP (5.0 mol%) were added to a vial containing a stir bar. The vial was twined with Teflon tape, toluene (1.0 ml) was added using a syringe, and the vial was fitted with a cap. The reaction mixture was stirred at the room temperature for corresponding time. To the mixture was added MeOH/H_2O (1/1, 1.0 ml), and then KHF_2 (10 eq) was added and the mixture was stirred vigorously for 10-30 min until the boronic ester was removed as evident from TLC analysis. The reaction mixture was evaporated and then re-dissolved in *n*-hexanes. The mixture was then extracted with MeOH/H_2O (1/1) twice and the combined aqueous phases was then evaporated and purified by column chromatography carefully over silica gel using *n*-hexane and ethyl acetate as eluents affording the desired diols. The products were further purified by preparative TLC when necessary.



5a

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.69 (dd, *J* = 10.2, 1.7 Hz, 1H), 5.98 (d, *J* = 10.2 Hz, 1H), 4.07 (ddd, *J* = 5.5, 4.0, 1.7 Hz, 1H), 2.72 (dd, *J* = 4.5, 3.4 Hz, 2H), 2.41 (br, 2H), 1.49 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.22, 151.58, 128.44, 73.67, 70.07, 42.75, 25.08. HRMS (ESI) m/z: calculated for $[C_7H_{10}O_3 + Na]^+$ 165.0528, found 165.0508. HPLC (Chiralpak AD column, 85:15 hexanes/isopropanol, 1 ml/min), tr = 9.3 min (major), 12.2 min (minor); ee = 88%.



5b

Colorless oil. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.51 – 7.49 (m, 2H), 7.42 (dd, *J* = 8.5, 6.8 Hz, 2H), 7.36 (td, *J* = 6.9, 6.3, 1.4 Hz, 1H), 6.76 (dd, *J* = 10.2, 1.7 Hz, 1H), 6.28 (d, *J* = 10.1 Hz, 1H), 4.26 (ddd, *J* = 5.8, 3.5, 1.8 Hz, 1H), 3.45 (br, 1H), 2.70 – 2.57 (m, 2H), 2.66 (br, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 197.06, 149.05, 140.66, 130.01, 128.78, 128.51, 126.02, 74.82, 41.71. HRMS (ESI) m/z: calculated for $[C_{12}H_{12}O_3 + Na]^+$ 227.0684, found 227.0680. HPLC (Chiralpak AD column, 85:15 hexanes/isopropanol, 1 ml/min), tr = 8.8 min (minor), 13.5 min (major); ee = 85%.

Mechanistic study

Procedure for titration experiments

To 4 vials, each one was added (*R*)-TRIP (0.01 mmol), tris(*m*-tolyl)boroxine (0 / 0.5 / 1.0 / 1.5 eq) and toluene-d_8 (1.0 ml) by syringe. The mixture was sonicated and transfered to an NMR tube. ^{1}H-NMR spectra were taken at 298.0 K in pre-warmed, tuned and shimmed NMR spectrometer.

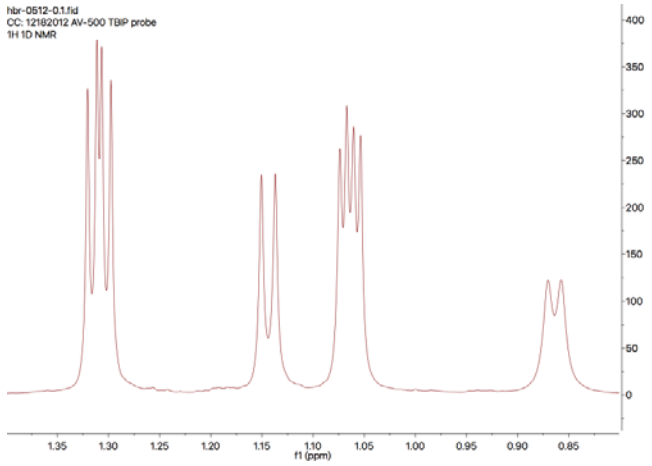


Figure S1. A spectrum from the titration experiments with no boroxine.

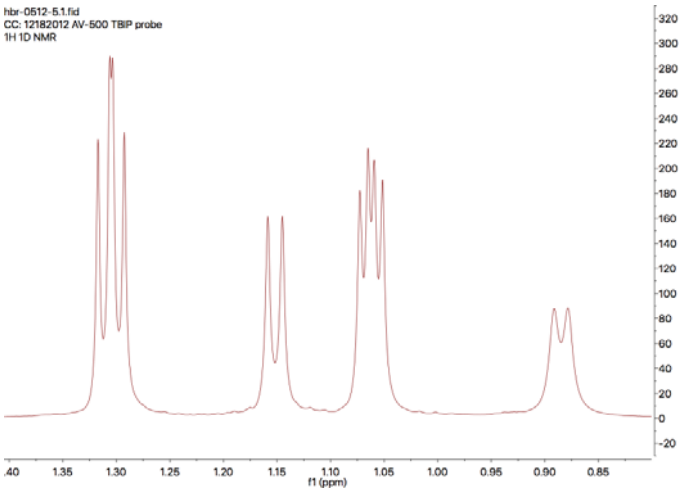


Figure S2. A spectrum from the titration experiments with 0.5 eq. boroxine.

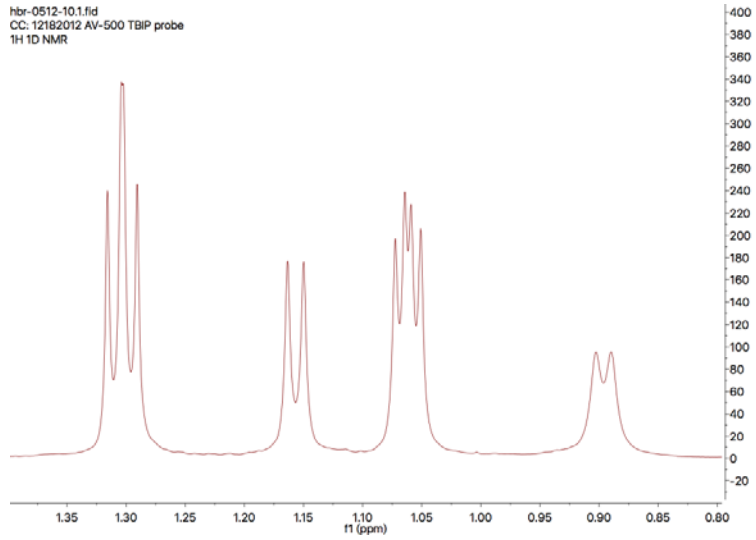


Figure S3. A spectrum from the titration experiments with 1.0 eq. boroxine.

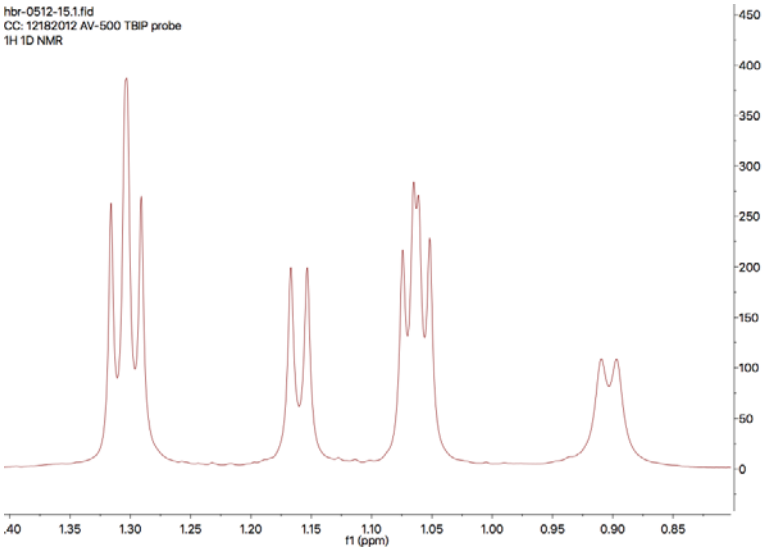


Figure S4. A spectrum from the titration experiments with 1.5 eq. boroxine.

Procedure for variable temperature NMR experiment

To an NMR tube, was added by syringe (*R*)-TRIP (0.01 mmol, 1 eq) and tris(*m*-tolyl)boroxine (0.005 mmol, 0.5 eq) as a solution in toluene-d_8 (1.0 ml). The NMR tube was fitted with a septum cap, cooled to -78 ^{o}C, and degassed and backfilled with N_{22} three times on a Schlenk line. ^{1}H-NMR spectra were taken with standard variable temperature techniques.

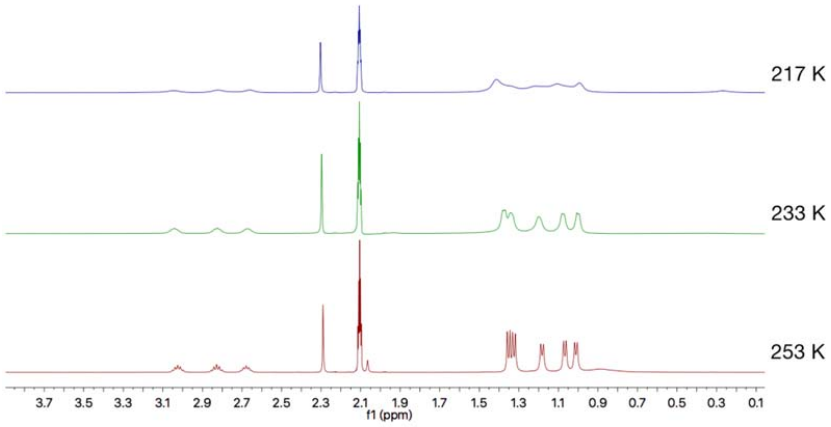


Figure S5. Variable temperature ^{1}H NMR experiment of (*R*)-TRIP and 0.5 eq boroxine.

Kinetics procedures

Dimethyl fumarate was used as an internal standard. All reactions were conducted at 298.0 K. One scan was used per time point in order to minimize integration error.

Procedure for kinetic analysis under typical reaction stoichiometries

To a vial, was added substrate **4a** (0.1 mmol, 1.0 eq), tris(*m*-tolyl)boroxine (0.03 mmol, 0.3 eq), (R)-TRIP (0.005 mmol, 0.05 eq) and dimethyl fumarate (0.025 mmol, 0.25 eq). Immediately prior to the kinetics experiment, by syringe, toluene-d_8 (1.0 mL) was added to the vial. After all the solid materials were dissolved, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed, tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 120-second intervals.

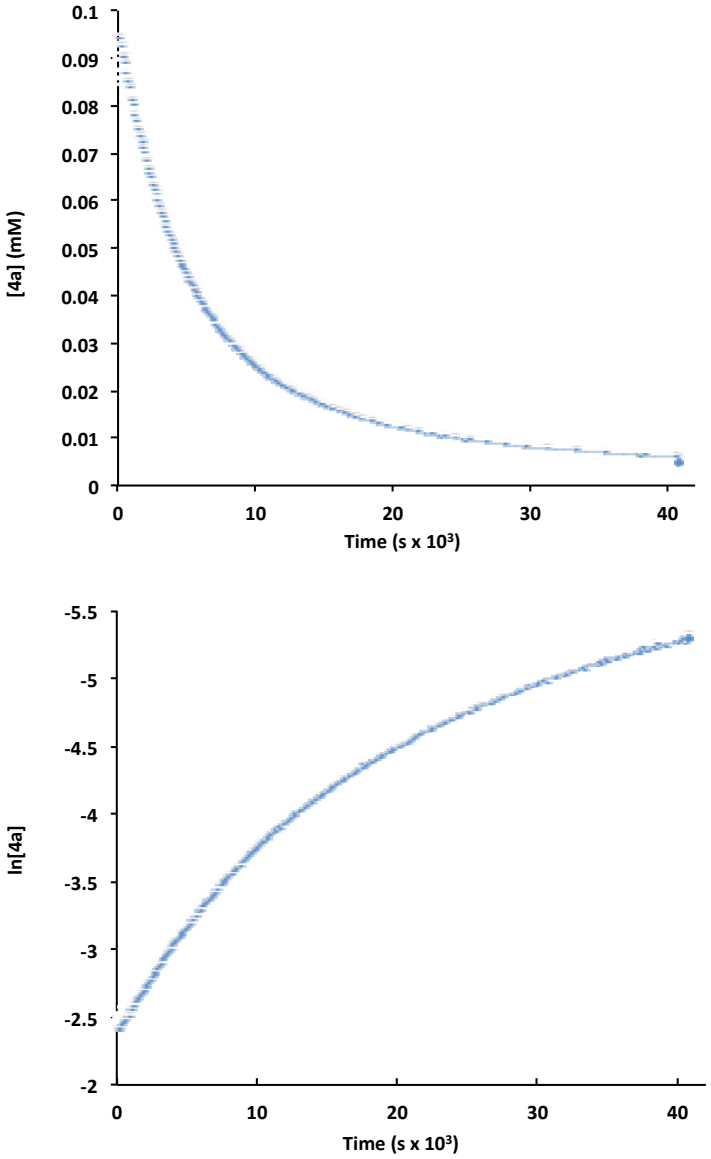


Figure S6. Kinetic plot used to determine product inhibition.

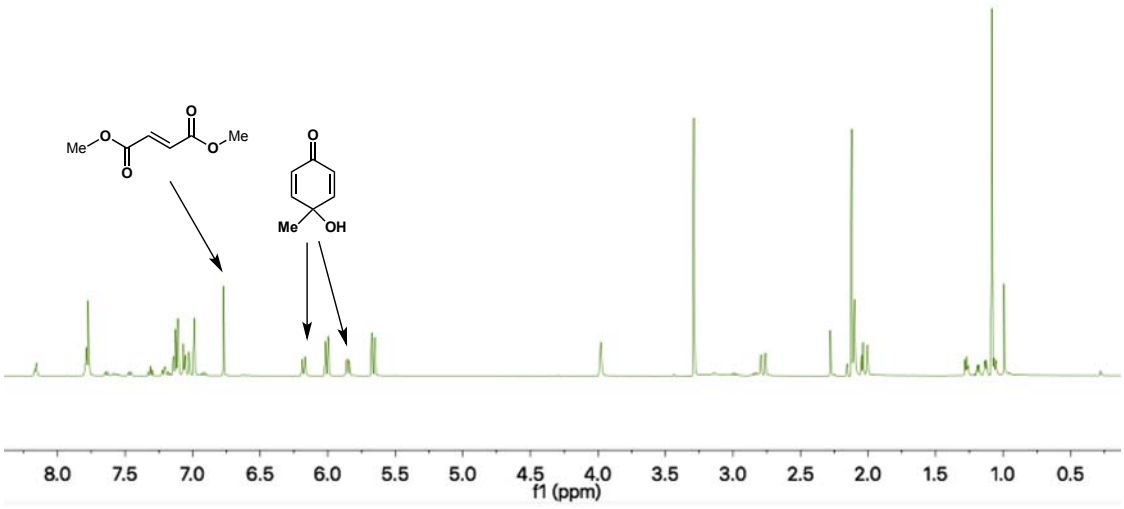
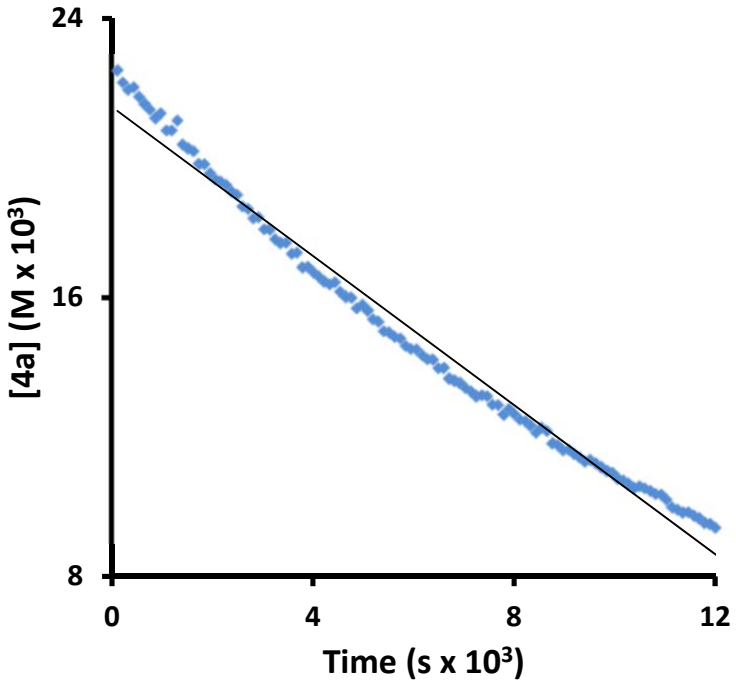


Figure S7. A representative spectrum from the kinetics analysis.

Procedure for kinetics analysis under saturation of boroxine

To a vial, was added substrate **4a** (0.025 mmol, 1.0 eq), tris(*m*-tolyl)boroxine (0.09 mmol, 3.6 eq), (*R*)-TRIP (1.2×10^{-3} mmol, 0.05 eq) and dimethyl fumarate (0.025 mmol, 1.0 eq). Immediately prior to the kinetics experiment, by syringe, toluene-d_8 (1.0 ml) was added to the vial. After all the solid materials were dissolved, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed, tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 108-second intervals.



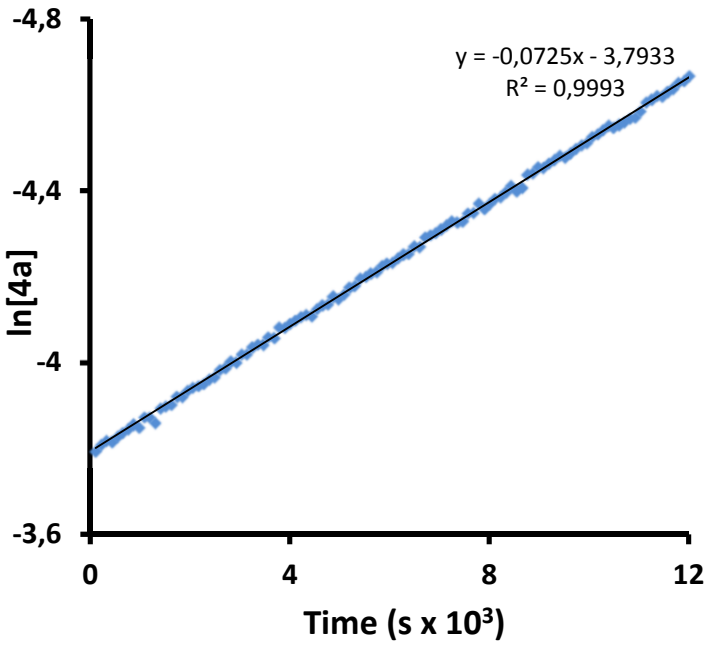


Figure S8. Kinetic plot used to determine a first order dependence on **4a** under saturation of boroxine.

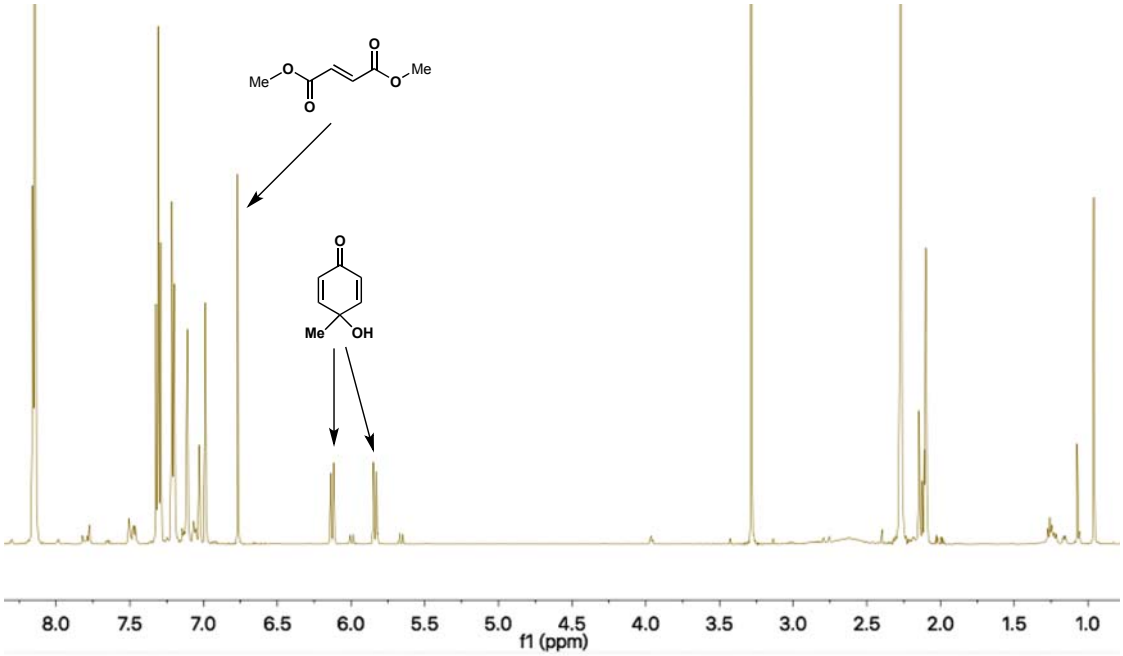


Figure S9. A representative spectrum from the kinetics analysis to determine the order of **4a** under saturation of boroxine.

Procedure to determine rate-catalyst loading relationship

For (*R*)-TRIP

A toluene-d_8 solution of substrate **4a** (0.025 M, 1.0 equiv.), dimethyl fumarate (0.025 M, 1.0 equiv.) and tris(*m*-tolyl)boroxine (0.09 M, 3.6 equiv.) was prepared. To 15 vials was added (*R*)-TRIP (5/10/15/20/25 mol%). 3 replicates were prepared for each catalyst loading. Immediately prior to the kinetics experiment, by syringe, aforementioned solution (1.0 mL) was added to a vial with catalyst. After all the solid materials were dissolved, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed, tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 15-second intervals. All data are recorded under 40% conversion of **4a**. Concentration of **4a** from every experiment was fitted into linear model and initial rates were extracted from the slopes.

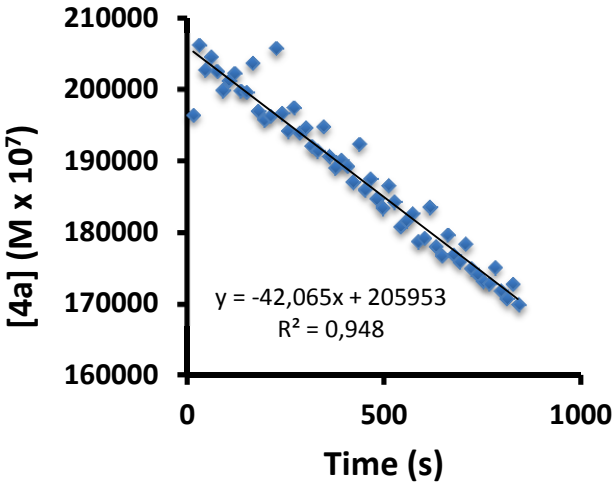


Figure S10. A representative plot of linear fit of concentration of **4a**.

The data acquired is listed below (the unit of rate is M/s * 10^6):

(*R*)-TRIP Load. (mol%)	5	10	15	20	25
Rate1	2.48	3.49	4.65	5.22	4.92
Rate2	2.33	3.87	4.21	4.85	5.26
Rate3	2.45	3.42	4.29	4.6	4.93
Mean Rate	2.42	3.593333333	4.383333333	4.89	5.036666667
Stand. Dev.	0.079372539	0.242143208	0.234378611	0.311929479	0.193476958
Stand. Err.	0.045825757	0.139801447	0.135318554	0.180092569	0.111703974

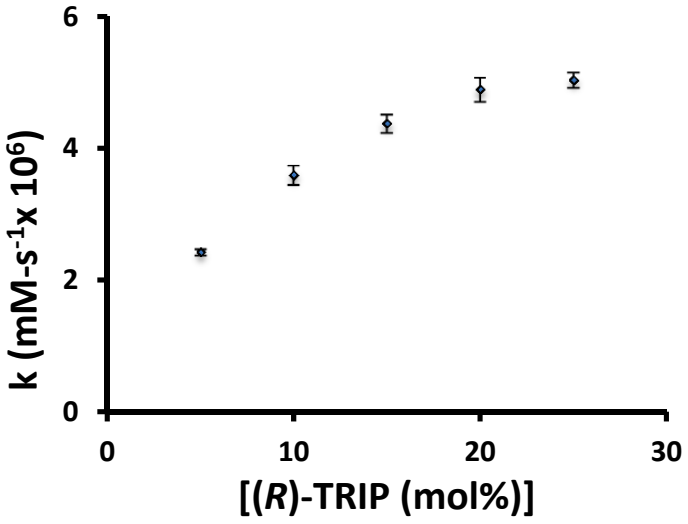


Figure S11. Initial rate-(*R*)-TRIP loading plot.

Procedure to determine reaction order in boroxine

A toluene-d_8 solution of substrate **4a** (0.031 M, 1.0 equiv.) and dimethyl fumarate (0.031 M, 1.0 equiv.) was prepared. To 30 vials was added tris(*m*-tolyl)boroxine 1/2/3/6/9/12/15 mg. 3 parallel replicates were prepared for each boroxine loading. Aforementioned solution (0.8 mL) toluene-d_8 solution was added to each vial. Immediately prior to the kinetics experiment, by syringe, 0.2 mL (*R*)-TRIP (0.00625 M) was added to each vial. After mixing, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed, tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 15-second intervals. All data are recorded under 20% conversion of **4a**. Concentration of **4a** from every experiment was fitted into linear model and initial rates were extracted from the slopes.

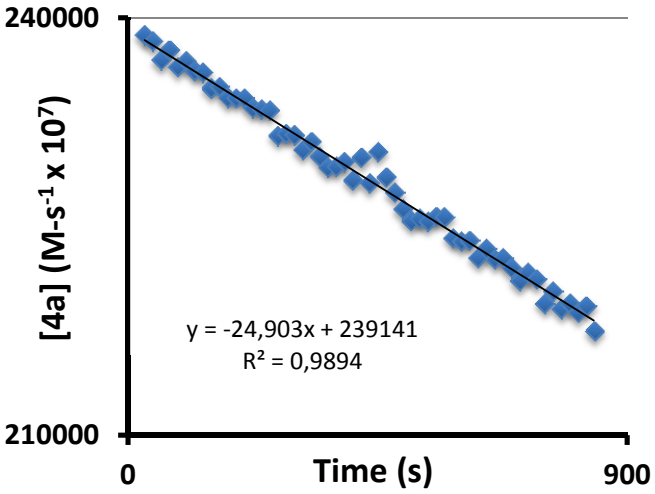


Figure S14. A representative plot of linear fit of concentration of **4a**.

The data acquired is listed below (the unit of rate is M/s * 10^7):

Boroxine Equiv.	0.11	0.22	0.33	0.67	1	1.33	1.67
Rate1	7.6	10.55	13.03	18.19	17.99	22.28	22.36
Rate2	8.6	12.32	13.1	16.66	19.63	22.44	22.77
Rate3	8.4	10.46	14.85	17.2	19.72	20.74	21.79
Mean Rate	8.2	11.11	13.66	17.35	19.1133	21.82	22.3066
Stand. Dev.	0.52915	1.0488	1.0311	0.77595	0.9738	0.93872	0.49217
Stand. Err.	0.30550	0.60555	0.59534	0.44799	0.56226	0.54197	0.28415

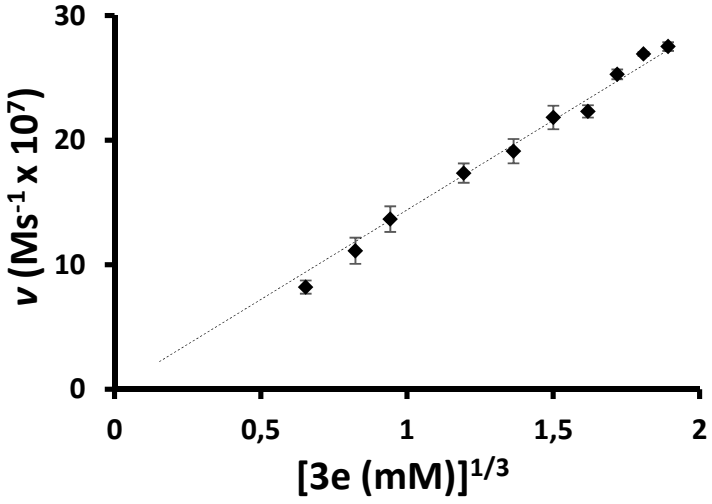
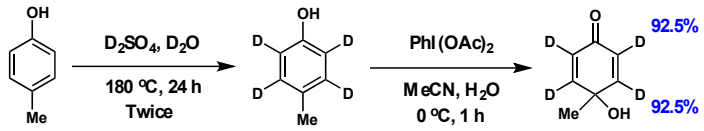


Figure S15. Initial rate-$[\mathbf{3e}]^{1/3}$ loading plot.

Isotope experiments

Preparation of 4a-d_4



2.2 g of *p*-cresol with 4 ml of D_2O and 1 ml of concentrated D_2SO_4 (> 99% D) were heated at 180 °C in a sealed tube for 24 h. After cooling to room temperature, the reaction mixture was extracted with EtOAc and the solvent was removed under reduced pressure. The residue was again heated with 4 ml of D_2O and 1 ml of concentrated D_2SO_4 (> 99% D) at 180 ℃ in a sealed tube for 24 h. After cooling to room temperature, the reaction mixture was extracted with EtOAc and the solvent was removed under reduced pressure. The residue was dissolved in the combined solvent (100 ml H_2O and 35 ml MeCN). The solution was then cooled to 0 ℃, followed by the addition of $PhI(OAc)_2$ (20 mmol, 6.4 g). The reaction mixture was stirred at 0 °C for 1 h. The solution was extracted with 50 ml EtOAc three times and the combined organic layer was dried with anhydrous Na_2SO_4. Yellow residue is obtained by removing the solvent under reduced pressure and was then purified by silica gel chromatography using hexanes/ethyl acetate eluent (4:1). **4a**-d_4 was obtained as light yellow solid (92.5% deuterium incorporation measured by NMR spectra). 1.4 g, 11.3 mmol, 58% yield. 1H NMR (500 MHz, Chloroform-*d*) δ 6.90 (t, *J* = 1.5 Hz, 0.15H), 6.15 (t, *J* = 1.5 Hz, 0.15H), 2.03 (br, 1H), 1.50 (s, 3H).

One-pot intermolecular competition experiment

To a vial, was added substrate **4a** (0.1 mmol, 1.0 eq), deuterated substrate **4a**-d_4 (0.1 mmol, 1.0 eq), tris(*m*-tolyl)boroxine (0.065 mmol, 0.3 eq) and toluene-d_8 (2.0 ml). The reaction mixture was sonicated. Isotope content in starting material was measured by taking ^{1}H-NMR of aforementioned solution. To another vial, was added (*R*)-TRIP (0.005 mmol), dimethyl fumarate (0.025 mmol) and 1 ml aforementioned solution. After all the solid materials were dissolved, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed (298.0 K), tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 108-second intervals.

Using the equation $KIE = \frac{\ln(1-F)}{\ln[(1-F)(R/R_0)]}$ (R/R_0 = ratio of isotope content in reaction mixture relative to the starting material; F = conversion), a KIE of 0.90 ± 0.01 was obtained (average result of the first 50 data points).

Similar procedure was also used to determine a KIE for diphenylphosphate. A KIE of 0.91 ± 0.01 was obtained (average result of the first 5 data points).

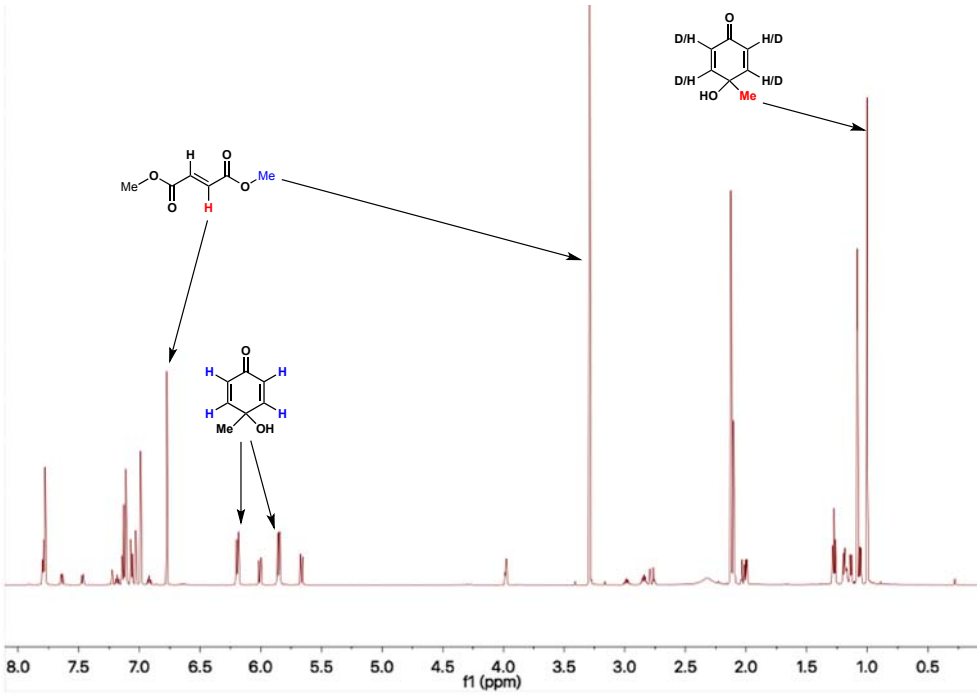


Figure 16. A representative spectrum from the one-pot intermolecular competition experiment to determine the isotope content.

k_H and k_D measurement under saturation of boroxine

To a vial, was added (*R*)-TRIP (0.004 mmol), tris(m-tolyl)boroxine (0.25 mmol) and toluene-d_8 (3.0 ml). The reaction mixture was sonicated. To another 2 vials, each one was added substrate **4a** or substrate **4a**-d_4 (0.025 mmol), dimethyl fumarate (0.025 mmol) and 1 mL aforementioned solution. After all the solid materials were dissolved, the solution was transferred to an NMR tube. The reaction was then placed into the pre-warmed (298.0 K), tuned and shimmed NMR spectrometer, and an automatic kinetics program was used to collect regular time points at 60-second intervals.

A KIE of 0.96, as the ratio of two rate constant k_H and k_D, was acquired.

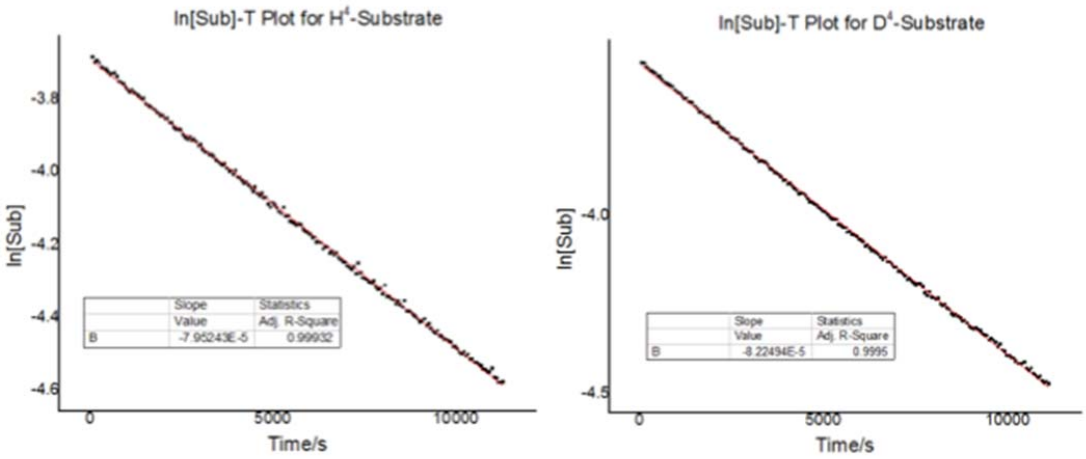


Figure S17. Kinetic plot used to determine k_H and k_D under saturation of boroxine.

DOSY Data of (*R*)-TRIP and Methylated (*R*)-TRIP

Preparation of methylated (*R*)-TRIP:

5 mg of (*R*)-TRIP in DCM (1.0 mL) was added Na_2CO_3 (10 equiv.). Filtered the mixture after being stirred for 30 min. The filtrate was added MeOTf (50 equiv.) and stirred overnight. The mixture was purified by preparation TLC and dissolved in toluene-d_8.

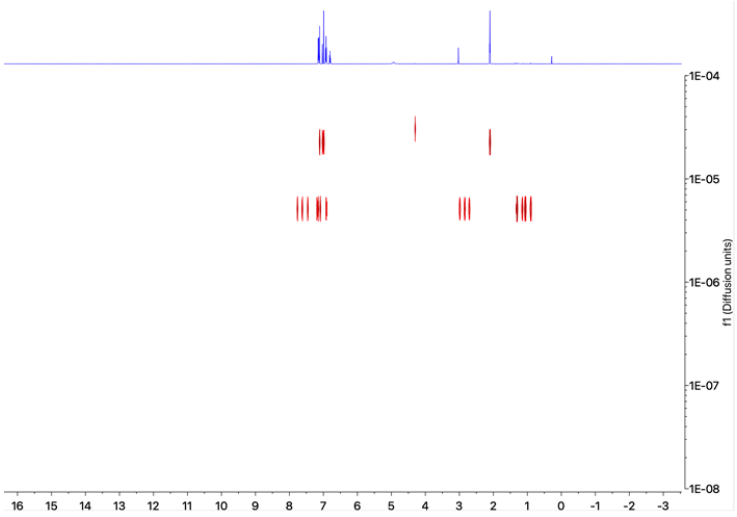


Figure S18. DOSY Data for (*R*)-TRIP.

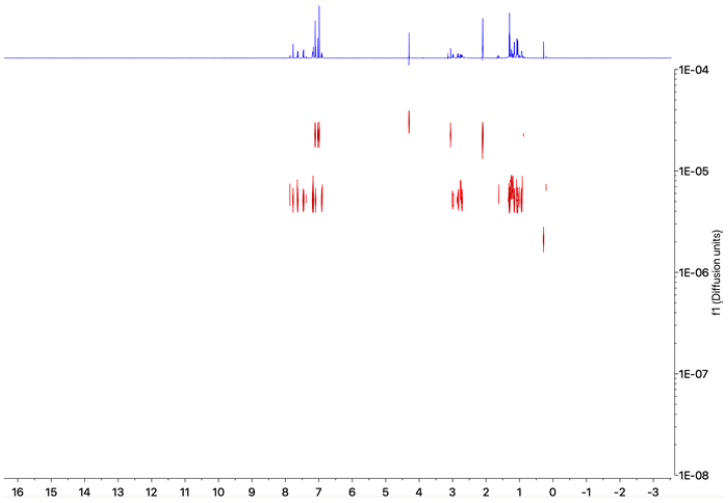
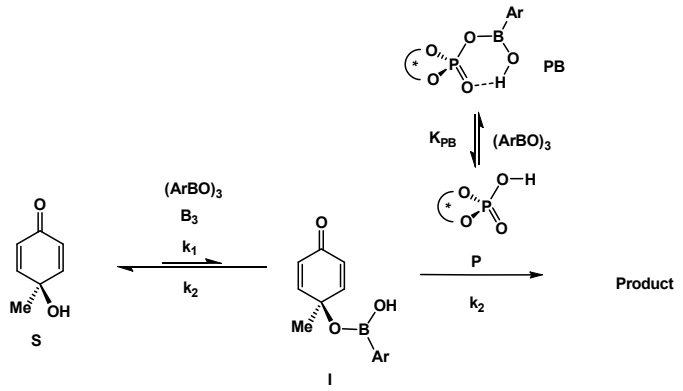


Figure S19. DOSY Data for Methylated (*R*)-TRIP.

Derivation of the Rate Law



Steady State Approximation on [I]

$$\frac{dI}{dt} = 0 = k_1[S][B_3]^{\frac{1}{3}} - k_{-1}[I] - k_2[P][I]$$

$$[I] = \frac{k_1[S][B_3]^{\frac{1}{3}}}{k_{-1} + k_2[P]}$$

$$Rate = k_2[I][P] = \frac{k_2 k_1[S][B_3]^{\frac{1}{3}}[P]}{k_{-1} + k_2[P]} = \frac{k_2 k_1[S][B_3]^{\frac{1}{3}}}{\frac{k_{-1}}{[P]} + k_2}$$

Equilibrium Approximation on P/PB

$$[P]_T = [P] + [PB]$$

$$K_{PB} = \frac{[P][B_3]^{\frac{1}{3}}}{[PB]}$$

$$[PB] = \frac{[P][B_3]^{\frac{1}{3}}}{K_{PB}}$$

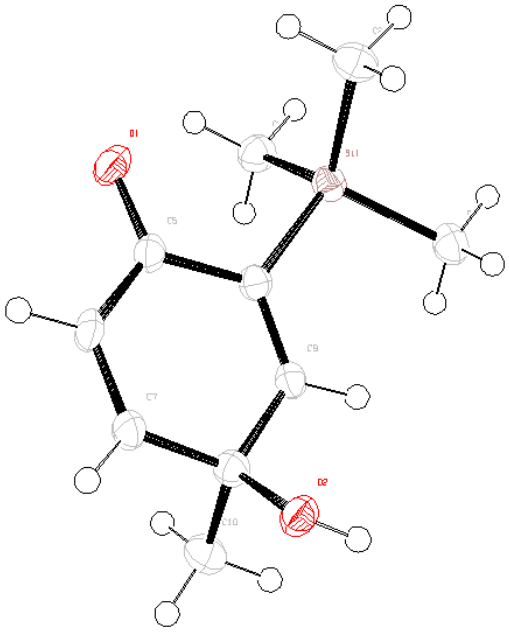
$$[P]_T = [P] + \frac{[P][B_3]^{\frac{1}{3}}}{K_{PB}} = [P]\left(1 + \frac{[B_3]^{\frac{1}{3}}}{K_{PB}}\right)$$

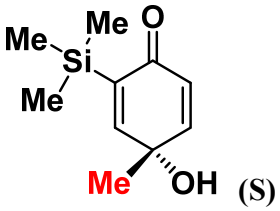
$$[P] = \frac{[P]_T}{1 + \frac{[B_3]^{\frac{1}{3}}}{K_{PB}}}$$

Thus,

$$Rate = \frac{k_2 k_1 [S][B_3]^{\frac{1}{3}}}{\frac{k_{-1}}{[P]} + k_2} = \frac{k_2 k_1 [S][B_3]^{\frac{1}{3}}}{\frac{k_{-1}}{[P]_T}\left(1 + \frac{[B_3]^{\frac{1}{3}}}{K_{PB}}\right) + k_2} = \frac{k_2 k_1 [S][B_3]^{\frac{1}{3}}[P]_T}{k_{-1}\left(1 + \frac{[B_3]^{\frac{1}{3}}}{K_{PB}}\right) + k_2}$$

Single X-ray structure data of enantioenriched 1g





(S)

Table 1. Crystal data and structure refinement for twin4.

Identification code	shelx
Empirical formula	C10 H16 O2 Si
Formula weight	196.32
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 6.8879(3) A alpha = 90 deg.
	b = 7.9921(4) A beta = 92.5410(10) deg.
	c = 10.5019(5) A gamma = 90 deg.
Volume	577.55(5) A^3
Z, Calculated density	2, 1.129 Mg/m^3
Absorption coefficient	0.173 mm^-1

F(000)	212
Crystal size	0.070 x 0.070 x 0.050 mm
Theta range for data collection	1.941 to 25.361 deg.
Limiting indices	-8<=h<=8, -9<=k<=9, -12<=l<=12
Reflections collected / unique	16375 / 16375 [R(int) = ?]
Completeness to theta = 25.000	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16375 / 1 / 124
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.0957
R indices (all data)	R1 = 0.0412, wR2 = 0.0973
Absolute structure parameter	-0.04(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.482 and -0.137 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for twin4. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4899(6)	2565(6)	4156(4)	30(1)
C(2)	1313(6)	1454(6)	2553(4)	29(1)
C(3)	891(6)	3909(6)	4750(4)	29(1)
C(4)	2905(6)	5034(5)	2347(4)	20(1)
C(5)	1216(6)	5763(5)	1634(4)	22(1)
C(6)	1556(6)	7064(5)	681(4)	25(1)
C(7)	3323(5)	7639(5)	501(4)	23(1)
C(8)	5065(6)	7114(6)	1284(4)	22(1)
C(9)	4655(6)	5677(5)	2156(4)	20(1)
C(10)	5836(6)	8601(5)	2079(4)	30(1)
O(1)	-445(4)	5261(4)	1821(3)	31(1)
O(2)	6484(4)	6639(4)	397(3)	25(1)
Si(1)	2467(2)	3223(1)	3457(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for twin4.

C(1)-Si(1)	1.874(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-Si(1)	1.861(5)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-Si(1)	1.858(4)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(9)	1.334(5)
C(4)-C(5)	1.475(5)
C(4)-Si(1)	1.891(4)
C(5)-O(1)	1.236(4)
C(5)-C(6)	1.469(6)
C(6)-C(7)	1.322(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.485(5)
C(7)-H(7)	0.9500
C(8)-O(2)	1.431(4)
C(8)-C(9)	1.504(6)

C(8)-C(10)	1.534(6)
C(9)-H(9)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
O(2)-H(2)	0.8400

Si(1)-C(1)-H(1A)	109.5
Si(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
Si(1)-C(2)-H(2A)	109.5
Si(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
Si(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
Si(1)-C(3)-H(3A)	109.5
Si(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
Si(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(9)-C(4)-C(5)	117.9(4)
C(9)-C(4)-Si(1)	123.9(3)
C(5)-C(4)-Si(1)	118.1(3)
O(1)-C(5)-C(6)	120.9(4)
O(1)-C(5)-C(4)	120.4(4)
C(6)-C(5)-C(4)	118.7(3)
C(7)-C(6)-C(5)	121.3(3)
C(7)-C(6)-H(6)	119.4
C(5)-C(6)-H(6)	119.4
C(6)-C(7)-C(8)	123.3(4)
C(6)-C(7)-H(7)	118.4
C(8)-C(7)-H(7)	118.4
O(2)-C(8)-C(7)	105.9(3)
O(2)-C(8)-C(9)	110.2(3)
C(7)-C(8)-C(9)	112.6(3)
O(2)-C(8)-C(10)	109.3(3)
C(7)-C(8)-C(10)	109.5(4)
C(9)-C(8)-C(10)	109.3(3)
C(4)-C(9)-C(8)	125.6(4)
C(4)-C(9)-H(9)	117.2
C(8)-C(9)-H(9)	117.2
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-O(2)-H(2)	109.5
C(3)-Si(1)-C(2)	110.30(19)
C(3)-Si(1)-C(1)	109.7(2)
C(2)-Si(1)-C(1)	109.9(2)
C(3)-Si(1)-C(4)	109.79(19)
C(2)-Si(1)-C(4)	110.06(19)
C(1)-Si(1)-C(4)	107.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for twin4.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	32(2)	25(2)	31(2)	3(2)	-2(2)	4(2)
C(2)	35(3)	27(2)	26(2)	1(2)	4(2)	-4(2)
C(3)	27(2)	30(3)	30(3)	-3(2)	3(2)	0(2)
C(4)	21(2)	20(2)	20(2)	-1(2)	2(2)	2(2)
C(5)	20(2)	21(2)	25(2)	-2(2)	0(2)	4(2)
C(6)	19(2)	27(2)	29(2)	6(2)	-4(2)	6(2)
C(7)	22(2)	23(2)	25(2)	7(2)	1(2)	3(2)
C(8)	22(2)	22(2)	23(2)	0(2)	2(2)	1(2)
C(9)	22(2)	17(2)	21(2)	-2(2)	-3(2)	3(2)
C(10)	34(2)	23(3)	34(3)	-3(2)	1(2)	-2(2)
O(1)	16(2)	36(2)	40(2)	8(2)	-1(1)	0(1)
O(2)	19(1)	29(2)	27(2)	3(2)	3(1)	2(1)
Si(1)	25(1)	21(1)	22(1)	2(1)	2(1)	1(1)

References

[1] Tobisu, M., Nakai, H., Chatani, N. J. Org. Chem. **2009**, *74*, 5471.
[2] Tello-Aburto, R., Kalstabakken, K. A., Volp, K. A., Harned, A. M. *Org. Biomol. Chem.* **2011**, *9*, 7849.

DFT

Results and Discussion

To further investigate the mechanism of this oxa-Michael reaction, we performed DFT calculations at the B3LYP-D3/def2-TZVPP/SMD(toluene)//B3LYP/6-31G(d) level of theory. The calculations indicate that a complexation of the phosphate catalyst to the boron is unlikely. Instead, the mixed boronic ester intermediate can be activated by the chiral phosphoric acid via a dual activation mode: i) hydrogen bonding between the hydroxyl proton of the mixed boronic ester and the P-O oxygen of the PA ii) and hydrogen bonding between the acidic proton of the PA and the carbonyl oxygen of the cyclohexadienone.

To elucidate the origin of enantioselectivity and particularly to explain the dependence of the observed enantioselectivity on the structure of the achiral boronic acid, we studied the desymmetrization reaction of 4-hydroxy-4-methylcyclohexa-2,5-dien-1-one using R-TRIP/1-Naphthalene boronic acid. Two conformations for the aryl moiety of the boronic acid were found, resulting in the location of a total of four TS structures: **TS(4*S*,5*R*)**, **TS'(4*S*,5*R*)**, **TS(4*R*,5*S*)**, **TS'(4*R*,5*S*)**. The first two lead to the formation of the major enantiomer (4*S*,5*R*) and are the lowest-energy transition states, which is in agreement with the sense of enantioselectivity observed.

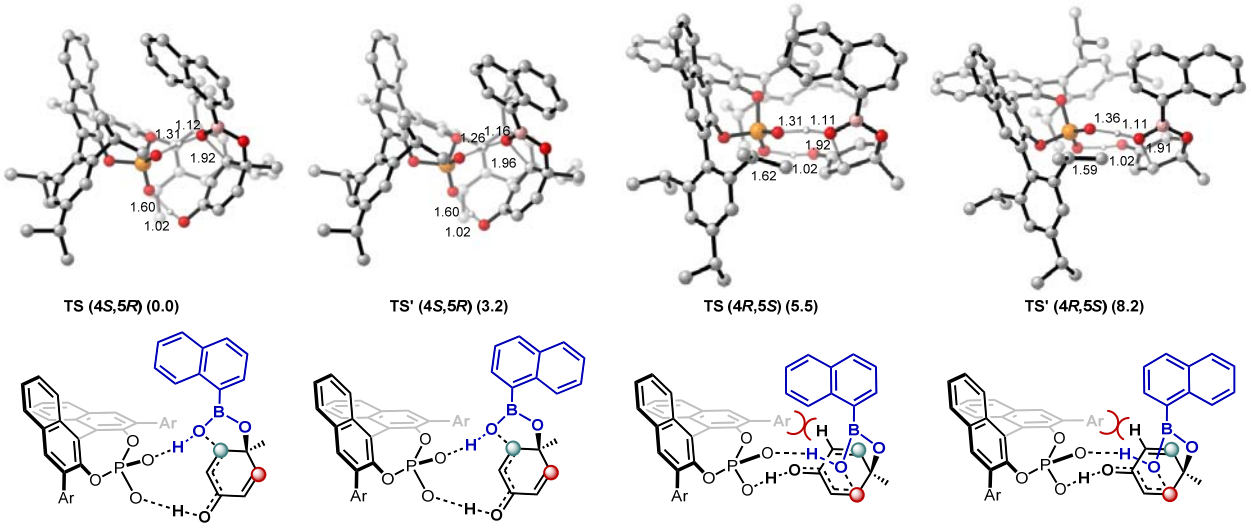


Figure 1. Structures and relative free energies (kcal/mol) computed at B3LYP-D3/def2-TZVPP/SMD(toluene)//B3LYP/6-31G(d) level of theory. Hydrogens attached to carbon atoms are omitted for clarity. Distances are shown for O···H···O hydrogen bond, C···O bond formation

In all the TS structures the cyclohexadienone moiety is located in the chiral pocket of the phosphoric acid, surrounded by the 6,6'-aryl substituents. For the latter two transition states the conformational requirement for the oxa-Michael addition to yield the (4R,5S)-product result in a steric clash between the carbonyl α'-proton and the aryl substituent of the PA (see "quadrant" and Goodman projections). This observation is in

agreement with the fact that bulky groups at the α-position result in higher selectivity.

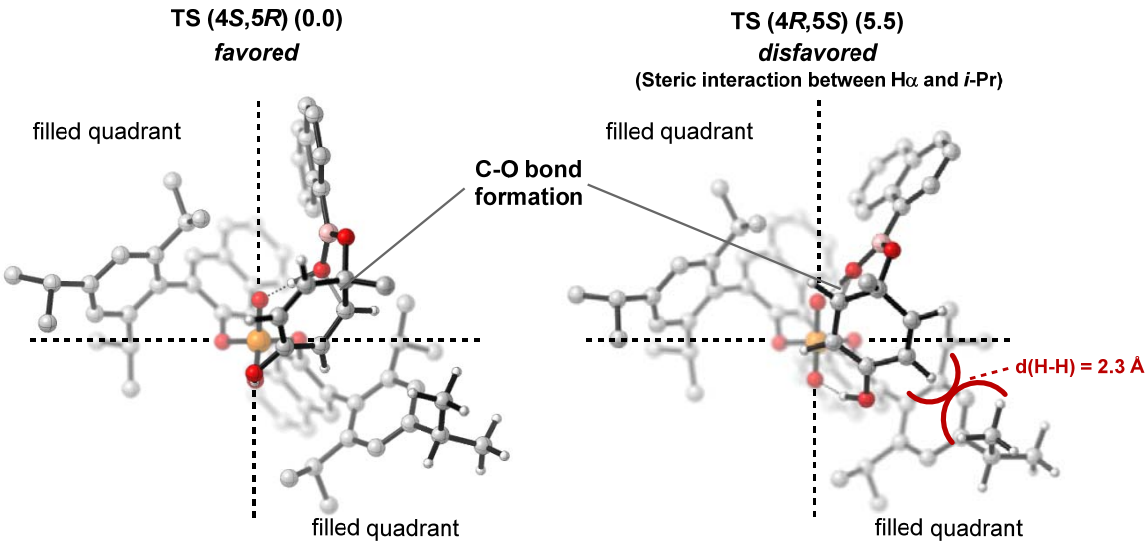


Figure 2. Quadrant projection of TS(4S,5R) and TS(4R,5S). Non-relevant hydrogen atoms are omitted for clarity.

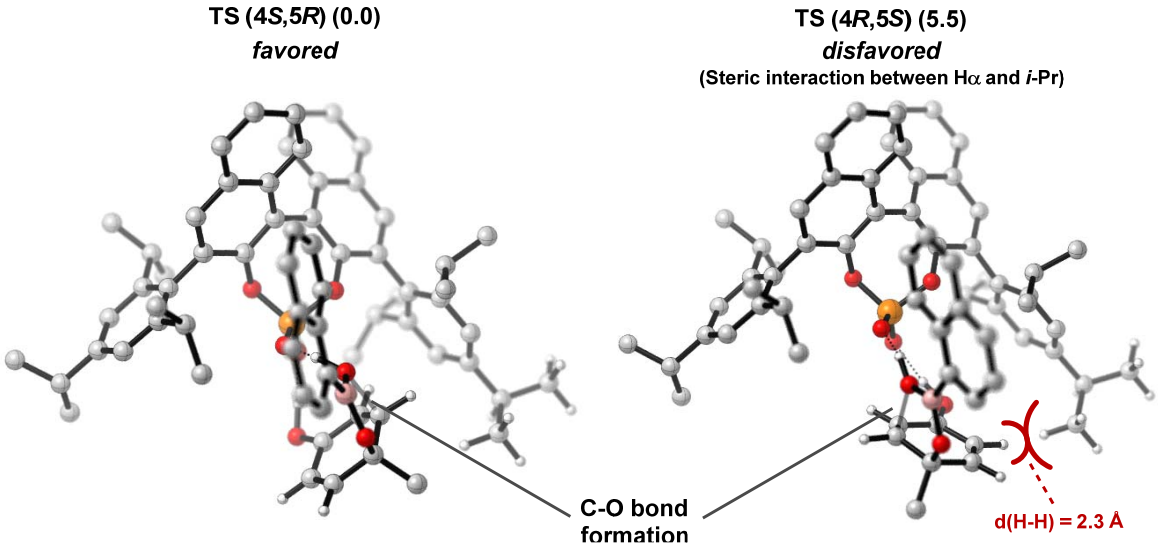


Figure 3. Goodman projection of TS(4S,5R) and TS(4R,5S). Non-relevant hydrogen atoms are omitted for clarity.

For both products, the shorter distance between the naphthyl moiety of the mixed boronic ester and the naphthyl backbone of the PA result in lower energy transition states. The energy difference between the two conformations of the BA is greater for the transition state leading to the formation of the major product (the difference in energies of TS'(4S,5R) and TS (4S,5R) is 3.2 kcal/mol) than the minor product (the difference in energies of TS'(4R,5S) and TS (4R,5S) is 2.7 kcal/mol). Thus, the use of naphthylboronic acid result in greater $\Delta\Delta G^{\ddagger}$.

DFT study shows that TRIP-Naphboronicester adduct is more stable than the two other adducts studied. The higher energy of the latter two adducts is probably due to the steric clash between the 3,3'-substituents of R-TRIP and the Naphtalene rings of the boroxine. Accordingly, the combined energy of the isolated species (*R)*-TRIP and Naphboroxine is lower in energy.

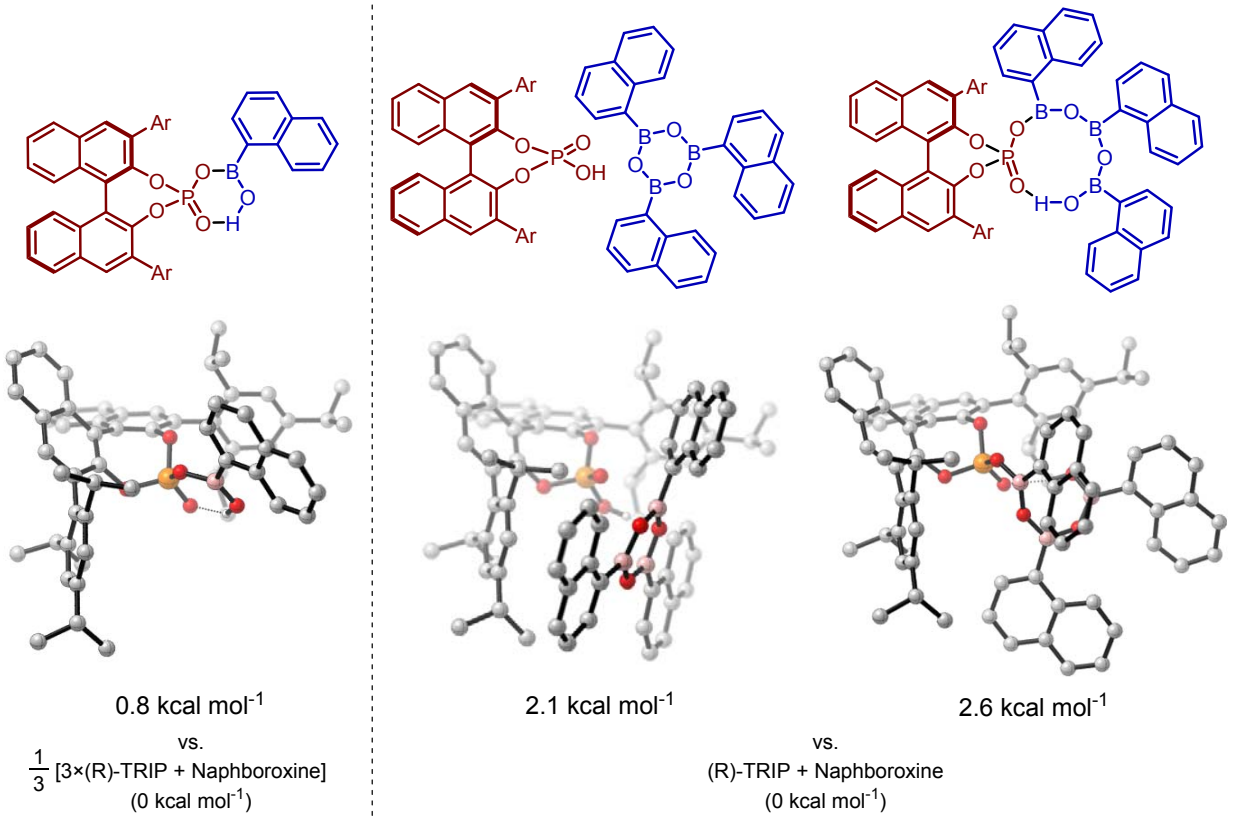
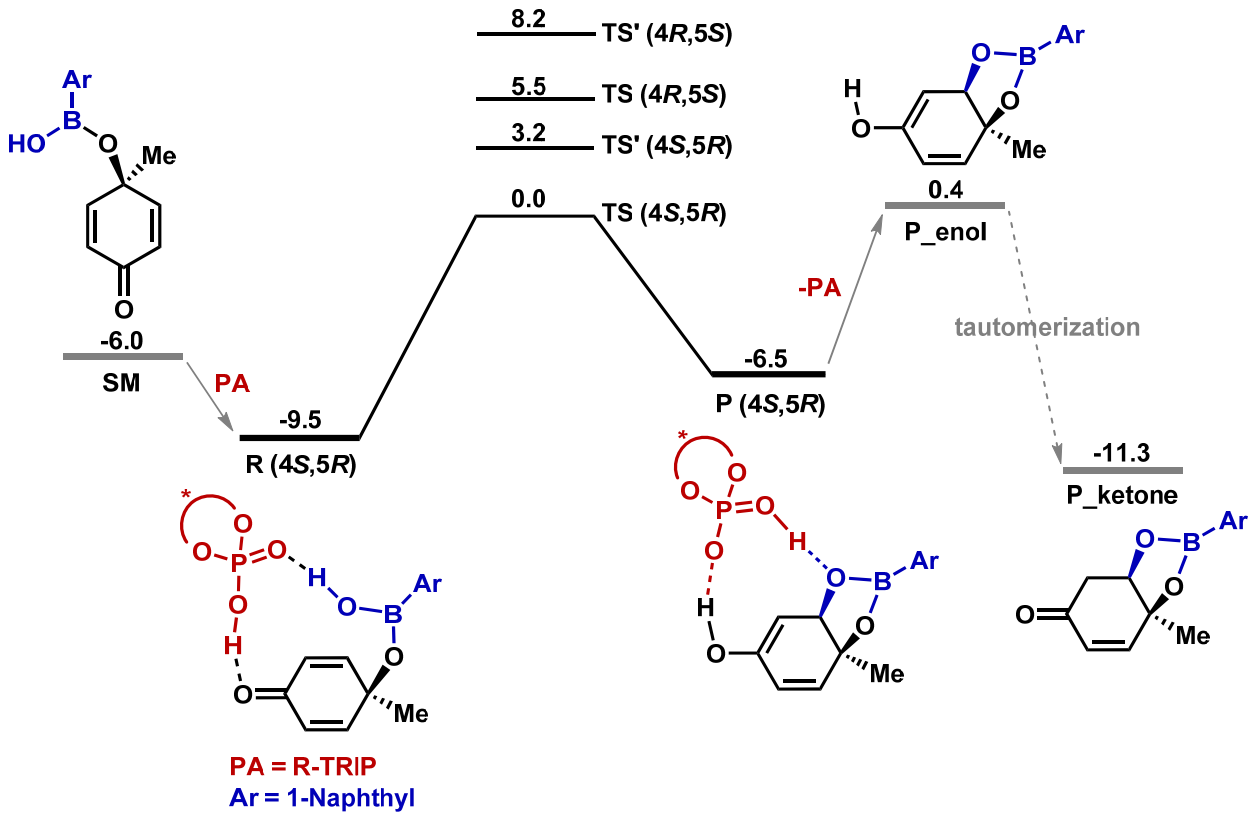


Figure 4. Relative free energies (the minimum is the combined isolated energies of (*R)*-TRIP + Naphboroxine; 0.0 kcal/mol) computed at B3LYP-D3/def2-TZVPP/SMD(toluene)//B3LYP/6-31G(d) level of theory. The energy of the (*R*)-TRIP-Naphboronicester adduct was compared to the energy of isolated 3 × (*R*)-TRIP plus 1 × Naphboroxine. To match the stoichiometry between the two cases, this energy difference (2.4 kcal/mol) was divided by 3 resulting in 0.8 kcal/mol.

Computational Details

Density functional theory (DFT) calculations were performed with Gaussian 09[1] and structural representations were generated with *CYLview*[2]. All the geometry optimizations were carried out at the B3LYP level of theory with the 6-31G(d) basis set. All of the optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition states (a single imaginary frequency corresponding to the desired reaction coordinate). Single-point energy calculations on the optimized geometries were then evaluated using t B3LYP-D3 and the triple-zeta valence quality def2-TZVPP basis set[4], within the SMD[5] model (toluene). Thermal corrections were calculated from the unscaled vibrational

frequencies at the B3LYP/6-31G(d) level on the optimized geometries. Entropic contributions to the reported free energies were calculated from partition functions evaluated using Truhlar's quasiharmonic approximation.[6] This method uses the same approximations as the usual harmonic one except that all vibrational frequencies lower than 100 cm^{-1} are set equal to 100 cm^{-1}.



TS(4*S*,5*R*)

SCF energy: -3491.04731413 Hartree
Free energy correction: 1.125146 Hartree
Quasiharmonic free energy correction: 1.147877 Hartree
Imaginary Frequency: 645.0 *i*cm^{-1}

C	-2.060877000	-2.015622000	1.713575000
C	-3.412537000	-1.667892000	1.777300000
C	-4.443915000	-2.595021000	2.397174000
C	-3.938891000	-4.013211000	2.519815000
C	-2.668295000	-4.358610000	2.263367000
C	-1.713447000	-3.361490000	1.788035000
O	-0.542219000	-3.825354000	1.418880000
C	-4.838758000	-2.063518000	3.788514000
O	-5.632591000	-2.604855000	1.589225000
B	-5.410833000	-2.333738000	0.243606000
O	-4.160927000	-1.851343000	-0.024198000
C	-6.591416000	-2.570482000	-0.754607000
C	-6.657000000	-2.044263000	-2.094996000
C	-7.794990000	-2.358840000	-2.915148000
C	-8.828930000	-3.178494000	-2.390515000
C	-8.758578000	-3.668490000	-1.107513000
C	-7.643154000	-3.358838000	-0.299958000
C	-5.650855000	-1.208517000	-2.656739000
C	-7.872569000	-1.845504000	-4.238290000
C	-6.875037000	-1.046516000	-4.746207000
C	-5.756016000	-0.725085000	-3.943237000
H	-1.326599000	-1.282828000	1.401796000
H	-3.666063000	-0.613318000	1.803583000
H	-4.674292000	-4.750072000	2.832548000
H	-2.316685000	-5.382986000	2.336806000
H	-0.145452000	-3.198835000	0.719732000
H	-3.971774000	-2.023242000	4.454860000
H	-5.264496000	-1.059943000	3.691729000
H	-5.596391000	-2.718599000	4.228181000
H	-9.681572000	-3.410575000	-3.025261000
H	-9.555100000	-4.293333000	-0.712360000
H	-7.603698000	-3.751629000	0.711608000
H	-4.785310000	-0.950140000	-2.059815000
H	-8.741350000	-2.097864000	-4.842396000
H	-6.938688000	-0.662058000	-5.760422000
H	-4.970854000	-0.092527000	-4.347214000
C	-0.587829000	0.448193000	-2.368077000
C	0.030824000	1.465755000	-1.585170000
C	0.823720000	2.380240000	-2.245538000
C	1.079301000	2.291255000	-3.637524000
C	0.449730000	1.258135000	-4.404865000
C	-0.464223000	0.360764000	-3.746966000
C	-1.230628000	-0.666259000	-4.514285000
C	-2.087346000	-0.308296000	-5.613476000
C	-2.661646000	-1.350378000	-6.411052000
C	-2.378767000	-2.704673000	-6.097905000
C	-1.642591000	-3.064825000	-4.988631000
C	-1.125440000	-2.009479000	-4.182947000
O	-0.404178000	-2.367169000	-3.048216000
O	-1.428648000	-0.440097000	-1.710772000
P	-1.036368000	-2.030761000	-1.582894000
O	0.050901000	-2.280372000	-0.576027000
O	-2.392670000	-2.720858000	-1.417420000
C	-0.191400000	1.562857000	-0.103485000
C	-1.404702000	2.101324000	0.390542000
C	-2.502444000	2.614637000	-0.541252000
C	-0.793677000	1.976293000	4.188375000
C	0.822903000	1.163353000	0.797968000
C	0.593075000	1.308140000	2.172953000
C	2.174243000	0.621255000	0.329484000
C	-1.992862000	1.153203000	4.695129000
C	-0.920355000	3.452564000	4.609433000
C	-0.594808000	1.830388000	2.685053000
C	-1.579650000	2.223455000	1.772846000
C	-3.884986000	2.017078000	-0.225076000
C	-2.548763000	4.155990000	-0.532208000
C	3.274811000	1.691056000	0.486277000
C	2.585116000	-0.680014000	1.041846000
C	-2.043887000	-6.733364000	-4.059424000
C	-2.349660000	-5.376281000	-4.225242000
C	-3.760931000	-4.895765000	-3.887481000
C	1.086990000	-4.138004000	-5.511131000
C	-0.780948000	-7.257989000	-4.330861000
C	0.203183000	-6.376522000	-4.785816000
C	-0.495169000	-8.741211000	-4.135041000
C	1.514805000	-4.567420000	-6.928253000
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C	-4.779507000	-5.341008000	-4.956127000
C	-4.215601000	-5.355960000	-2.489485000
C	-0.148956000	-9.438372000	-5.464295000
C	0.603257000	-8.982210000	-3.082482000
C	-3.508161000	-1.009493000	-7.500259000
C	-2.431165000	1.037459000	-5.922297000
C	-3.809621000	0.303621000	-7.780101000
C	-3.272655000	1.334001000	-6.972810000
C	0.789795000	1.151013000	-5.782195000
C	1.966162000	3.197908000	-4.278327000
C	1.667383000	2.035192000	-6.370337000
C	2.253952000	3.079335000	-5.617973000
H	1.288461000	3.184153000	-1.680662000
H	-2.769307000	-3.482527000	-6.748356000
H	-3.343750000	-2.247592000	-0.742539000
H	-2.252041000	2.309583000	-1.561048000
H	0.106531000	1.572846000	4.671762000
H	1.370833000	1.005993000	2.870284000
H	2.091082000	0.385154000	-0.735201000
H	-2.067165000	1.207234000	5.787908000
H	-1.894932000	0.099559000	4.409742000
H	-2.936580000	1.528632000	4.280744000
H	-0.048360000	4.031291000	4.286183000
H	-1.003876000	3.540009000	5.699517000
H	-1.810576000	3.916845000	4.168668000
H	-2.505713000	2.654336000	2.146312000
H	-4.621524000	2.353881000	-0.964171000
H	-4.250621000	2.328359000	0.761293000
H	-3.857138000	0.923086000	-0.252872000
H	-3.306491000	4.523889000	-1.234690000
H	-1.581409000	4.581734000	-0.821265000
H	-2.798476000	4.541307000	0.463775000
H	4.232816000	1.314991000	0.107556000
H	3.413262000	1.961940000	1.540212000
H	3.030808000	2.607727000	-0.061597000
H	3.528610000	-1.049864000	0.622956000
H	1.827699000	-1.453836000	0.899639000
H	2.743170000	-0.531412000	2.116725000
H	-2.818983000	-7.406282000	-3.700372000
H	-3.752151000	-3.802336000	-3.872822000
H	0.719353000	-3.111298000	-5.590986000
H	1.197388000	-6.759286000	-5.003905000
H	-1.419083000	-9.199356000	-3.755569000
H	2.292539000	-3.897032000	-7.314053000
H	0.667790000	-4.541677000	-7.623250000
H	1.920202000	-5.586089000	-6.935330000
H	1.986126000	-3.769997000	-3.554680000
H	3.062039000	-3.427116000	-4.924513000
H	2.747544000	-5.101432000	-4.445818000
H	-5.777105000	-4.953029000	-4.718182000
H	-4.844787000	-6.434971000	-5.008447000
H	-4.505419000	-4.978501000	-5.953121000
H	-5.188308000	-4.912012000	-2.249351000
H	-3.497185000	-5.042945000	-1.726890000

H	-4.329946000	-6.445222000	-2.433142000
H	-0.005250000	-10.515121000	-5.312141000
H	0.776146000	-9.036678000	-5.894624000
H	-0.946715000	-9.300902000	-6.202512000
H	0.748619000	-10.056129000	-2.913111000
H	0.342854000	-8.516519000	-2.125808000
H	1.563855000	-8.563584000	-3.405482000
H	-3.925921000	-1.813274000	-8.101754000
H	-2.032927000	1.838411000	-5.309905000
H	-4.463863000	0.551406000	-8.611509000
H	-3.527561000	2.369619000	-7.181189000
H	0.359278000	0.351449000	-6.373292000
H	2.425459000	3.981943000	-3.680914000
H	1.915701000	1.924812000	-7.422474000
H	2.939247000	3.773895000	-6.095957000

TS'(4*S*,5*R*)

SCF energy: -3491.04304057 Hartree
Free energy correction: 1.125279 Hartree
Quasiharmonic free energy correction: 1.148745 Hartree
Imaginary Frequency: 400.5 *i*cm^{-1}

C	-2.054881000	-2.083531000	1.764108000
C	-3.412082000	-1.747719000	1.850446000
C	-4.426965000	-2.701525000	2.461959000
C	-3.911467000	-4.119849000	2.530157000
C	-2.643201000	-4.446049000	2.241827000
C	-1.699377000	-3.427019000	1.785895000
O	-0.532137000	-3.873109000	1.383916000
C	-4.811538000	-2.214586000	3.869951000
O	-5.628552000	-2.697712000	1.661184000
B	-5.417809000	-2.381059000	0.329854000
O	-4.160691000	-1.878894000	0.088513000
C	-6.505214000	-2.499323000	-0.783306000
C	-7.804204000	-3.107799000	-0.631986000
C	-8.690217000	-3.153770000	-1.762618000
C	-8.273401000	-2.598575000	-3.001512000
C	-7.034713000	-2.016033000	-3.133093000
C	-6.162014000	-1.971117000	-2.024463000
H	-1.331456000	-1.335250000	1.463613000
H	-3.668491000	-0.695929000	1.925676000
H	-4.635725000	-4.872094000	2.831912000
H	-2.283815000	-5.469740000	2.277423000
H	-3.935076000	-2.182550000	4.524212000
H	-5.249926000	-1.213640000	3.808555000
H	-5.553730000	-2.891199000	4.303388000
H	-3.391573000	-2.237790000	-0.641675000
H	-8.957006000	-2.641126000	-3.846770000
H	-6.721332000	-1.590822000	-4.082350000
H	-5.187066000	-1.510135000	-2.151506000
C	-0.657628000	0.456338000	-2.369055000
C	-0.040530000	1.484159000	-1.598040000
C	0.731291000	2.406946000	-2.271216000
C	0.967513000	2.317127000	-3.666690000
C	0.339534000	1.274318000	-4.422480000
C	-0.554049000	0.367324000	-3.749605000
C	-1.319306000	-0.671622000	-4.502537000
C	-2.195336000	-0.328662000	-5.591411000
C	-2.769312000	-1.380972000	-6.375901000
C	-2.466373000	-2.730690000	-6.060607000
C	-1.707953000	-3.076872000	-4.961832000
C	-1.192226000	-2.012188000	-4.167157000
O	-0.451270000	-2.356602000	-3.041945000
O	-1.476293000	-0.437662000	-1.695446000
P	-1.078452000	-2.028461000	-1.570065000
O	0.020894000	-2.270274000	-0.572404000
O	-2.428461000	-2.719991000	-1.391826000
C	-0.242142000	1.572717000	-0.113177000
C	-1.463004000	2.072565000	0.402414000
C	-2.584533000	2.570921000	-0.509248000
C	-0.802676000	1.913696000	4.191177000
C	0.793958000	1.191258000	0.771044000
C	0.577231000	1.312015000	2.150494000
C	2.154286000	0.693044000	0.281216000
C	-1.973446000	1.053072000	4.701966000
C	-0.962006000	3.380478000	4.633819000
C	-0.618732000	1.793057000	2.683680000
C	-1.624668000	2.171299000	1.788162000
C	-3.942580000	1.914313000	-0.203542000
C	-2.687475000	4.108772000	-0.456810000
C	3.232380000	1.780398000	0.469305000
C	2.592836000	-0.623502000	0.948009000
C	-2.025015000	-6.751329000	-4.018281000
C	-2.356567000	-5.399343000	-4.175531000
C	-3.764946000	-4.941028000	-3.798308000
C	1.023751000	-4.105029000	-5.550970000
C	-0.761229000	-7.255179000	-4.323170000
C	0.195995000	-6.357629000	-4.803234000
C	-0.445898000	-8.733468000	-4.135369000
C	1.429086000	-4.532487000	-6.975235000
C	2.246043000	-4.050891000	-4.614700000
C	-0.081701000	-5.000791000	-4.991044000
C	-1.375888000	-4.514725000	-4.679708000
C	-4.805570000	-5.393380000	-4.842318000
C	-4.176224000	-5.413256000	-2.390966000
C	-0.118469000	-9.423934000	-5.472884000
C	0.680527000	-8.955753000	-3.108598000
H	1.195683000	3.217166000	-1.714953000
H	-2.854551000	-3.516181000	-6.703526000
H	-0.150956000	-3.223550000	0.694853000
H	-2.328691000	2.304475000	-1.538397000
H	0.113659000	1.527385000	4.657979000
H	1.372114000	1.023138000	2.834215000
H	2.072821000	0.490769000	-0.790379000
H	-2.037198000	1.093805000	5.796013000
H	-1.849967000	0.005399000	4.404587000
H	-2.931469000	1.407371000	4.301867000
H	-0.109207000	3.985613000	4.307744000
H	-1.033917000	3.451457000	5.725943000
H	-1.869175000	3.827641000	4.210214000
H	-2.557459000	2.572416000	2.177836000
H	-4.698060000	2.256937000	-0.920818000
H	-4.306349000	2.174901000	0.798199000
H	-3.879191000	0.823958000	-0.275562000
H	-3.460199000	4.467449000	-1.147665000
H	-1.737417000	4.578022000	-0.735600000
H	-2.948806000	4.457712000	0.549524000
H	4.195668000	1.439179000	0.071430000
H	3.372719000	2.017243000	1.531158000
H	2.964157000	2.710384000	-0.044136000
H	3.548399000	-0.953722000	0.523175000
H	1.854892000	-1.408955000	0.770305000
H	2.739222000	-0.511138000	2.029004000
H	-2.779021000	-7.436973000	-3.638875000
H	-3.767476000	-3.847447000	-3.777433000
H	0.635120000	-3.085836000	-5.626883000
H	1.190415000	-6.724148000	-5.046934000
H	-1.352844000	-9.207607000	-3.735157000
H	2.184710000	-3.848546000	-7.380626000
H	0.566785000	-4.526588000	-7.651641000
H	1.854540000	-5.542917000	-6.987291000
H	1.956890000	-3.709699000	-3.616143000
H	2.998455000	-3.357429000	-5.010009000
H	2.721890000	-5.033894000	-4.515034000
H	-5.802341000	-5.022460000	-4.574249000
H	-4.856940000	-6.487664000	-4.900201000
H	-4.563209000	-5.020683000	-5.843866000
H	-5.148099000	-4.983093000	-2.123850000
H	-3.442336000	-5.091939000	-1.646858000

H	-4.274421000	-6.504034000	-2.336443000
H	0.046609000	-10.498221000	-5.325093000
H	0.789730000	-9.006620000	-5.923819000
H	-0.935042000	-9.299408000	-6.192607000
H	0.850100000	-10.027025000	-2.945102000
H	0.433194000	-8.496958000	-2.145146000
H	1.625243000	-8.518038000	-3.452391000
C	-8.266025000	-3.674766000	0.589074000
C	-9.971811000	-3.752778000	-1.629891000
C	-10.381237000	-4.290315000	-0.432119000
H	-11.363736000	-4.745645000	-0.341389000
C	-9.515822000	-4.247772000	0.685217000
H	-10.625577000	-3.777276000	-2.498849000
H	-9.841482000	-4.672044000	1.631646000
H	-7.617565000	-3.646976000	1.455509000
C	-3.631206000	-1.054506000	-7.457508000
C	-2.554911000	1.011366000	-5.904759000
C	-3.945640000	0.254088000	-7.743093000
C	-3.408724000	1.293891000	-6.948488000
C	0.661944000	1.167664000	-5.804103000
C	1.834872000	3.232147000	-4.322126000
C	1.521168000	2.060212000	-6.406618000
C	2.105844000	3.113192000	-5.665262000
H	-2.158665000	1.819436000	-5.300607000
H	-3.675144000	2.325887000	-7.160528000
H	-4.611485000	0.490824000	-8.568498000
H	-4.048168000	-1.865618000	-8.049892000
H	0.232451000	0.361780000	-6.387261000
H	1.756234000	1.949681000	-7.461801000
H	2.776499000	3.814270000	-6.154403000
H	2.293188000	4.023064000	-3.733046000

TS(*4R*,*5S*)

SCF energy: -3491.03909333 Hartree
Free energy correction: 1.125540 Hartree
Quasiharmonic free energy correction: 1.148346 Hartree
Imaginary Frequency: 324.0 $i$cm^{-1}

C	-3.030210000	-2.246715000	1.039312000
C	-4.055798000	-1.881993000	1.822374000
C	-4.549503000	-2.723951000	2.975079000
C	-3.865074000	-4.080907000	3.028920000
C	-2.675736000	-4.332480000	2.336120000
C	-2.362363000	-3.529445000	1.246195000
O	-1.488033000	-3.872536000	0.328220000
C	-4.320506000	-1.979687000	4.303118000
O	-5.966511000	-2.909359000	2.819809000
B	-6.329582000	-4.088950000	2.173938000
O	-5.273018000	-4.939419000	2.048038000
C	-7.826485000	-4.253648000	1.750100000
C	-8.420920000	-5.429413000	1.163435000
C	-9.821686000	-5.415244000	0.836758000
C	-10.590185000	-4.250625000	1.096362000
C	-10.012402000	-3.135053000	1.654601000
C	-8.638677000	-3.145851000	1.975094000
C	-3.382242000	-7.720023000	-2.459872000
C	-2.795119000	-7.017917000	-3.552523000
C	-2.504508000	-7.742414000	-4.689973000
C	-2.689121000	-9.145021000	-4.763099000
C	-3.244183000	-9.838858000	-3.640070000
C	-3.669039000	-9.078563000	-2.492478000
C	-4.346674000	-9.748791000	-1.343106000
C	-5.535097000	-10.540400000	-1.519727000
C	-6.017521000	-11.319093000	-0.418430000
C	-5.324498000	-11.279398000	0.818757000
C	-4.252765000	-10.438140000	1.036729000
C	-3.817579000	-9.643388000	-0.064460000
O	-2.756229000	-8.771206000	0.150448000
O	-3.765813000	-6.971456000	-1.357545000
P	-3.079211000	-7.167728000	0.120184000
O	-1.757032000	-6.464162000	0.248105000
O	-4.207860000	-6.875479000	1.102021000
C	-2.467809000	-5.554504000	-3.496342000
C	-3.493626000	-4.581844000	-3.569748000
C	-4.972991000	-4.959424000	-3.642588000
C	-1.437189000	-1.329305000	-3.706677000
C	-1.112791000	-5.147098000	-3.450833000
C	-0.820691000	-3.779030000	-3.513008000
C	0.054322000	-6.131905000	-3.349775000
C	-1.827502000	-0.557679000	-2.432226000
C	-2.023169000	-0.656717000	-4.961575000
C	-1.811507000	-2.803178000	-3.611471000
C	-3.143030000	-3.228886000	-3.622850000
C	-5.781627000	-4.362441000	-2.475740000
C	-5.586797000	-4.567218000	-5.001281000
C	0.932347000	-6.097726000	-4.616440000
C	0.904203000	-5.897554000	-2.085918000
C	-3.540261000	-9.977304000	4.746901000
C	-4.201453000	-9.911059000	3.513631000
C	-5.601809000	-9.298671000	3.475019000
C	-1.493459000	-11.566345000	1.293122000
C	-2.259649000	-10.510476000	4.885399000
C	-1.633618000	-10.995793000	3.734541000
C	-1.579035000	-10.562610000	6.246938000
C	-1.262679000	-13.079007000	1.482339000
C	-0.167307000	-10.831075000	1.021121000
C	-2.247981000	-10.965683000	2.479677000
C	-3.550152000	-10.416887000	2.363453000
C	-6.642140000	-10.225410000	4.135556000
C	-5.647065000	-7.900495000	4.119909000
C	-1.323130000	-12.011155000	6.704763000
C	-0.277898000	-9.738657000	6.272301000
C	-7.695898000	-6.620007000	0.879442000
C	-10.423110000	-6.563859000	0.255105000
C	-9.684698000	-7.694094000	-0.005776000
C	-8.307021000	-7.716965000	0.310224000
C	-7.184222000	-12.114021000	-0.584059000
C	-6.281810000	-10.557832000	-2.730221000
C	-7.873311000	-12.120466000	-1.774879000
C	-7.420982000	-11.322894000	-2.852336000
C	-3.316345000	-11.258596000	-3.708096000
C	-2.295144000	-9.876147000	-5.916431000
C	-2.907866000	-11.940993000	-4.832937000
C	-2.405677000	-11.246149000	-5.957915000
H	-2.701711000	-1.648157000	0.196378000
H	-4.592384000	-0.951392000	1.656207000
H	-4.067380000	-4.656925000	3.926983000
H	-2.150938000	-5.268630000	2.478553000
H	-1.411255000	-4.885778000	0.310522000
H	-3.252943000	-1.819797000	4.483214000
H	-4.824670000	-1.009564000	4.271598000
H	-4.741673000	-2.560570000	5.129700000
H	-4.845563000	-5.805819000	1.511618000
H	-11.648041000	-4.257970000	0.842222000
H	-10.605657000	-2.245729000	1.849819000
H	-8.199106000	-2.256564000	2.415562000
H	-2.080183000	-7.227587000	-5.548227000
H	-5.665877000	-11.921171000	1.626427000
H	-5.051554000	-6.046930000	-3.561823000
H	-0.342851000	-1.281870000	-3.791473000
H	0.219957000	-3.462336000	-3.491254000
H	-0.356629000	-7.141350000	-3.268595000
H	-1.515448000	0.491935000	-2.497866000
H	-1.349784000	-1.002015000	-1.551903000
H	-2.913683000	-0.575245000	-2.277940000
H	-1.722055000	-1.187817000	-5.871040000
H	-1.677127000	0.380937000	-5.041218000
H	-3.119010000	-0.638824000	-4.933566000
H	-3.936177000	-2.488233000	-3.695394000

H	-6.825177000	-4.694990000	-2.523980000
H	-5.781524000	-3.265919000	-2.502428000
H	-5.370917000	-4.682010000	-1.513283000
H	-6.632653000	-4.892582000	-5.058146000
H	-5.040714000	-5.029980000	-5.831048000
H	-5.566819000	-3.481515000	-5.153877000
H	1.730228000	-6.847050000	-4.549179000
H	1.406074000	-5.117869000	-4.750203000
H	0.345916000	-6.307175000	-5.518400000
H	1.725899000	-6.623337000	-2.045755000
H	0.298864000	-6.023009000	-1.183894000
H	1.347881000	-4.894856000	-2.071245000
H	-4.042901000	-9.596818000	5.633302000
H	-5.886765000	-9.170763000	2.427379000
H	-2.111831000	-11.452970000	0.398904000
H	-0.636240000	-11.420922000	3.814247000
H	-2.270350000	-10.107525000	6.969804000
H	-0.771934000	-13.504309000	0.598443000
H	-2.209294000	-13.609780000	1.634643000
H	-0.622510000	-13.284028000	2.348579000
H	-0.340545000	-9.764840000	0.849748000
H	0.321266000	-11.246950000	0.131478000
H	0.531438000	-10.934785000	1.860200000
H	-7.645318000	-9.787441000	4.067525000
H	-6.414635000	-10.382029000	5.197081000
H	-6.670005000	-11.210446000	3.656764000
H	-6.640778000	-7.457539000	3.983479000
H	-4.913003000	-7.238880000	3.652780000
H	-5.447749000	-7.938909000	5.197512000
H	-0.886370000	-12.028428000	7.710777000
H	-0.626697000	-12.523954000	6.030702000
H	-2.253266000	-12.589516000	6.725574000
H	0.163101000	-9.741709000	7.276538000
H	-0.462242000	-8.698410000	5.982427000
H	0.467058000	-10.149318000	5.580533000
H	-6.640857000	-6.677491000	1.106924000
H	-11.484049000	-6.528502000	0.017396000
H	-10.151764000	-8.566458000	-0.454641000
H	-7.720893000	-8.606607000	0.097790000
H	-7.529485000	-12.708978000	0.258214000
H	-5.952263000	-9.945132000	-3.561472000
H	-8.768257000	-12.726413000	-1.887133000
H	-7.979624000	-11.309936000	-3.784314000
H	-3.687428000	-11.812528000	-2.854356000
H	-1.887085000	-9.327460000	-6.762047000
H	-2.966844000	-13.025927000	-4.852652000
H	-2.094469000	-11.796205000	-6.841760000

TS'(4*R*,5*S*)

SCF energy: -3491.03555633 Hartree
Free energy correction: 1.125740 Hartree
Quasiharmonic free energy correction: 1.149160 Hartree
Imaginary Frequency: 224.6 *i*cm^{-1}

C	-2.540909000	-2.211627000	1.028236000
C	-3.448924000	-1.816326000	1.931388000
C	-3.907566000	-2.692511000	3.073283000
C	-3.310566000	-4.093387000	3.004255000
C	-2.221489000	-4.388044000	2.177615000
C	-1.972705000	-3.557065000	1.091116000
O	-1.256829000	-3.923548000	0.055349000
C	-3.544488000	-2.044297000	4.419344000
O	-5.348915000	-2.773598000	3.001475000
B	-5.828238000	-3.888453000	2.329877000
O	-4.849059000	-4.829068000	2.153587000
C	-7.299564000	-4.059185000	1.842987000
C	-8.398546000	-3.195508000	2.198517000
C	-9.698710000	-3.454717000	1.644485000
C	-9.875174000	-4.549026000	0.757053000
C	-8.820508000	-5.366625000	0.427433000
C	-7.542841000	-5.120573000	0.975752000
C	-3.173480000	-7.848102000	-2.745065000
C	-2.478146000	-7.212102000	-3.815327000
C	-2.063437000	-8.006014000	-4.864227000
C	-2.229518000	-9.412821000	-4.860785000
C	-2.898232000	-10.037931000	-3.759484000
C	-3.448845000	-9.208550000	-2.717332000
C	-4.243043000	-9.809036000	-1.605297000
C	-5.391219000	-10.637726000	-1.859765000
C	-5.970300000	-11.370072000	-0.774513000
C	-5.412815000	-11.245351000	0.523257000
C	-4.392551000	-10.360218000	0.805849000
C	-3.860411000	-9.610483000	-0.285332000
O	-2.838237000	-8.714317000	-0.007362000
O	-3.673616000	-7.035941000	-1.738780000
P	-3.105295000	-7.108231000	-0.201162000
O	-1.753251000	-6.463046000	-0.047229000
O	-4.285801000	-6.660970000	0.643110000
C	-2.176521000	-5.743135000	-3.816043000
C	-3.208794000	-4.797402000	-4.026824000
C	-4.663125000	-5.211481000	-4.250934000
C	-1.221378000	-1.500060000	-4.029818000
C	-0.838697000	-5.303656000	-3.667784000
C	-0.570925000	-3.931172000	-3.743408000
C	0.338677000	-6.257294000	-3.447878000
C	-1.703705000	-0.749094000	-2.773925000
C	-1.746353000	-0.828271000	-5.311258000
C	-1.569009000	-2.981564000	-3.957240000
C	-2.882970000	-3.439087000	-4.088871000
C	-5.614872000	-4.590436000	-3.211822000
C	-5.118282000	-4.883880000	-5.687167000
C	1.310930000	-6.228872000	-4.644169000
C	1.082942000	-5.976445000	-2.128540000
C	-4.107396000	-9.717351000	4.546767000
C	-4.635252000	-9.739489000	3.249018000
C	-6.056360000	-9.214965000	3.038447000
C	-1.623174000	-11.333973000	1.406696000
C	-2.822813000	-10.170068000	4.842999000
C	-2.052328000	-10.663896000	3.787212000
C	-2.291012000	-10.129780000	6.269758000
C	-1.367013000	-12.828329000	1.688176000
C	-0.298365000	-10.562520000	1.253443000
C	-2.528569000	-10.718341000	2.474347000
C	-3.837496000	-10.248392000	2.196109000
C	-7.105702000	-10.175849000	3.633242000
C	-6.249059000	-7.799133000	3.611302000
C	-1.988951000	-11.540383000	6.810270000
C	-1.059097000	-9.214247000	6.399285000
C	-8.271594000	-2.093065000	3.089908000
C	-10.792761000	-2.616979000	1.991199000
C	-10.628573000	-1.559091000	2.854357000
C	-9.353222000	-1.299875000	3.407029000
C	-7.093570000	-12.206206000	-1.016578000
C	-6.004277000	-10.740797000	-3.138964000
C	-7.652394000	-12.295417000	-2.270430000
C	-7.106536000	-11.543128000	-3.337003000
C	-2.952322000	-11.459960000	-3.738909000
C	-1.709038000	-10.213225000	-5.913565000
C	-2.420111000	-12.209836000	-4.764731000
C	-1.804918000	-11.584391000	-5.874090000
H	-2.247035000	-1.587429000	0.190689000
H	-3.919109000	-0.838221000	1.872070000
H	-3.455771000	-4.693024000	3.897575000
H	-1.761243000	-5.367556000	2.214911000
H	-1.285011000	-4.941361000	-0.016595000
H	-2.458829000	-1.964225000	4.532906000
H	-3.980721000	-1.042913000	4.476281000
H	-3.947310000	-2.645045000	5.240911000
H	-4.624963000	-5.618255000	1.450524000

H	-10.865100000	-4.729016000	0.343291000
H	-8.960631000	-6.203046000	-0.251431000
H	-6.730922000	-5.785571000	0.695152000
H	-1.554618000	-7.543995000	-5.706487000
H	-5.820210000	-11.856924000	1.323602000
H	-4.730214000	-6.296888000	-4.137613000
H	-0.125135000	-1.429479000	-4.049369000
H	0.456383000	-3.589361000	-3.635761000
H	-0.053766000	-7.274602000	-3.375719000
H	-1.405006000	0.305972000	-2.808218000
H	-1.276041000	-1.199788000	-1.871406000
H	-2.796528000	-0.787918000	-2.687440000
H	-1.386879000	-1.347877000	-6.206080000
H	-1.411925000	0.214823000	-5.364270000
H	-2.842113000	-0.824881000	-5.344622000
H	-3.680474000	-2.720510000	-4.262193000
H	-6.641007000	-4.939424000	-3.380091000
H	-5.625775000	-3.495536000	-3.274615000
H	-5.322430000	-4.873856000	-2.196492000
H	-6.143271000	-5.236417000	-5.855298000
H	-4.467982000	-5.362872000	-6.427791000
H	-5.101307000	-3.804201000	-5.877746000
H	2.116347000	-6.959288000	-4.500524000
H	1.773889000	-5.241948000	-4.762930000
H	0.799385000	-6.468271000	-5.583531000
H	1.925450000	-6.670357000	-2.018192000
H	0.416779000	-6.115872000	-1.272876000
H	1.486514000	-4.957569000	-2.094036000
H	-4.721482000	-9.331514000	5.357497000
H	-6.236182000	-9.148856000	1.962031000
H	-2.137393000	-11.280376000	0.444025000
H	-1.049180000	-11.030617000	3.990877000
H	-3.085194000	-9.701932000	6.897416000
H	-0.764355000	-13.270652000	0.885551000
H	-2.307335000	-13.387175000	1.755211000
H	-0.824951000	-12.973781000	2.630092000
H	-0.483801000	-9.512413000	1.010525000
H	0.302689000	-10.999593000	0.446791000
H	0.301621000	-10.603532000	2.170684000
H	-8.119818000	-9.802572000	3.445211000
H	-6.980770000	-10.273452000	4.718583000
H	-7.029488000	-11.179928000	3.202132000
H	-7.244273000	-7.419270000	3.351947000
H	-5.508064000	-7.107523000	3.203675000
H	-6.168198000	-7.785117000	4.704913000
H	-1.666050000	-11.493981000	7.857517000
H	-1.189157000	-12.023684000	6.236680000
H	-2.874255000	-12.183080000	6.753517000
H	-0.730895000	-9.150183000	7.443881000
H	-1.281225000	-8.200592000	6.047618000
H	-0.217098000	-9.593576000	5.808448000
H	-7.302512000	-1.878142000	3.522360000
H	-11.767696000	-2.832070000	1.559568000
H	-11.472254000	-0.925211000	3.113722000
H	-9.225417000	-0.464925000	4.091362000
H	-7.512891000	-12.764643000	-0.182891000
H	-5.602207000	-10.164325000	-3.964346000
H	-8.516799000	-12.931125000	-2.441829000
H	-7.563414000	-11.595299000	-4.321641000
H	-3.409688000	-11.961148000	-2.894663000
H	-1.216547000	-9.716091000	-6.746035000
H	-2.469085000	-13.294411000	-4.717024000
H	-1.396790000	-12.187444000	-6.680572000

R(4*S*,5*R*)

SCF energy: -3491.06489731 Hartree

Free energy correction: 1.124922 Hartree

Quasiharmonic free energy correction: 1.150333 Hartree

6	-2.169514000	-1.716509000	2.284359000
6	-3.427334000	-1.430978000	2.648377000
6	-4.461898000	-2.479053000	2.989140000
6	-3.888291000	-3.876813000	3.000198000
6	-2.626886000	-4.163432000	2.651879000
6	-1.743956000	-3.113909000	2.119466000
8	-0.700201000	-3.421881000	1.520562000
6	-5.067402000	-2.165663000	4.369664000
8	-5.572899000	-2.410111000	2.064938000
5	-5.423168000	-2.577184000	0.690647000
8	-4.162648000	-2.761561000	0.241735000
6	-6.754969000	-2.584674000	-0.149434000
6	-6.857289000	-2.166068000	-1.523550000
6	-8.107552000	-2.316324000	-2.216502000
6	-9.224306000	-2.860046000	-1.527976000
6	-9.122741000	-3.229762000	-0.207827000
6	-7.891667000	-3.085667000	0.470843000
6	-5.775439000	-1.578040000	-2.239749000
6	-8.210831000	-1.911484000	-3.574804000
6	-7.135355000	-1.365215000	-4.236506000
6	-5.907625000	-1.191193000	-3.556120000
1	-1.457916000	-0.940773000	2.016954000
1	-3.771920000	-0.399830000	2.686309000
1	-4.581803000	-4.663869000	3.291235000
1	-2.242396000	-5.178890000	2.631123000
1	-0.259856000	-2.759934000	0.048552000
1	-4.300614000	-2.193863000	5.150484000
1	-5.525330000	-1.171800000	4.353693000
1	-5.845324000	-2.898236000	4.606817000
1	-10.163857000	-2.972581000	-2.064843000
1	-9.983239000	-3.637859000	0.316109000
1	-7.829820000	-3.386718000	1.512769000
1	-4.828092000	-1.414683000	-1.740263000
1	-9.164738000	-2.037848000	-4.082419000
1	-7.227109000	-1.058860000	-5.275089000
1	-5.062069000	-0.746192000	-4.073542000
6	-0.569271000	0.352846000	-2.465698000
6	-0.014363000	1.334275000	-1.595106000
6	0.809563000	2.285537000	-2.162463000
6	1.163518000	2.266490000	-3.533787000
6	0.601357000	1.265271000	-4.388011000
6	-0.348921000	0.335519000	-3.836421000
6	-1.046473000	-0.652889000	-4.710303000
6	-1.822756000	-0.248557000	-5.851679000
6	-2.319573000	-1.257929000	-6.738293000
6	-2.057619000	-2.623736000	-6.459097000
6	-1.407599000	-3.032427000	-5.312317000
6	-0.943752000	-2.007862000	-4.440264000
8	-0.289736000	-2.397752000	-3.265570000
8	-1.452042000	-0.572012000	-1.908501000
15	-1.124234000	-2.170105000	-1.895169000
8	0.029840000	-2.418824000	-0.848954000
8	-2.388627000	-2.930661000	-1.762926000
6	-0.310839000	1.417981000	-0.123282000
6	-1.523642000	1.998794000	0.318323000
6	-2.637485000	2.396020000	-0.649241000
6	-0.888614000	2.278570000	4.106694000
6	0.677736000	1.048806000	0.820099000
6	0.447615000	1.320408000	2.175506000
6	1.995326000	0.385754000	0.414979000
6	-2.151507000	1.654851000	4.727325000
6	-0.863591000	3.803804000	4.328016000
6	-0.720868000	1.933407000	2.631747000
6	-1.701380000	2.244765000	1.684628000
6	-3.956373000	1.668576000	-0.326770000

6	-2.837239000	3.923435000	-0.690474000
6	3.170284000	1.383224000	0.473198000
6	2.318634000	-0.858187000	1.265086000
6	-1.978011000	-6.707783000	-4.524749000
6	-2.232230000	-5.338659000	-4.674832000
6	-3.652494000	-4.824581000	-4.434347000
6	1.328942000	-4.168073000	-5.648105000
6	-0.712045000	-7.262548000	-4.709973000
6	0.330000000	-6.399708000	-5.059258000
6	-0.483389000	-8.757319000	-4.528038000
6	1.857233000	-4.569090000	-7.039634000
6	2.453258000	-4.200507000	-4.595110000
6	0.134090000	-5.026822000	-5.233422000
6	-1.162986000	-4.489705000	-5.045622000
6	-4.587188000	-5.174493000	-5.610004000
6	-4.248640000	-5.337206000	-3.109809000
6	-0.002158000	-9.429361000	-5.827793000
6	0.481413000	-9.051343000	-3.363732000
6	-3.074461000	-0.872827000	-7.879252000
6	-2.153561000	1.107410000	-6.125429000
6	-3.360722000	0.449992000	-8.124957000
6	-2.904575000	1.445901000	-7.229636000
6	1.039766000	1.221032000	-5.741023000
6	2.082090000	3.209969000	-4.068436000
6	1.946524000	2.137894000	-6.225147000
6	2.465001000	3.153492000	-5.387867000
1	1.219006000	3.069466000	-1.531310000
1	-2.400491000	-3.374113000	-7.165969000
1	-3.919891000	-2.909428000	-0.689560000
1	-2.340975000	2.086738000	-1.655292000
1	-0.022680000	1.856634000	4.634938000
1	1.212890000	1.056309000	2.901524000
1	1.895619000	0.048467000	-0.621143000
1	-2.203063000	1.877275000	5.799785000
1	-2.158440000	0.566591000	4.604068000
1	-3.063283000	2.052702000	4.265407000
1	0.055946000	4.246165000	3.929590000
1	-0.922529000	4.042396000	5.396846000
1	-1.710560000	4.289704000	3.829038000
1	-2.625100000	2.715857000	2.012693000
1	-4.713081000	1.888414000	-1.088842000
1	-4.364495000	1.981434000	0.642143000
1	-3.806837000	0.584517000	-0.298820000
1	-3.612787000	4.189343000	-1.418767000
1	-1.912096000	4.436399000	-0.976376000
1	-3.148139000	4.315066000	0.285346000
1	4.102369000	0.896076000	0.162467000
1	3.313028000	1.762003000	1.492644000
1	3.005802000	2.244541000	-0.182246000
1	3.189734000	-1.376456000	0.848170000
1	1.484131000	-1.564036000	1.284971000
1	2.563056000	-0.592913000	2.300660000
1	-2.797149000	-7.365794000	-4.245217000
1	-3.609344000	-3.734624000	-4.356406000
1	0.995150000	-3.129425000	-5.726557000
1	1.327507000	-6.806142000	-5.207156000
1	-1.454437000	-9.201633000	-4.269669000
1	2.678532000	-3.908415000	-7.343192000
1	1.068694000	-4.502452000	-7.797732000
1	2.238248000	-5.597107000	-7.045242000
1	2.083050000	-3.875758000	-3.617955000
1	3.271899000	-3.533241000	-4.891328000
1	2.871735000	-5.207832000	-4.482710000
1	-5.590021000	-4.767370000	-5.433607000
1	-4.679730000	-6.261024000	-5.729832000
1	-4.219310000	-4.767940000	-6.558585000
1	-5.208786000	-4.843276000	-2.920576000
1	-3.580039000	-5.119311000	-2.273151000
1	-4.436124000	-6.417421000	-3.133693000
1	0.098061000	-10.512745000	-5.689401000
1	0.975670000	-9.042486000	-6.138719000
1	-0.706155000	-9.253483000	-6.648623000
1	0.582339000	-10.132339000	-3.207781000
1	0.123625000	-8.602282000	-2.430974000
1	1.481409000	-8.649099000	-3.564723000
1	-3.434556000	-1.650447000	-8.548505000
1	-1.817548000	1.881311000	-5.444823000
1	-3.945414000	0.731670000	-8.996317000
1	-3.152588000	2.487980000	-7.412011000
1	0.662338000	0.444854000	-6.395855000
1	2.488619000	3.970431000	-3.405967000
1	2.270937000	2.076283000	-7.260341000
1	3.173672000	3.874833000	-5.785181000

P(4*S*,5*R*)

SCF energy: -3491.06382799 Hartree
Free energy correction: 1.130953 Hartree
Quasiharmonic free energy correction: 1.154020 Hartree

6	-2.191087000	-1.926786000	1.645778000
6	-3.647293000	-1.641290000	1.668752000
6	-4.522816000	-2.545103000	2.576106000
6	-3.904590000	-3.899936000	2.834473000
6	-2.619638000	-4.166384000	2.571079000
6	-1.732967000	-3.158057000	1.973668000
8	-0.467106000	-3.582617000	1.783226000
6	-4.901012000	-1.864112000	3.890727000
8	-5.734417000	-2.743622000	1.796193000
5	-5.493768000	-2.406905000	0.486122000
8	-4.231171000	-1.855367000	0.308754000
6	-6.568736000	-2.659589000	-0.613454000
6	-6.555796000	-2.108166000	-1.944239000
6	-7.617410000	-2.446124000	-2.852392000
6	-8.657692000	-3.310368000	-2.419620000
6	-8.663219000	-3.824278000	-1.143994000
6	-7.620632000	-3.494428000	-0.251491000
6	-5.540462000	-1.228636000	-2.414301000
6	-7.612668000	-1.912036000	-4.169712000
6	-6.607262000	-1.072201000	-4.588880000
6	-5.564425000	-0.726992000	-3.697855000
1	-1.528125000	-1.169744000	1.242149000
1	-3.841381000	-0.587415000	1.891571000
1	-4.565512000	-4.649786000	3.262454000
1	-2.183052000	-5.140777000	2.770314000
1	-0.082423000	-3.077969000	1.027590000
1	-4.002095000	-1.640657000	4.474816000
1	-5.435485000	-0.928990000	3.690851000
1	-5.550433000	-2.514092000	4.485419000
1	-9.453320000	-3.557825000	-3.119188000
1	-9.463529000	-4.483849000	-0.819569000
1	-7.638222000	-3.907685000	0.752666000
1	-4.733315000	-0.951856000	-1.747865000
1	-8.424412000	-2.181942000	-4.841756000
1	-6.606019000	-0.673629000	-5.599575000
1	-4.773719000	-0.061421000	-4.031916000
6	-0.581991000	0.421939000	-2.382671000
6	0.024711000	1.434839000	-1.587937000
6	0.819147000	2.352117000	-2.244126000
6	1.086158000	2.266700000	-3.634097000
6	0.463994000	1.235926000	-4.410013000
6	-0.452178000	0.335649000	-3.759873000
6	-1.221218000	-0.682881000	-4.536294000
6	-2.077989000	-0.306135000	-5.629546000
6	-2.659244000	-1.335055000	-6.438685000
6	-2.384299000	-2.694460000	-6.142724000
6	-1.648603000	-3.074907000	-5.039463000
6	-1.124223000	-2.030684000	-4.226243000
8	-0.395725000	-2.413624000	-3.094662000

8	-1.421746000	-0.491384000	-1.737049000
15	-0.948430000	-2.046536000	-1.624071000
8	0.096190000	-2.321076000	-0.607384000
8	-2.338418000	-2.797674000	-1.515288000
6	-0.212808000	1.545823000	-0.108784000
6	-1.409566000	2.137117000	0.363263000
6	-2.492421000	2.650896000	-0.585391000
6	-0.828349000	2.073261000	4.166146000
6	0.778259000	1.122792000	0.808268000
6	0.547079000	1.312383000	2.176698000
6	2.099785000	0.497328000	0.358434000
6	-2.024136000	1.248304000	4.678609000
6	-0.969243000	3.555903000	4.558190000
6	-0.621632000	1.894989000	2.667680000
6	-1.586939000	2.299780000	1.741055000
6	-3.884842000	2.079382000	-0.262083000
6	-2.517842000	4.192336000	-0.608008000
6	3.238176000	1.538880000	0.373747000
6	2.503000000	-0.732770000	1.191885000
6	-2.085966000	-6.750862000	-4.161223000
6	-2.378483000	-5.388904000	-4.308397000
6	-3.785838000	-4.899968000	-3.965903000
6	1.070591000	-4.168189000	-5.580810000
6	-0.828211000	-7.284262000	-4.439939000
6	0.164802000	-6.406574000	-4.882813000
6	-0.557851000	-8.772971000	-4.265686000
6	1.478066000	-4.575796000	-7.010486000
6	2.284299000	-4.176824000	-4.631874000
6	-0.071048000	-5.040123000	-5.056829000
6	-1.359625000	-4.524323000	-4.771108000
6	-4.805601000	-5.308888000	-5.048107000
6	-4.253989000	-5.388215000	-2.581683000
6	-0.221973000	-9.453961000	-5.605965000
6	0.539805000	-9.040512000	-3.218859000
6	-3.504539000	-0.976013000	-7.523177000
6	-2.413159000	1.045525000	-5.921329000
6	-3.797707000	0.342310000	-7.786416000
6	-3.253772000	1.359493000	-6.967185000
6	0.811363000	1.133598000	-5.785622000
6	1.975772000	3.177100000	-4.265933000
6	1.691805000	2.020933000	-6.364391000
6	2.272137000	3.062881000	-5.603970000
1	1.273032000	3.158901000	-1.675319000
1	-2.780376000	-3.461763000	-6.801942000
1	-2.974535000	-2.455309000	-0.830357000
1	-2.242177000	2.321748000	-1.598173000
1	0.072051000	1.686336000	4.662320000
1	1.303996000	0.991319000	2.887477000
1	1.973926000	0.155089000	-0.673409000
1	-2.106781000	1.320698000	5.769747000
1	-1.914476000	0.191547000	4.410642000
1	-2.967292000	1.608336000	4.249674000
1	-0.100800000	4.136636000	4.228587000
1	-1.058278000	3.661884000	5.646080000
1	-1.861870000	4.005098000	4.106699000
1	-2.501987000	2.765526000	2.099092000
1	-4.612425000	2.400779000	-1.016705000
1	-4.252544000	2.423683000	0.712015000
1	-3.870467000	0.984600000	-0.251390000
1	-3.268184000	4.556604000	-1.320244000
1	-1.543775000	4.599339000	-0.901614000
1	-2.765641000	4.600373000	0.379206000
1	4.176716000	1.086517000	0.031234000
1	3.400730000	1.924194000	1.387777000
1	3.019659000	2.393383000	-0.274979000
1	3.375051000	-1.217106000	0.737715000
1	1.695492000	-1.466568000	1.234581000
1	2.780243000	-0.462244000	2.217603000
1	-2.867451000	-7.420731000	-3.810999000
1	-3.766115000	-3.807003000	-3.928335000
1	0.717348000	-3.134690000	-5.637139000
1	1.154636000	-6.796497000	-5.107425000
1	-1.485919000	-9.226376000	-3.890989000
1	2.261666000	-3.909414000	-7.391237000
1	0.624759000	-4.524841000	-7.696300000
1	1.868414000	-5.599831000	-7.040415000
1	1.997092000	-3.855649000	-3.626034000
1	3.060915000	-3.495812000	-5.000873000
1	2.729950000	-5.175634000	-4.555103000
1	-5.798179000	-4.911240000	-4.805690000
1	-4.885663000	-6.400404000	-5.122947000
1	-4.522502000	-4.930043000	-6.036390000
1	-5.212166000	-4.923317000	-2.325387000
1	-3.527136000	-5.126440000	-1.807563000
1	-4.400802000	-6.474555000	-2.558920000
1	-0.090482000	-10.534300000	-5.469784000
1	0.707162000	-9.056857000	-6.031908000
1	-1.019296000	-9.296610000	-6.340690000
1	0.672089000	-10.118175000	-3.063991000
1	0.287126000	-8.584604000	-2.255515000
1	1.504904000	-8.629837000	-3.538651000
1	-3.927152000	-1.769643000	-8.134485000
1	-2.009896000	1.837020000	-5.300159000
1	-4.450838000	0.604441000	-8.614167000
1	-3.502741000	2.398936000	-7.162731000
1	0.384838000	0.336079000	-6.382408000
1	2.430074000	3.959789000	-3.663228000
1	1.947127000	1.915247000	-7.415229000
1	2.959640000	3.759797000	-6.075107000

(*R*)-TRIP

SCF energy: -2583.16295529 Hartree
Free energy correction: 0.864285 Hartree
Quasiharmonic free energy correction: 0.879163 Hartree

C	-0.496826000	0.532580000	-2.664498000
C	0.039503000	1.530345000	-1.800679000
C	0.863887000	2.475554000	-2.375190000
C	1.242502000	2.421083000	-3.740354000
C	0.709039000	1.391057000	-4.580634000
C	-0.251953000	0.472010000	-4.027794000
C	-0.947204000	-0.538236000	-4.878938000
C	-1.688076000	-0.160329000	-6.054142000
C	-2.205917000	-1.189972000	-6.904663000
C	-2.019305000	-2.550179000	-6.550427000
C	-1.411993000	-2.927795000	-5.370497000
C	-0.905356000	-1.883761000	-4.546906000
O	-0.263042000	-2.264140000	-3.360886000
O	-1.388835000	-0.378155000	-2.095064000
P	-1.019638000	-1.950669000	-1.966572000
O	0.261812000	-2.072599000	-0.998973000
O	-2.196534000	-2.739834000	-1.564438000
C	-0.271022000	1.555986000	-0.332485000
C	-1.572357000	1.895836000	0.114433000
C	-2.697506000	2.279750000	-0.846806000
C	-1.144751000	1.702484000	3.933252000
C	0.745533000	1.273866000	0.613583000
C	0.429333000	1.333450000	1.977204000
C	2.185928000	0.936670000	0.220176000
C	-2.169117000	0.627403000	4.343752000
C	-1.601892000	3.101532000	4.387774000
C	-0.845808000	1.656220000	2.440450000
C	-1.829271000	1.934942000	1.487539000
C	-3.948749000	1.399340000	-0.670725000
C	-3.047339000	3.775926000	-0.713631000
C	3.136624000	2.104642000	0.554717000
C	2.698593000	-0.365583000	0.863920000
C	-2.271761000	-6.471656000	-4.300495000

C	-2.422478000	-5.110454000	-4.594539000
C	-3.817307000	-4.492386000	-4.486163000
C	1.243201000	-4.286028000	-5.533502000
C	-1.042386000	-7.125173000	-4.374922000
C	0.069968000	-6.373867000	-4.764376000
C	-0.926883000	-8.607182000	-4.042466000
C	1.762444000	-4.851633000	-6.870357000
C	2.344746000	-4.304820000	-4.456708000
C	-0.020613000	-5.014645000	-5.075773000
C	-1.281344000	-4.374397000	-4.992175000
C	-4.735692000	-4.997464000	-5.617583000
C	-4.466705000	-4.732529000	-3.109743000
C	-0.465844000	-9.434559000	-5.257203000
C	-0.012604000	-8.852788000	-2.827366000
H	1.266061000	3.272857000	-1.756136000
H	-2.396639000	-3.318890000	-7.219389000
H	-0.023698000	-2.376115000	-0.120919000
H	-2.342049000	2.129713000	-1.869872000
H	-0.205053000	1.478176000	4.456660000
H	1.208034000	1.122989000	2.706824000
H	2.218450000	0.785611000	-0.862072000
H	-2.330713000	0.640714000	5.428376000
H	-1.827167000	-0.374516000	4.062003000
H	-3.138335000	0.796300000	3.859917000
H	-0.859387000	3.864603000	4.129890000
H	-1.752907000	3.124213000	5.473655000
H	-2.549735000	3.384422000	3.914953000
H	-2.828989000	2.199919000	1.821875000
H	-4.708008000	1.669679000	-1.414342000
H	-4.400009000	1.528181000	0.320314000
H	-3.707012000	0.340386000	-0.800624000
H	-3.818932000	4.055533000	-1.441177000
H	-2.168648000	4.406562000	-0.890134000
H	-3.430340000	4.010565000	0.286597000
H	4.156304000	1.879632000	0.219412000
H	3.171836000	2.289146000	1.635150000
H	2.818487000	3.035500000	0.072775000
H	3.715994000	-0.579258000	0.515529000
H	2.067769000	-1.215057000	0.588368000
H	2.733932000	-0.301415000	1.957534000
H	-3.145857000	-7.043400000	-3.997845000
H	-3.718510000	-3.409304000	-4.603159000
H	0.989121000	-3.237292000	-5.713395000
H	1.039206000	-6.861510000	-4.836746000
H	-1.933104000	-8.955079000	-3.771313000
H	2.637599000	-4.285862000	-7.212382000
H	0.994160000	-4.795166000	-7.649683000
H	2.061335000	-5.901959000	-6.773474000
H	1.985336000	-3.864504000	-3.521740000
H	3.216172000	-3.730257000	-4.793748000
H	2.684324000	-5.325556000	-4.244302000
H	-5.719003000	-4.515263000	-5.558624000
H	-4.889823000	-6.081103000	-5.548066000
H	-4.314089000	-4.787587000	-6.607296000
H	-5.435763000	-4.220643000	-3.063343000
H	-3.835008000	-4.341394000	-2.308471000
H	-4.651779000	-5.797565000	-2.925073000
H	-0.442495000	-10.503180000	-5.011588000
H	0.542099000	-9.144783000	-5.577270000
H	-1.139095000	-9.294701000	-6.110061000
H	0.010112000	-9.918546000	-2.569328000
H	-0.361605000	-8.295691000	-1.951199000
H	1.017243000	-8.538360000	-3.034375000
C	-2.920306000	-0.831321000	-8.079864000
C	-1.967159000	1.191982000	-6.395309000
C	-3.151847000	0.487762000	-8.392333000
C	-2.681205000	1.506001000	-7.530651000
C	1.184820000	1.307970000	-5.918458000
C	2.168248000	3.354428000	-4.280575000
C	2.098941000	2.215702000	-6.406368000
C	2.586847000	3.260450000	-5.587162000
H	-1.622878000	1.985006000	-5.741930000
H	-2.889523000	2.546765000	-7.763154000
H	-3.706863000	0.749813000	-9.288802000
H	-3.295871000	-1.625842000	-8.720105000
H	0.829203000	0.509115000	-6.558170000
H	2.452260000	2.124328000	-7.429802000
H	3.300999000	3.974867000	-5.987140000
H	2.552821000	4.137494000	-3.631522000

NaphBoroxine

SCF energy: -1457.08021200 Hartree
Free energy correction: 0.382939 Hartree
Quasiharmonic free energy correction: 0.391205 Hartree

C	8.379411000	-2.078170000	-4.064883000
C	7.857077000	-1.619098000	-2.837642000
C	8.221898000	-0.398693000	-2.275987000
C	9.196373000	0.407393000	-2.973471000
C	9.722103000	-0.059013000	-4.227856000
C	9.288488000	-1.306359000	-4.748891000
C	9.688534000	1.648190000	-2.479786000
C	10.617876000	2.383947000	-3.183755000
C	11.116183000	1.925926000	-4.424709000
C	10.675896000	0.725393000	-4.930630000
B	7.510000000	-0.021978000	-0.938780000
O	6.671640000	-0.956018000	-0.346587000
C	7.353420000	3.878984000	3.896675000
C	7.117653000	2.761697000	3.066837000
C	7.273386000	2.812943000	1.685851000
C	7.650062000	4.068436000	1.086477000
C	7.886858000	5.206263000	1.931165000
C	7.737600000	5.074838000	3.337288000
C	7.770297000	4.256226000	-0.319067000
C	8.124376000	5.477026000	-0.852332000
C	8.376695000	6.586371000	-0.012603000
C	8.255357000	6.449727000	1.350690000
B	7.069625000	1.467643000	0.921732000
O	7.651975000	1.202753000	-0.308074000
C	4.257211000	-2.513155000	3.762185000
C	4.982297000	-1.602762000	2.964139000
C	5.178354000	-1.795903000	1.600515000
C	4.583530000	-2.955720000	0.983128000
C	3.843880000	-3.881363000	1.796111000
C	3.705583000	-3.633787000	3.187431000
C	4.664196000	-3.226653000	-0.411653000
C	4.071556000	-4.342792000	-0.961687000
C	3.361970000	-5.258710000	-0.151335000
C	3.250777000	-5.026562000	1.199597000
B	6.073117000	-0.739301000	0.879817000
O	6.319698000	0.468643000	1.513222000
H	8.058939000	-3.036610000	-4.464058000
H	7.144162000	-2.244943000	-2.310721000
H	9.696346000	-1.643349000	-5.699551000
H	9.330965000	2.013999000	-1.527222000
H	10.973102000	3.326687000	-2.775686000
H	11.847239000	2.517278000	-4.969402000
H	11.055748000	0.352449000	-5.879163000
H	7.232597000	3.788091000	4.972709000
H	6.816619000	1.824757000	3.526062000
H	7.926059000	5.943589000	3.964414000
H	7.572420000	3.421965000	-0.980002000
H	8.205691000	5.588745000	-1.930394000
H	8.656592000	7.542767000	-0.445895000
H	8.433578000	7.297122000	2.008905000
H	4.140206000	-2.325447000	4.826048000
H	5.410640000	-0.722960000	3.434503000
H	3.146402000	-4.346478000	3.789910000

H	5.195460000	-2.531497000	-1.048569000
H	4.147838000	-4.520406000	-2.031352000
H	2.902293000	-6.136247000	-0.597876000
H	2.698354000	-5.715277000	1.834904000

(*R*)-TRIP-NaphBoronicester

SCF energy: -3068.86657049 Hartree
Free energy correction: 0.998745 Hartree
Quasiharmonic free energy correction: 1.021065 Hartree

C	0.727878000	0.543831000	-2.697327000
C	0.837353000	1.955793000	-2.559969000
C	0.144539000	2.721753000	-3.474372000
C	-0.584397000	2.147356000	-4.546658000
C	-0.672575000	0.721814000	-4.660706000
C	-0.049812000	-0.093373000	-3.648956000
C	-0.211500000	-1.578363000	-3.639992000
C	-1.518766000	-2.183208000	-3.635665000
C	-1.630156000	-3.595033000	-3.845126000
C	-0.455084000	-4.365514000	-4.033883000
C	0.808861000	-3.824298000	-3.920703000
C	0.887603000	-2.424746000	-3.662635000
O	2.176350000	-1.890649000	-3.546751000
O	1.398497000	-0.248545000	-1.756053000
P	2.688689000	-1.090949000	-2.245798000
O	2.794814000	-2.118146000	-1.034324000
O	3.941022000	-0.355274000	-2.544972000
C	1.650199000	2.588920000	-1.469006000
C	1.180672000	2.561883000	-0.132924000
C	-0.147655000	1.913364000	0.257847000
C	3.948359000	4.520003000	1.683046000
C	2.863798000	3.248200000	-1.777697000
C	3.574370000	3.863130000	-0.738895000
C	3.425960000	3.337693000	-3.197589000
C	4.462003000	3.501298000	2.718522000
C	3.164526000	5.655930000	2.367063000
C	3.136357000	3.846483000	0.584767000
C	1.933910000	3.190105000	0.862085000
C	0.023529000	0.830867000	1.339629000
C	-1.174367000	2.977068000	0.696854000
C	3.305716000	4.772558000	-3.750248000
C	4.880230000	2.838489000	-3.293325000
C	3.496491000	-6.487751000	-3.501169000
C	2.387582000	-5.679254000	-3.219946000
C	1.608937000	-5.939218000	-1.929842000
C	2.442881000	-3.463455000	-6.398287000
C	4.268774000	-6.330677000	-4.650951000
C	3.897878000	-5.324818000	-5.547139000
C	5.467976000	-7.231947000	-4.913705000
C	2.010086000	-4.153595000	-7.707627000
C	3.588096000	-2.464414000	-6.650914000
C	2.797551000	-4.492855000	-5.324217000
C	2.031934000	-4.667575000	-4.143087000
C	0.766162000	-7.227131000	-2.032103000
C	2.523808000	-6.003757000	-0.693226000
C	5.274339000	-8.087744000	-6.180051000
C	6.782966000	-6.432825000	-4.982236000
C	-2.916033000	-4.199816000	-3.860428000
C	-2.711009000	-1.445794000	-3.396224000
C	-4.050812000	-3.453758000	-3.642504000
C	-3.941421000	-2.065430000	-3.394959000
C	-1.342508000	0.183119000	-5.793700000
C	-1.211097000	2.966916000	-5.524052000
C	-1.922664000	1.005357000	-6.734511000
C	-1.871398000	2.411798000	-6.595028000
O	4.937275000	-1.400503000	-0.196585000
C	1.618835000	-3.705970000	2.731364000
C	2.079016000	-3.098649000	1.542693000
C	3.423996000	-2.825447000	1.318455000
C	4.376912000	-3.191816000	2.337043000
C	3.907993000	-3.820662000	3.541083000
C	2.518386000	-4.059812000	3.709064000
C	5.778005000	-2.975443000	2.207855000
C	6.653262000	-3.352382000	3.203453000
C	6.184099000	-3.967903000	4.386989000
C	4.837465000	-4.195815000	4.548141000
B	3.788297000	-2.082305000	-0.004751000
H	0.180560000	3.804483000	-3.389930000
H	-0.556730000	-5.422346000	-4.263272000
H	-0.562972000	1.420116000	-0.625822000
H	4.827228000	4.971325000	1.202342000
H	4.507049000	4.372054000	-0.970622000
H	2.827013000	2.687995000	-3.842179000
H	5.094082000	3.995187000	3.466467000
H	5.051574000	2.712281000	2.239550000
H	3.631773000	3.020244000	3.249205000
H	2.822623000	6.397828000	1.637004000
H	3.792713000	6.167675000	3.106027000
H	2.281707000	5.271758000	2.891912000
H	1.565980000	3.169936000	1.884842000
H	-0.938994000	0.348854000	1.549806000
H	0.392874000	1.252336000	2.281690000
H	0.728751000	0.058618000	1.017060000
H	-2.139117000	2.509367000	0.928648000
H	-1.337346000	3.720465000	-0.091609000
H	-0.837579000	3.511075000	1.593192000
H	3.672982000	4.818823000	-4.782567000
H	3.896183000	5.477530000	-3.152821000
H	2.267677000	5.124389000	-3.743896000
H	5.215855000	2.869772000	-4.337105000
H	4.960202000	1.807423000	-2.940589000
H	5.567182000	3.463889000	-2.710966000
H	3.770348000	-7.267431000	-2.794695000
H	0.918857000	-5.103412000	-1.776544000
H	1.583062000	-2.883723000	-6.052075000
H	4.478110000	-5.187025000	-6.456016000
H	5.545853000	-7.920546000	-4.061158000
H	1.708286000	-3.406873000	-8.452125000
H	1.163724000	-4.829142000	-7.539773000
H	2.826796000	-4.743593000	-8.139824000
H	3.872643000	-1.948769000	-5.728940000
H	3.276935000	-1.709685000	-7.383159000
H	4.478975000	-2.962954000	-7.050599000
H	0.188654000	-7.383229000	-1.112827000
H	1.407499000	-8.104574000	-2.178242000
H	0.062919000	-7.190004000	-2.871034000
H	1.922452000	-6.070717000	0.220345000
H	3.150487000	-5.111710000	-0.613624000
H	3.182106000	-6.879809000	-0.716493000
H	6.121898000	-8.769521000	-6.319555000
H	5.200649000	-7.460909000	-7.076724000
H	4.359803000	-8.687642000	-6.116681000
H	7.638365000	-7.106641000	-5.112311000
H	6.941359000	-5.851819000	-4.067303000
H	6.779852000	-5.732182000	-5.825616000
H	-2.982817000	-5.271168000	-4.033467000
H	-2.645149000	-0.382723000	-3.195282000
H	-5.028181000	-3.928126000	-3.647232000
H	-4.836258000	-1.481844000	-3.196881000
H	-1.384835000	-0.891515000	-5.924126000
H	-1.143478000	4.046488000	-5.414341000
H	-2.420126000	0.567726000	-7.595664000
H	-2.340157000	3.048136000	-7.340439000
H	4.951944000	-0.929332000	-1.058667000
H	0.556501000	-3.890092000	2.867139000
H	1.354059000	-2.832557000	0.779390000
H	2.178593000	-4.530010000	4.629503000
H	6.153279000	-2.497789000	1.311608000

H	7.718134000	-3.173914000	3.077939000
H	6.887019000	-4.258887000	5.163074000
H	4.460771000	-4.670137000	5.451679000

(*R*)-TRIP-NaphBoroxine (bounded)

SCF energy: -4040.26872982 Hartree
Free energy correction: 1.270880 Hartree
Quasiharmonic free energy correction: 1.300029 Hartree

C	0.304604000	0.699345000	-2.806226000
C	0.221830000	2.110415000	-2.641305000
C	-0.536055000	2.795973000	-3.569963000
C	-1.140162000	2.160098000	-4.682973000
C	-1.044632000	0.738491000	-4.817865000
C	-0.364577000	-0.007102000	-3.791865000
C	-0.387996000	-1.498003000	-3.774592000
C	-1.643021000	-2.204809000	-3.775673000
C	-1.635298000	-3.626698000	-3.931629000
C	-0.396266000	-4.303904000	-4.031683000
C	0.817471000	-3.658807000	-3.902702000
C	0.782643000	-2.242088000	-3.746070000
O	2.017600000	-1.580804000	-3.672922000
O	1.063266000	-0.034548000	-1.874867000
P	2.455320000	-0.641056000	-2.433355000
O	2.827430000	-1.594600000	-1.207996000
O	3.499670000	0.330923000	-2.835172000
C	0.875516000	2.849013000	-1.510220000
C	0.349116000	2.739334000	-0.199734000
C	-0.843411000	1.843307000	0.135552000
C	2.541955000	5.257939000	1.709080000
C	1.954698000	3.729035000	-1.766665000
C	2.471185000	4.481130000	-0.704634000
C	2.560429000	3.919628000	-3.158993000
C	3.149376000	4.408525000	2.839980000
C	1.497483000	6.247425000	2.260891000
C	1.966152000	4.397136000	0.592279000
C	0.908048000	3.513371000	0.820686000
C	-0.484838000	0.772446000	1.183080000
C	-2.062844000	2.672307000	0.585116000
C	2.156639000	5.282973000	-3.758017000
C	4.093500000	3.771745000	-3.173070000
C	3.549808000	-6.156712000	-3.048822000
C	2.392877000	-5.376316000	-2.930065000
C	1.492003000	-5.604439000	-1.713503000
C	2.609220000	-3.455366000	-6.284372000
C	4.408504000	-6.068801000	-4.143664000
C	4.082807000	-5.154435000	-5.150466000
C	5.628371000	-6.975724000	-4.244012000
C	2.263060000	-4.307015000	-7.522908000
C	3.723337000	-2.443126000	-6.604045000
C	2.941997000	-4.348477000	-5.087598000
C	2.090320000	-4.450849000	-3.958843000
C	0.810276000	-6.986926000	-1.782729000
C	2.238990000	-5.447118000	-0.377492000
C	5.495857000	-7.972844000	-5.411585000
C	6.944138000	-6.184038000	-4.341964000
C	-2.866192000	-4.336653000	-3.963428000
C	-2.898798000	-1.560404000	-3.596954000
C	-4.063903000	-3.679029000	-3.810111000
C	-4.074138000	-2.278516000	-3.610129000
C	-1.598338000	0.136529000	-5.981284000
C	-1.825458000	2.911784000	-5.675704000
C	-2.237411000	0.895523000	-6.936666000
C	-2.366684000	2.295601000	-6.779525000
C	7.568240000	-2.511443000	-5.084696000
C	6.795357000	-2.129794000	-3.964443000
C	7.376785000	-1.678883000	-2.786301000
C	8.813927000	-1.660100000	-2.694337000
C	9.598366000	-2.066318000	-3.826560000
C	8.940630000	-2.474059000	-5.017669000
C	9.506371000	-1.290065000	-1.508185000
C	10.883286000	-1.300386000	-1.449275000
C	11.649812000	-1.684982000	-2.573893000
C	11.016279000	-2.061905000	-3.735654000
B	6.406144000	-1.133323000	-1.684945000
O	5.168379000	-1.735737000	-1.552660000
C	6.100885000	1.693798000	3.637770000
C	5.690482000	1.357512000	2.326971000
C	6.581841000	1.304676000	1.264082000
C	7.956934000	1.644325000	1.509461000
C	8.373087000	1.999326000	2.837611000
C	7.416757000	2.003692000	3.887526000
C	8.934748000	1.686051000	0.475857000
C	10.241978000	2.034699000	0.738009000
C	10.647982000	2.366794000	2.051997000
C	9.729397000	2.350126000	3.076082000
B	6.004184000	0.827123000	-0.117780000
O	6.729071000	-0.057596000	-0.912267000
C	3.271156000	-2.179063000	3.019825000
C	3.232176000	-1.910910000	1.634383000
C	4.199425000	-2.393751000	0.758657000
C	5.246929000	-3.233114000	1.284406000
C	5.285862000	-3.501854000	2.694588000
C	4.284596000	-2.950904000	3.537499000
C	6.237240000	-3.848130000	0.468048000
C	7.220806000	-4.645303000	1.013169000
C	7.269126000	-4.881614000	2.406214000
C	6.314948000	-4.324646000	3.225587000
B	4.119378000	-1.900079000	-0.717709000
O	4.775528000	1.270131000	-0.485806000
H	-0.651572000	3.870366000	-3.460149000
H	-0.403193000	-5.379006000	-4.187157000
H	-1.142778000	1.312966000	-0.773069000
H	3.356386000	5.850218000	1.270485000
H	3.298428000	5.160134000	-0.895632000
H	2.162041000	3.138463000	-3.812794000
H	3.601164000	5.051922000	3.604867000
H	3.924375000	3.736972000	2.457777000
H	2.383658000	3.795905000	3.331714000
H	1.092656000	6.882992000	1.465458000
H	1.945298000	6.896619000	3.022891000
H	0.656495000	5.719185000	2.726204000
H	0.492752000	3.433763000	1.822502000
H	-1.342496000	0.114050000	1.367371000
H	-0.200828000	1.223834000	2.141059000
H	0.350305000	0.155738000	0.836019000
H	-2.926229000	2.019735000	0.763496000
H	-2.343551000	3.408103000	-0.176754000
H	-1.859202000	3.216764000	1.514518000
H	2.560793000	5.392281000	-4.771830000
H	2.546024000	6.109620000	-3.151573000
H	1.068791000	5.399911000	-3.813500000
H	4.462272000	3.834257000	-4.203794000
H	4.401352000	2.809560000	-2.760139000
H	4.587687000	4.564099000	-2.599183000
H	3.783261000	-6.871764000	-2.263382000
H	0.701460000	-4.849124000	-1.725936000
H	1.714106000	-2.876233000	-6.042189000
H	4.723975000	-5.082395000	-6.025509000
H	5.666084000	-7.562578000	-3.315845000
H	1.966918000	-3.663878000	-8.360450000
H	1.436204000	-4.994472000	-7.312252000
H	3.120540000	-4.907204000	-7.849277000
H	3.933832000	-1.801723000	-5.743009000
H	3.422390000	-1.798558000	-7.438633000
H	4.653988000	-2.943698000	-6.897049000
H	0.126937000	-7.120572000	-0.935489000
H	1.550402000	-7.795095000	-1.746374000

H	0.233903000	-7.111023000	-2.706190000
H	1.545028000	-5.587490000	0.459934000
H	2.678424000	-4.451296000	-0.280879000
H	3.043265000	-6.182807000	-0.264001000
H	6.351228000	-8.658817000	-5.432690000
H	5.462447000	-7.452289000	-6.376195000
H	4.581261000	-8.569375000	-5.322525000
H	7.803628000	-6.865177000	-4.333227000
H	7.052971000	-5.483358000	-3.507998000
H	6.993979000	-5.600469000	-5.268126000
H	-2.839049000	-5.415542000	-4.095389000
H	-2.927758000	-0.489877000	-3.432774000
H	-4.999414000	-4.231140000	-3.827076000
H	-5.018989000	-1.763458000	-3.460096000
H	-1.501420000	-0.933605000	-6.122256000
H	-1.897606000	3.989490000	-5.551677000
H	-2.642171000	0.413985000	-7.822582000
H	-2.880306000	2.880568000	-7.537363000
H	7.070512000	-2.827183000	-5.997371000
H	5.712969000	-2.171758000	-4.040006000
H	9.545351000	-2.763042000	-5.874725000
H	8.936662000	-0.995311000	-0.635635000
H	11.381989000	-1.009665000	-0.528518000
H	12.735105000	-1.687561000	-2.515648000
H	11.593478000	-2.369588000	-4.604918000
H	5.371344000	1.705623000	4.443363000
H	4.645660000	1.118259000	2.151243000
H	7.744510000	2.264902000	4.891584000
H	8.640203000	1.436029000	-0.536947000
H	10.965482000	2.058033000	-0.072711000
H	11.681599000	2.640475000	2.247195000
H	10.027143000	2.613687000	4.088756000
H	2.503233000	-1.769102000	3.669871000
H	2.428369000	-1.292872000	1.245171000
H	4.331169000	-3.158314000	4.604330000
H	6.208015000	-3.703471000	-0.605492000
H	7.964915000	-5.099155000	0.364305000
H	8.052587000	-5.508609000	2.822877000
H	6.329962000	-4.510590000	4.297055000
H	4.441964000	0.966900000	-1.358124000

(*R*)-TRIP-NaphBoroxine (unbounded)

SCF energy: -4040.26976988 Hartree
Free energy correction: 1.268280 Hartree
Quasiharmonic free energy correction: 1.300239 Hartree

C	0.550153000	0.141351000	-2.913823000
C	0.743755000	1.523680000	-2.632858000
C	0.364392000	2.418293000	-3.612465000
C	-0.122087000	1.997621000	-4.875689000
C	-0.310284000	0.600762000	-5.129306000
C	-0.040364000	-0.339877000	-4.072876000
C	-0.381206000	-1.786563000	-4.208752000
C	-1.715870000	-2.209869000	-4.548663000
C	-1.955542000	-3.597007000	-4.811297000
C	-0.897405000	-4.527753000	-4.661093000
C	0.351281000	-4.157546000	-4.206524000
C	0.573865000	-2.767134000	-3.985698000
O	1.863303000	-2.388582000	-3.613244000
O	0.910421000	-0.767680000	-1.912604000
P	2.189579000	-1.727724000	-2.167640000
O	1.880677000	-2.824946000	-1.046420000
O	3.549842000	-1.153734000	-2.160328000
C	1.321750000	2.000704000	-1.333164000
C	0.561986000	1.907930000	-0.141087000
C	-0.852459000	1.328410000	-0.108840000
C	2.949423000	3.521546000	2.407142000
C	2.608928000	2.587955000	-1.304841000
C	3.103154000	3.064742000	-0.083735000
C	3.485863000	2.731258000	-2.549168000
C	3.066764000	2.425036000	3.481946000
C	2.140030000	4.723985000	2.929427000
C	2.375905000	2.982495000	1.103292000
C	1.105992000	2.401083000	1.047668000
C	-0.965709000	0.127465000	0.849026000
C	-1.892758000	2.413538000	0.233945000
C	3.640716000	4.209530000	-2.958198000
C	4.862846000	2.064991000	-2.372989000
C	2.246416000	-7.074924000	-2.675831000
C	1.251658000	-6.109547000	-2.882109000
C	0.024555000	-6.127325000	-1.966941000
C	2.754190000	-4.349251000	-5.985863000
C	3.388725000	-7.161268000	-3.472270000
C	3.520140000	-6.241037000	-4.516629000
C	4.435061000	-8.239947000	-3.222437000
C	2.656989000	-5.152672000	-7.298801000
C	4.071846000	-3.554804000	-5.919154000
C	2.558532000	-5.259771000	-4.773535000
C	1.412949000	-5.184442000	-3.943197000
C	-0.860875000	-7.357206000	-2.255189000
C	0.387233000	-6.069430000	-0.471713000
C	4.530830000	-9.223503000	-4.404703000
C	5.816081000	-7.645493000	-2.888254000
C	-3.259118000	-4.024992000	-5.182269000
C	-2.824471000	-1.320322000	-4.605814000
C	-4.302697000	-3.132367000	-5.254324000
C	-4.081379000	-1.769758000	-4.946199000
C	-0.721006000	0.207912000	-6.433098000
C	-0.405532000	2.938807000	-5.902336000
C	-0.967001000	1.143678000	-7.413544000
C	-0.823173000	2.525166000	-7.145600000
H	0.473853000	3.482978000	-3.424459000
H	-1.092771000	-5.575036000	-4.874797000
H	2.711097000	-3.152907000	-0.638894000
H	-1.098349000	0.964000000	-1.110411000
H	3.965747000	3.877130000	2.191215000
H	4.092543000	3.515950000	-0.056779000
H	2.991915000	2.213006000	-3.375487000
H	3.539223000	2.823739000	4.388314000
H	3.667931000	1.583272000	3.122163000
H	2.082163000	2.034884000	3.766427000
H	2.089198000	5.522113000	2.180659000
H	2.598493000	5.136174000	3.836707000
H	1.112052000	4.433415000	3.177664000
H	0.515222000	2.334114000	1.957980000
H	-1.975095000	-0.299704000	0.805719000
H	-0.776005000	0.420718000	1.888386000
H	-0.251057000	-0.656208000	0.580672000
H	-2.906591000	1.995842000	0.205825000
H	-1.847104000	3.245362000	-0.478000000
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H	4.239027000	4.293297000	-3.873490000
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H	2.668934000	4.681992000	-3.143002000
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H	4.745912000	1.010379000	-2.108055000
H	5.461993000	2.563333000	-1.601475000
H	2.121790000	-7.793186000	-1.868361000
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H	1.940409000	-3.619440000	-6.002456000
H	4.392451000	-6.296882000	-5.163117000
H	4.103551000	-8.813656000	-2.345734000
H	2.745382000	-4.484860000	-8.164266000
H	1.698671000	-5.679110000	-7.371658000
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H	0.989410000	-5.185825000	-0.245141000
H	0.943449000	-6.957989000	-0.149531000
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H	4.879093000	-8.719131000	-5.313864000
H	3.556786000	-9.673725000	-4.625225000
H	6.535326000	-8.441918000	-2.662938000
H	5.764779000	-6.980439000	-2.019044000
H	6.215618000	-7.065685000	-3.728546000
H	-3.417842000	-5.080271000	-5.391036000
H	-2.677761000	-0.274489000	-4.364244000
H	-5.297210000	-3.471650000	-5.530414000
H	-4.912244000	-1.070044000	-4.972801000
H	-0.826307000	-0.846501000	-6.659721000
H	-0.268333000	3.995855000	-5.687732000
H	-1.269168000	0.816231000	-8.404589000
H	-1.028295000	3.253024000	-7.925704000
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C	7.093826000	-1.177749000	-3.049540000
C	7.987295000	-0.437723000	-2.283383000
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C	9.544917000	-0.452014000	-4.214903000
C	8.581128000	-1.191442000	-4.951103000
C	10.250360000	0.658226000	-2.152474000
C	11.453054000	0.986839000	-2.739944000
C	11.730630000	0.609916000	-4.074474000
C	10.793601000	-0.096672000	-4.792230000
B	7.508417000	-0.023094000	-0.859526000
O	6.681793000	-0.870557000	-0.140818000
C	7.313044000	4.422475000	3.538633000
C	7.128636000	3.210147000	2.840747000
C	7.602094000	3.009743000	1.547051000
C	8.299029000	4.096583000	0.899597000
C	8.485465000	5.331363000	1.612903000
C	7.981025000	5.460856000	2.933507000
C	8.813648000	4.022497000	-0.426128000
C	9.470668000	5.089504000	-1.000791000
C	9.654717000	6.297298000	-0.289819000
C	9.168399000	6.411370000	0.991356000
B	7.331675000	1.601205000	0.928893000
O	7.848238000	1.191618000	-0.287793000
C	4.698830000	-2.011886000	4.334453000
C	5.319560000	-1.183253000	3.375297000
C	5.457431000	-1.553063000	2.041490000
C	4.928974000	-2.831062000	1.634316000
C	4.304225000	-3.678079000	2.612453000
C	4.204793000	-3.238182000	3.958832000
C	4.985408000	-3.307271000	0.291250000
C	4.470763000	-4.543184000	-0.053804000
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C	3.789043000	-4.945423000	2.225420000
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H	6.127628000	-1.448423000	-2.632514000
H	8.813036000	-1.472400000	-5.976386000
H	10.057782000	0.955679000	-1.128284000
H	12.196745000	1.539011000	-2.171225000
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H	6.928773000	4.528805000	4.549510000
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H	8.132685000	6.401619000	3.458586000
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H	9.297207000	7.334582000	1.552009000
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H	5.714891000	-0.223853000	3.693313000
H	3.728511000	-3.891095000	4.686898000
H	5.448420000	-2.687329000	-0.464577000
H	4.537386000	-4.887807000	-1.083187000
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SM

SCF energy: -907.866633037 Hartree
Free energy correction: 0.236897 Hartree
Quasiharmonic free energy correction: 0.241415 Hartree

6	-1.523960000	-2.820256000	3.256058000
6	-2.624644000	-2.058657000	3.350264000
6	-4.022663000	-2.628416000	3.445228000
6	-4.062377000	-4.110482000	3.149785000
6	-2.965378000	-4.875638000	3.056180000
6	-1.602556000	-4.300581000	3.161295000
8	-0.596915000	-4.999962000	3.142018000
6	-4.556281000	-2.390448000	4.876621000
8	-4.931202000	-1.917982000	2.589828000
5	-4.833645000	-1.793911000	1.212274000
8	-3.774205000	-2.290697000	0.501692000
6	-6.027878000	-1.052830000	0.508065000
6	-6.052861000	-0.633486000	-0.872881000
6	-7.222212000	0.030081000	-1.383906000
6	-8.330056000	0.258299000	-0.526230000
6	-8.294933000	-0.143146000	0.787711000
6	-7.146263000	-0.790279000	1.291558000
6	-4.967441000	-0.832307000	-1.773838000
6	-7.259211000	0.453462000	-2.739975000
6	-6.189815000	0.240883000	-3.577588000
6	-5.035087000	-0.408301000	-3.083442000
1	-0.524974000	-2.393227000	3.239425000
1	-2.558725000	-0.973817000	3.413796000
1	-5.059521000	-4.537700000	3.060777000
1	-3.020436000	-5.947625000	2.888776000
1	-3.927439000	-2.893195000	5.616457000
1	-4.573905000	-1.316317000	5.085753000
1	-5.578972000	-2.772920000	4.952493000
1	-3.085996000	-2.694480000	1.050723000
1	-9.207450000	0.759101000	-0.930170000
1	-9.145077000	0.034794000	1.441097000
1	-7.136326000	-1.095945000	2.333052000
1	-4.076667000	-1.331095000	-1.415663000
1	-8.155030000	0.952887000	-3.102577000
1	-6.228422000	0.569197000	-4.612901000
1	-4.189316000	-0.575465000	-3.745689000

P_enol

SCF energy: -907.859592679 Hartree
Free energy correction: 0.241503 Hartree
Quasiharmonic free energy correction: 0.244578 Hartree

6	-2.235315000	-1.916244000	1.522761000
6	-3.701417000	-1.645682000	1.642684000
6	-4.511544000	-2.631706000	2.548546000
6	-3.815103000	-3.949237000	2.795118000
6	-2.517973000	-4.142192000	2.533473000
6	-1.703966000	-3.083200000	1.930267000
8	-0.385787000	-3.420985000	1.830313000
6	-4.919567000	-1.991328000	3.876585000
8	-5.707198000	-2.901959000	1.777075000
5	-5.539426000	-2.407241000	0.498928000
8	-4.361044000	-1.718148000	0.346152000

6	-6.626413000	-2.639078000	-0.595792000
6	-6.570586000	-2.126065000	-1.940262000
6	-7.648720000	-2.413137000	-2.845654000
6	-8.745317000	-3.196638000	-2.398533000
6	-8.786583000	-3.682007000	-1.112477000
6	-7.727960000	-3.399709000	-0.221967000
6	-5.488799000	-1.338732000	-2.426972000
6	-7.603628000	-1.910497000	-4.174118000
6	-6.541153000	-1.152281000	-4.607425000
6	-5.475888000	-0.866824000	-3.721604000
1	-1.623889000	-1.156258000	1.040792000
1	-3.858385000	-0.620128000	2.001787000
1	-4.432487000	-4.739617000	3.214522000
1	-2.022510000	-5.086712000	2.738326000
1	0.090137000	-2.701031000	1.385243000
1	-4.031705000	-1.727634000	4.461771000
1	-5.503500000	-1.082917000	3.690922000
1	-5.531767000	-2.681668000	4.465512000
1	-9.554082000	-3.406375000	-3.095486000
1	-9.628988000	-4.281518000	-0.777624000
1	-7.774986000	-3.789790000	0.790703000
1	-4.665977000	-1.114338000	-1.759048000
1	-8.429684000	-2.138766000	-4.844184000
1	-6.516836000	-0.772963000	-5.625642000
1	-4.637161000	-0.268025000	-4.067788000

P_ketone

SCF energy: -3491.06382799 Hartree
Free energy correction: 0.241886 Hartree
Quasiharmonic free energy correction: 0.244983 Hartree

6	-2.288202000	-1.645952000	1.765731000
6	-3.805714000	-1.511182000	1.789895000
6	-4.556796000	-2.559419000	2.653127000
6	-3.852413000	-3.897373000	2.693191000
6	-2.625405000	-4.136542000	2.208108000
6	-1.780417000	-3.075037000	1.619633000
8	-0.706556000	-3.324661000	1.096904000
6	-4.912374000	-2.065901000	4.052934000
8	-5.779770000	-2.776145000	1.902388000
5	-5.563288000	-2.349431000	0.602715000
8	-4.357549000	-1.691498000	0.471665000
6	-6.608666000	-2.611430000	-0.518377000
6	-6.497179000	-2.154462000	-1.879971000
6	-7.548151000	-2.463504000	-2.809465000
6	-8.671992000	-3.211137000	-2.368677000
6	-8.766313000	-3.642980000	-1.066252000
6	-7.734425000	-3.340734000	-0.151998000
6	-5.386861000	-1.404841000	-2.360819000
6	-7.449485000	-2.018953000	-4.155510000
6	-6.360106000	-1.296392000	-4.582839000
6	-5.321501000	-0.989371000	-3.673139000
1	-1.863515000	-1.033493000	0.965464000
1	-4.076489000	-0.499929000	2.122336000
1	-4.448217000	-4.708341000	3.109549000
1	-2.196149000	-5.135139000	2.213179000
1	-4.007058000	-1.849432000	4.631060000
1	-5.516954000	-1.155578000	3.987067000
1	-5.489861000	-2.823978000	4.591287000
1	-9.459488000	-3.437606000	-3.084396000
1	-9.629395000	-4.215570000	-0.737469000
1	-7.822560000	-3.689049000	0.873136000
1	-4.582640000	-1.163129000	-1.676675000
1	-8.255446000	-2.263508000	-4.843887000
1	-6.293874000	-0.961959000	-5.614705000
1	-4.461097000	-0.419587000	-4.014539000
1	-1.886103000	-1.258073000	2.713363000

References for DFT

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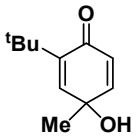
Spectral Data



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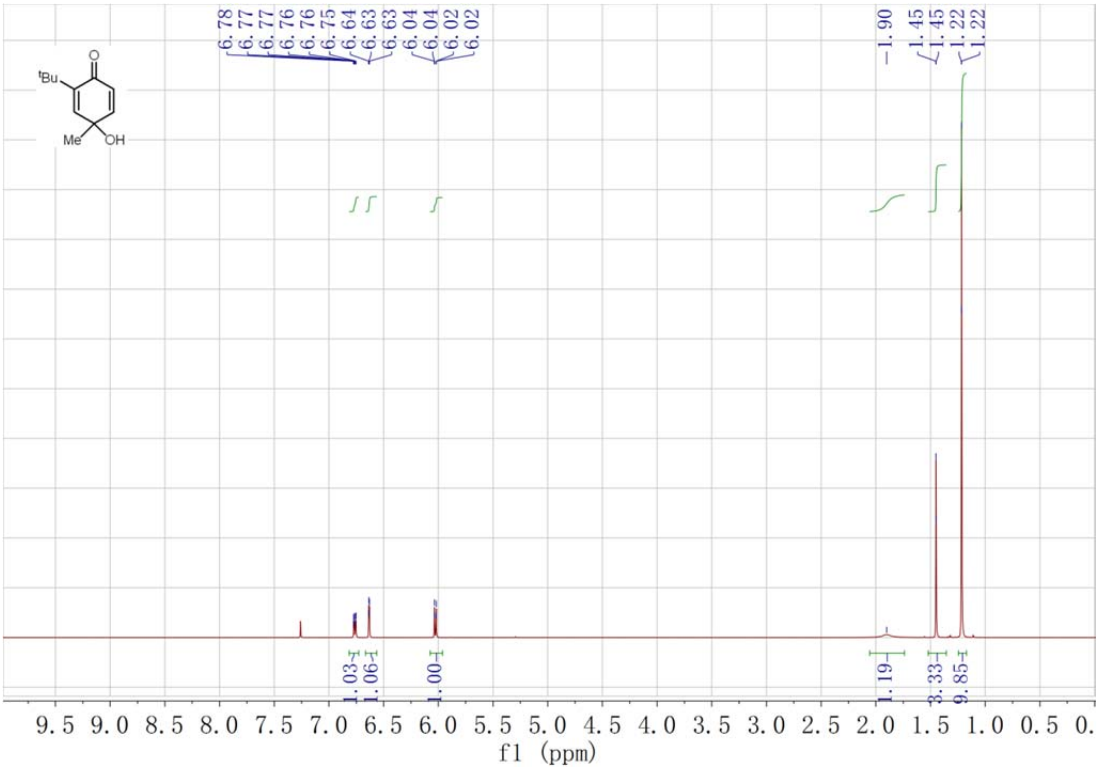

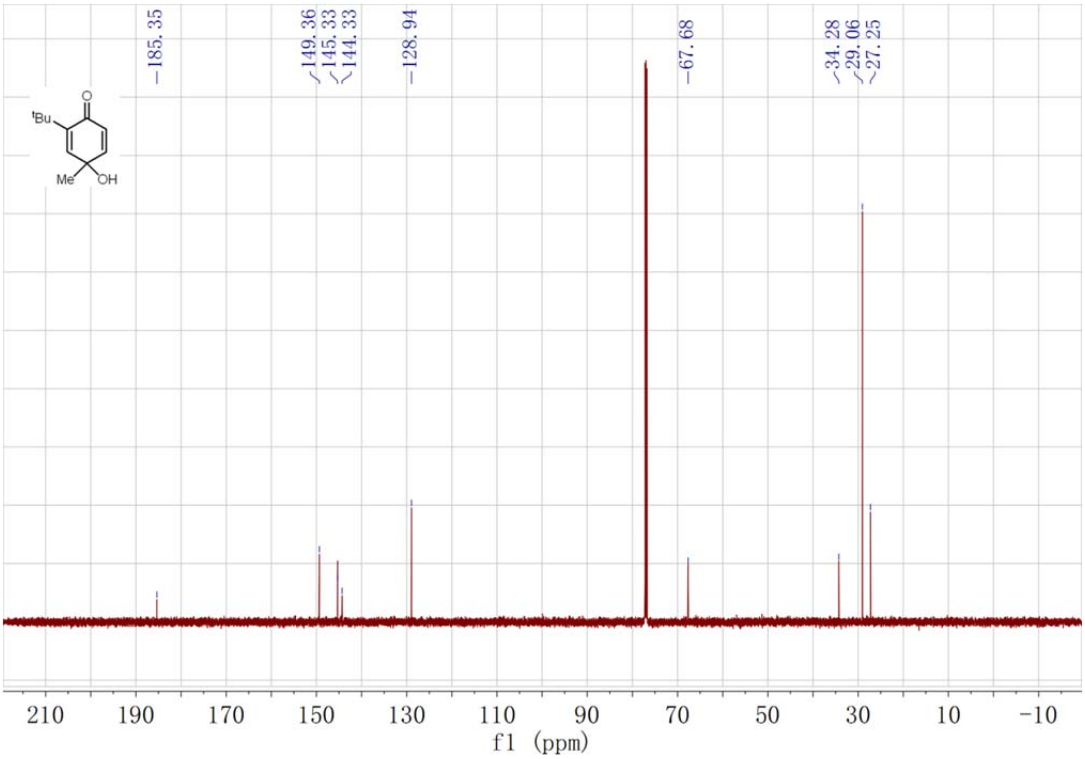

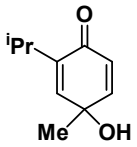
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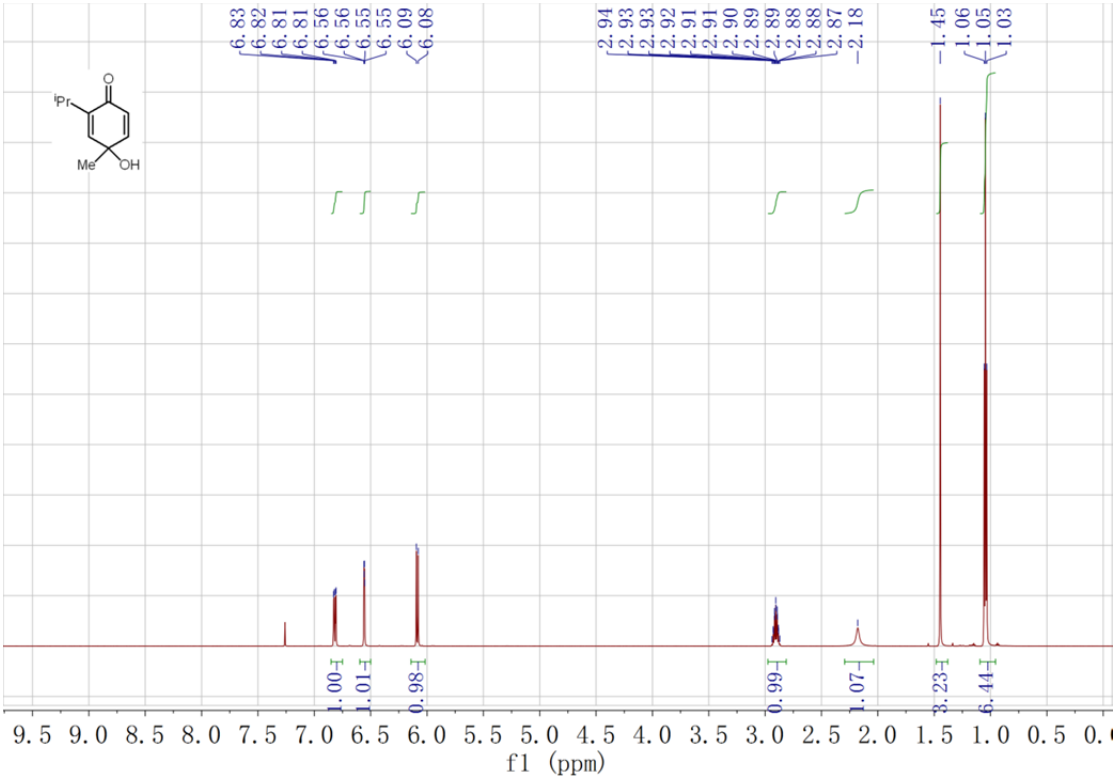
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2.87
2.18
1.45
1.06
1.05
1.03
1.00
1.01
0.98
0.99
1.07
3.23
6.44
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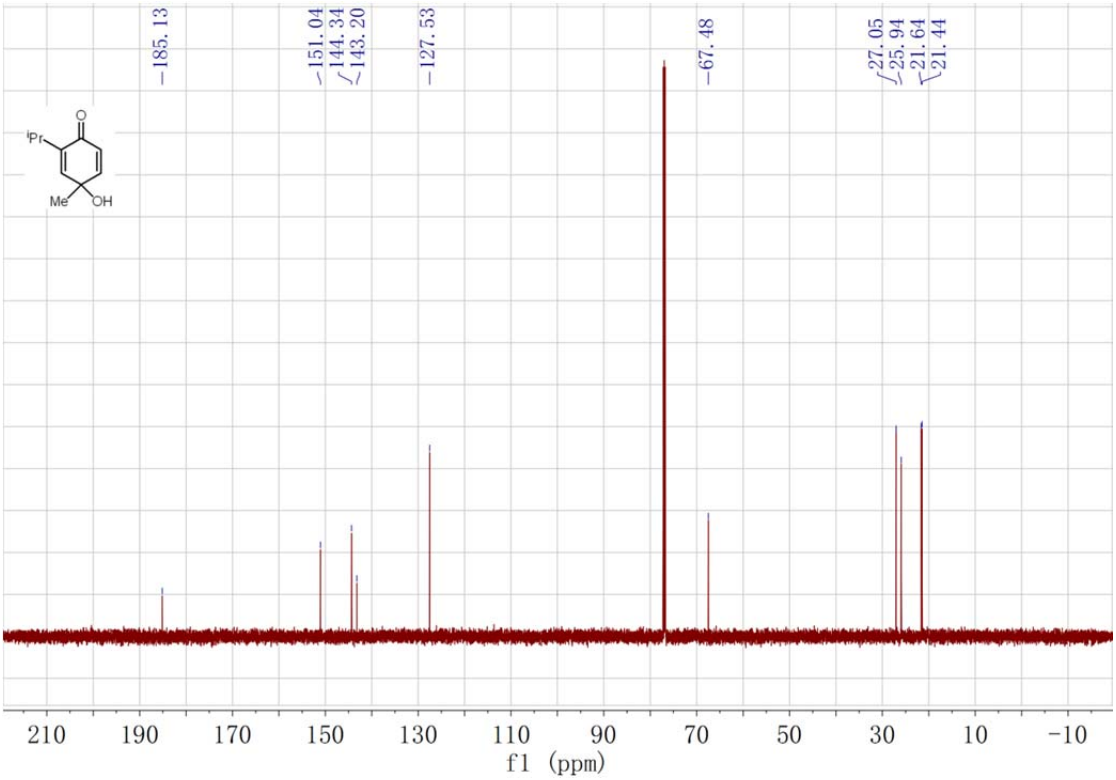
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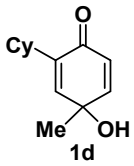
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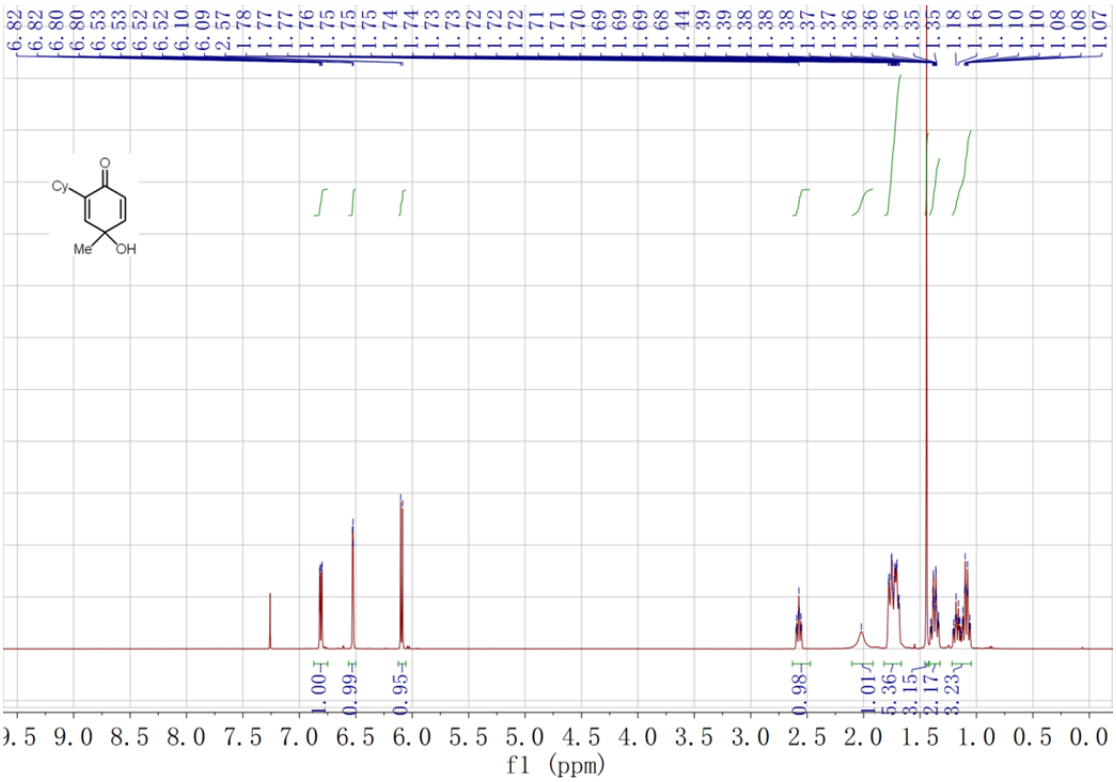
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1.00 0.99 0.95 0.98 1.01 5.36 3.15 2.17 3.23
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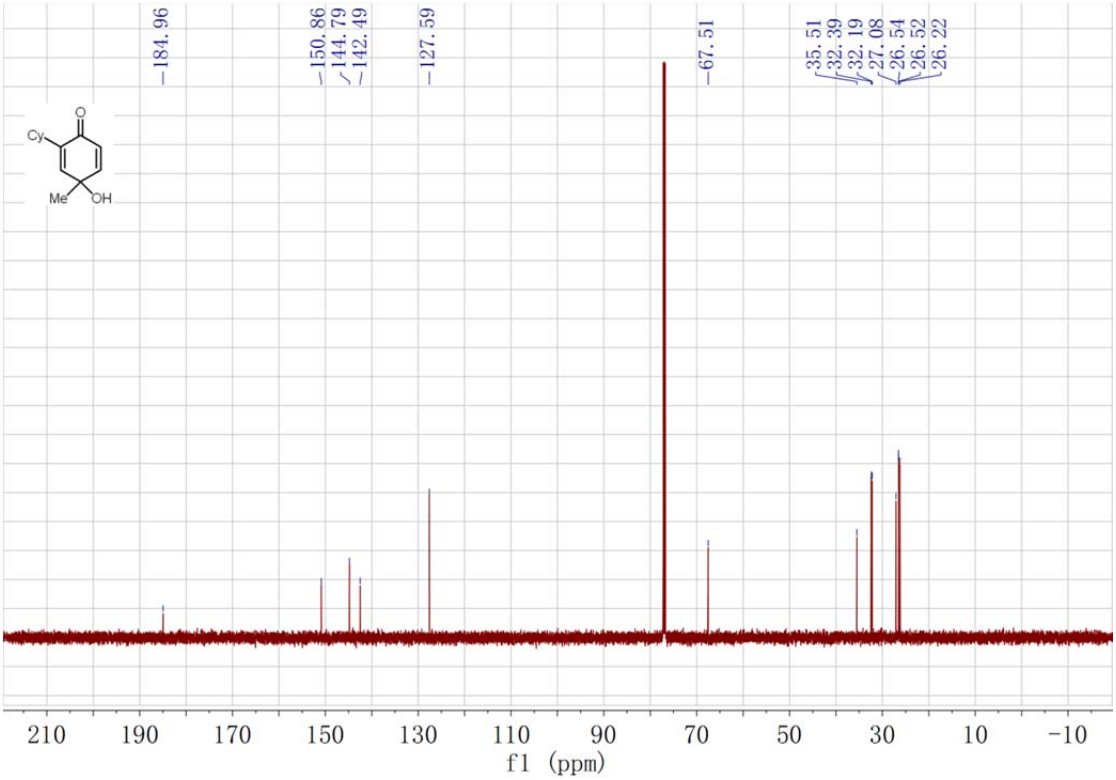
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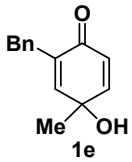
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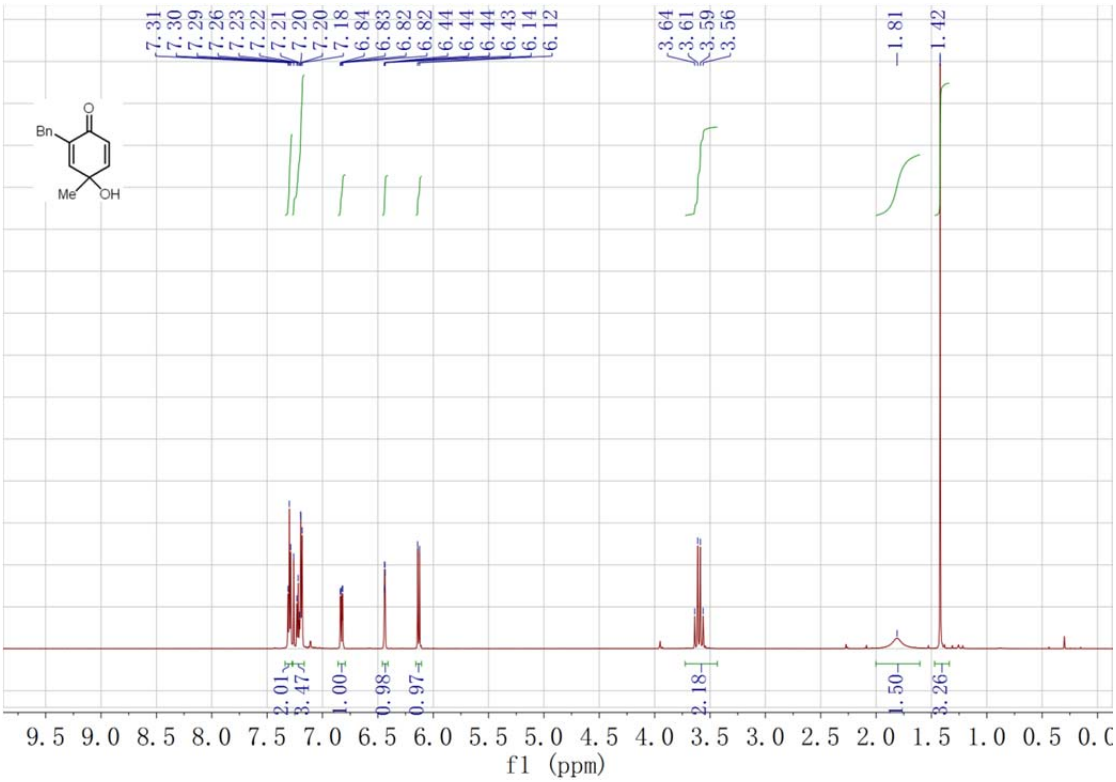
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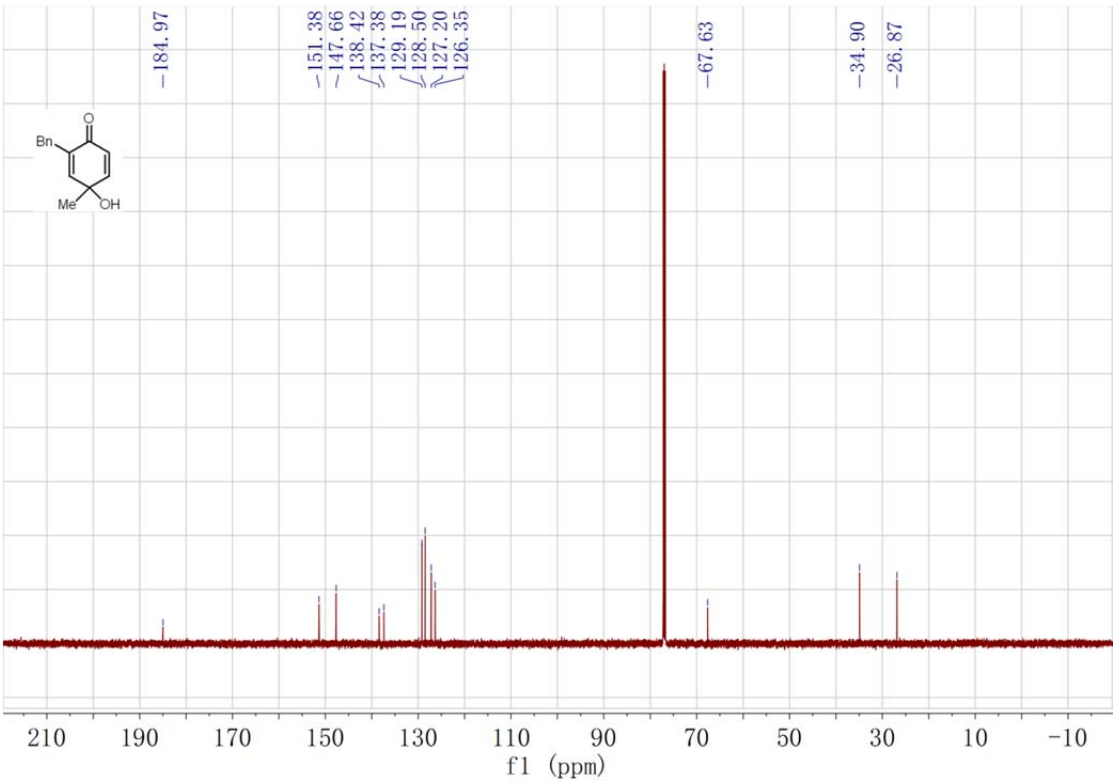
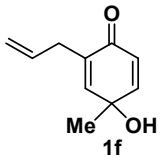
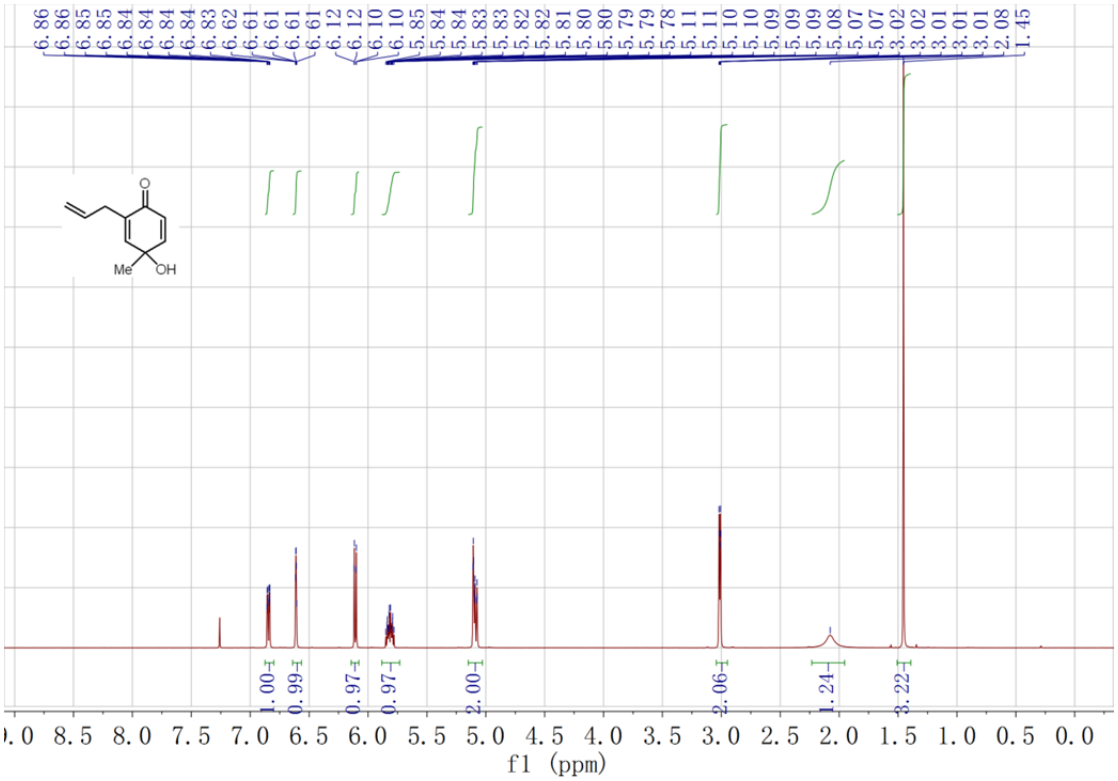
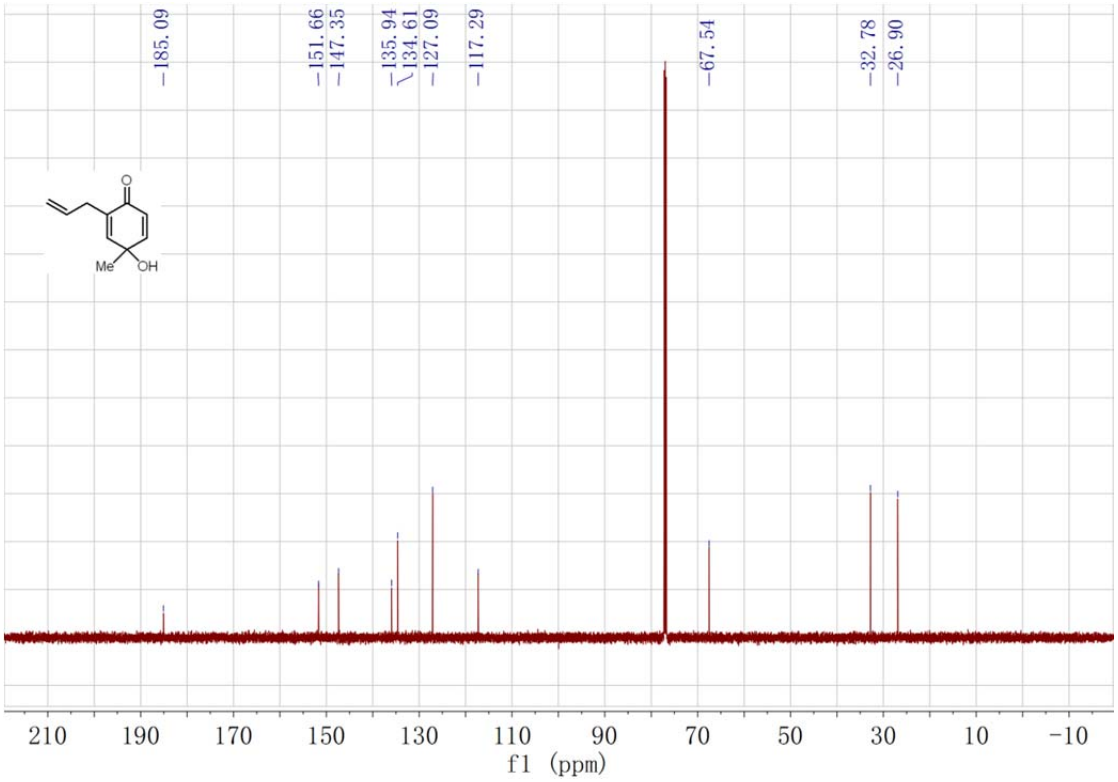
2.18
1.50
3.26
f1 (ppm)

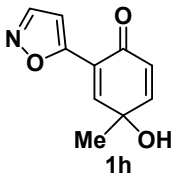

184.97
151.38
147.66
138.42
137.38
129.19
128.50
127.20
126.35
67.63
34.90
26.87
f1 (ppm)


O
Me
OH

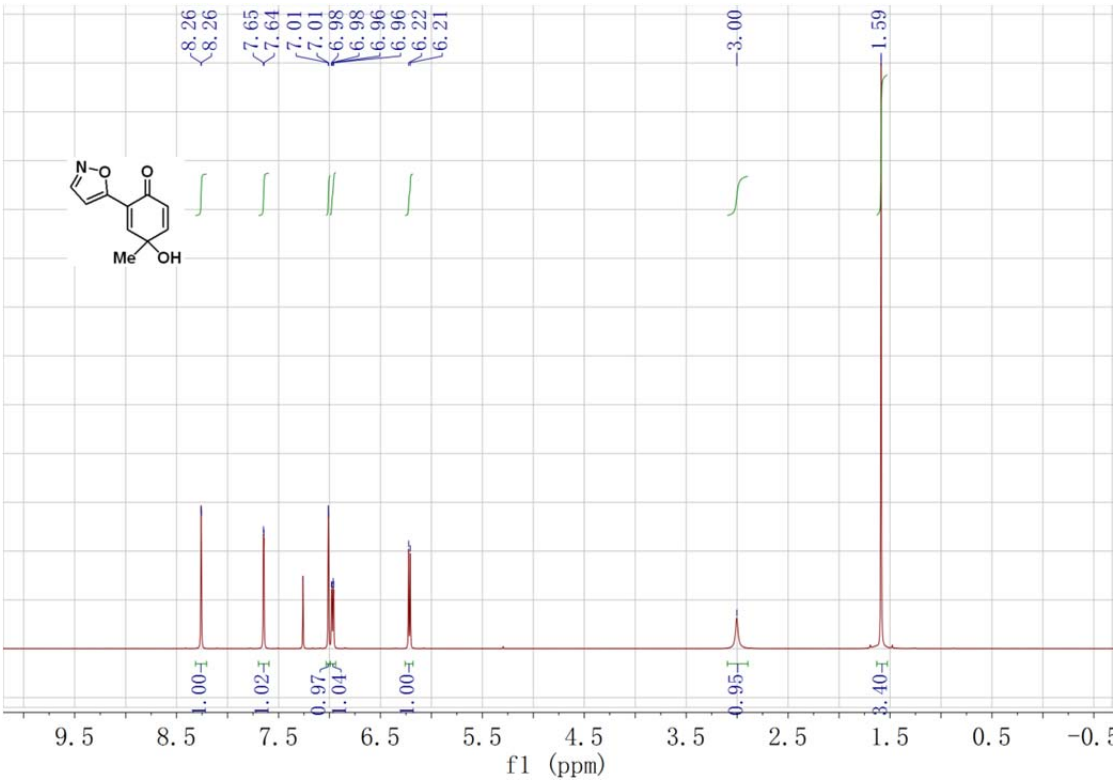
1f

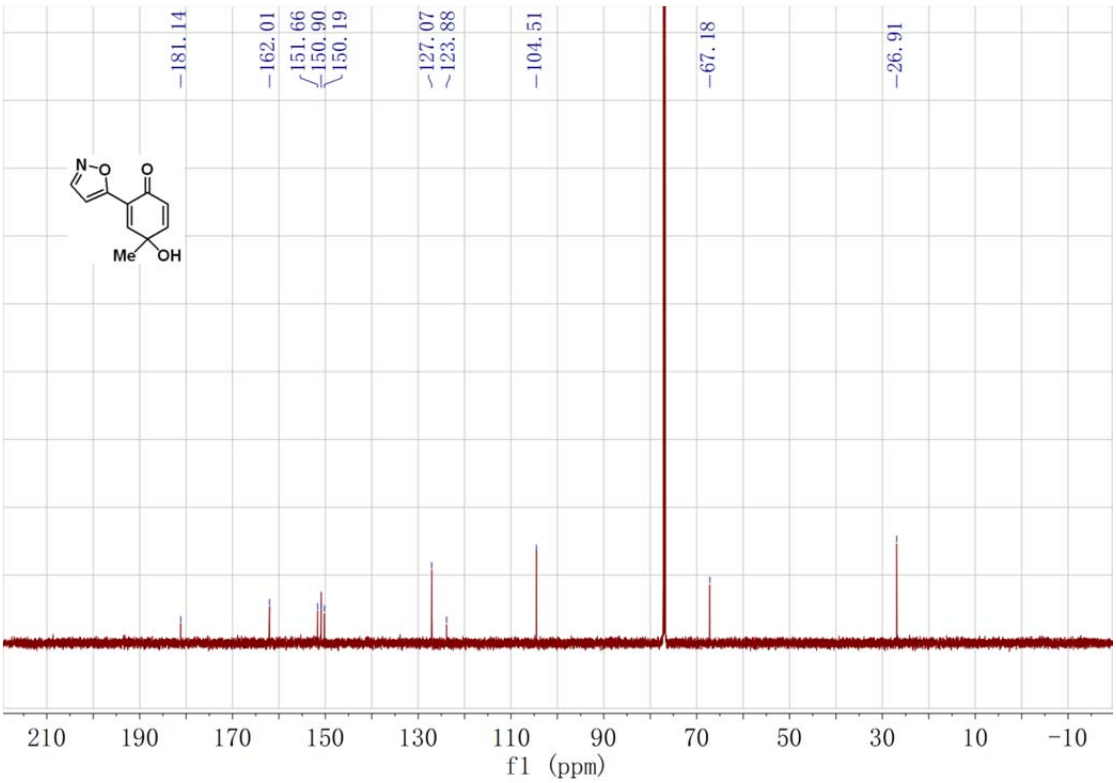

6.86 6.86 6.85 6.85 6.84 6.84 6.84 6.84 6.83 6.62 6.61 6.61 6.61 6.61 6.12 6.12 6.10 6.10 5.85 5.84 5.84 5.83 5.83 5.82 5.82 5.81 5.80 5.80 5.79 5.79 5.78 5.11 5.11 5.10 5.10 5.09 5.09 5.09 5.08 5.07 5.07 3.02 3.02 3.01 3.01 3.01 3.01 2.08 1.45
1.00 0.99 0.97 0.97 2.00 2.06 1.24 3.22
f1 (ppm)

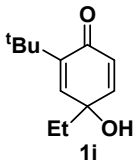

185.09
151.66
147.35
135.94
134.61
127.09
117.29
67.54
32.78
26.90
f1 (ppm)


O
N
O
Me
OH

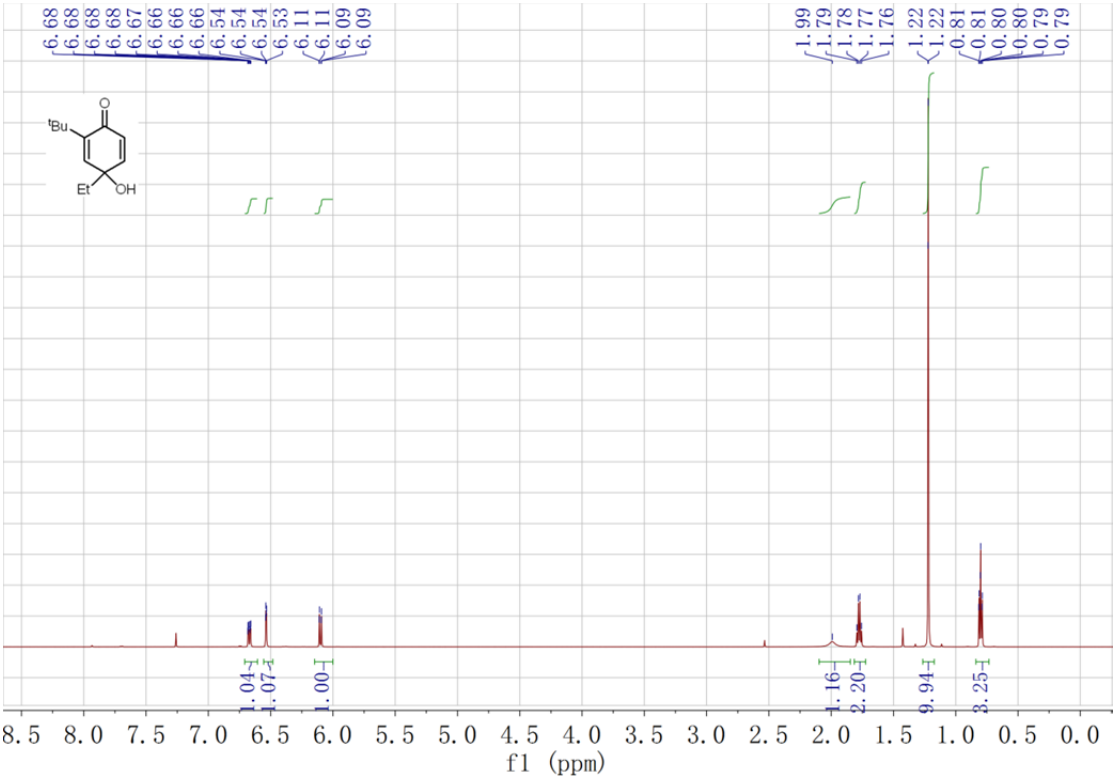
1h

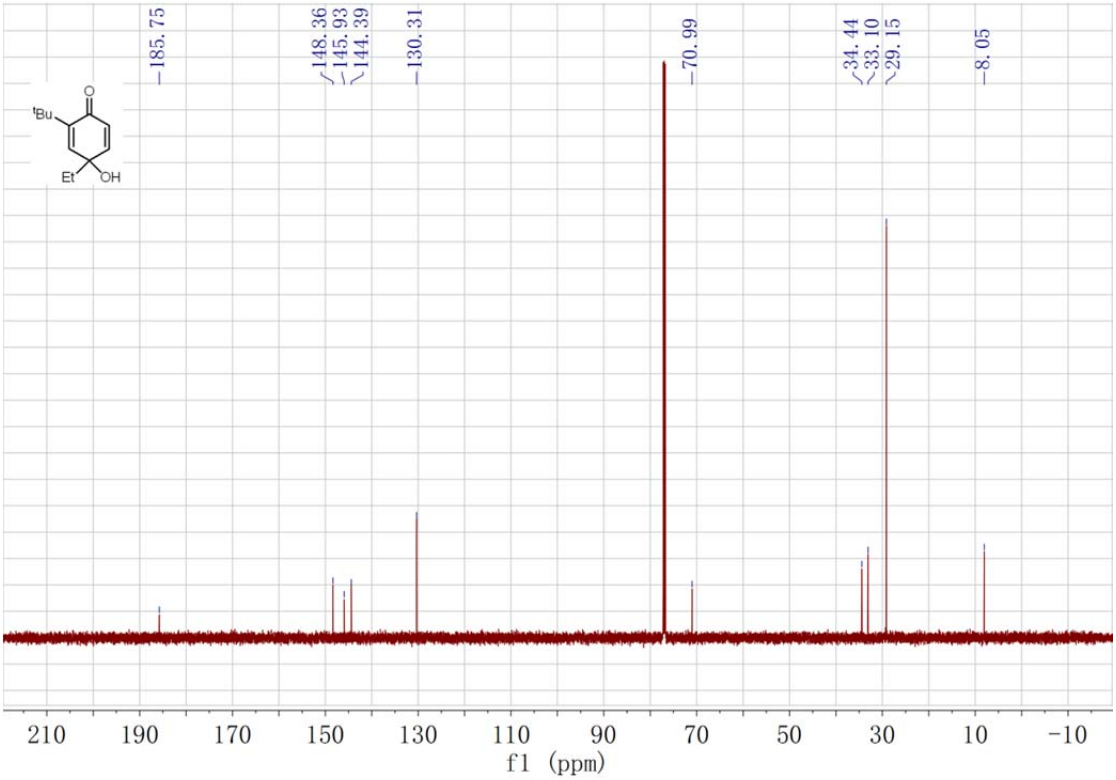

8.26
8.26
7.65
7.64
7.01
7.01
6.98
6.98
6.96
6.96
6.22
6.21
3.00
1.59
1.00
1.02
0.97
1.04
1.00
0.95
3.40
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

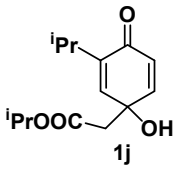

181.14
162.01
151.66
150.90
150.19
127.07
123.88
104.51
67.18
26.91
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


O
tBu
Et
OH

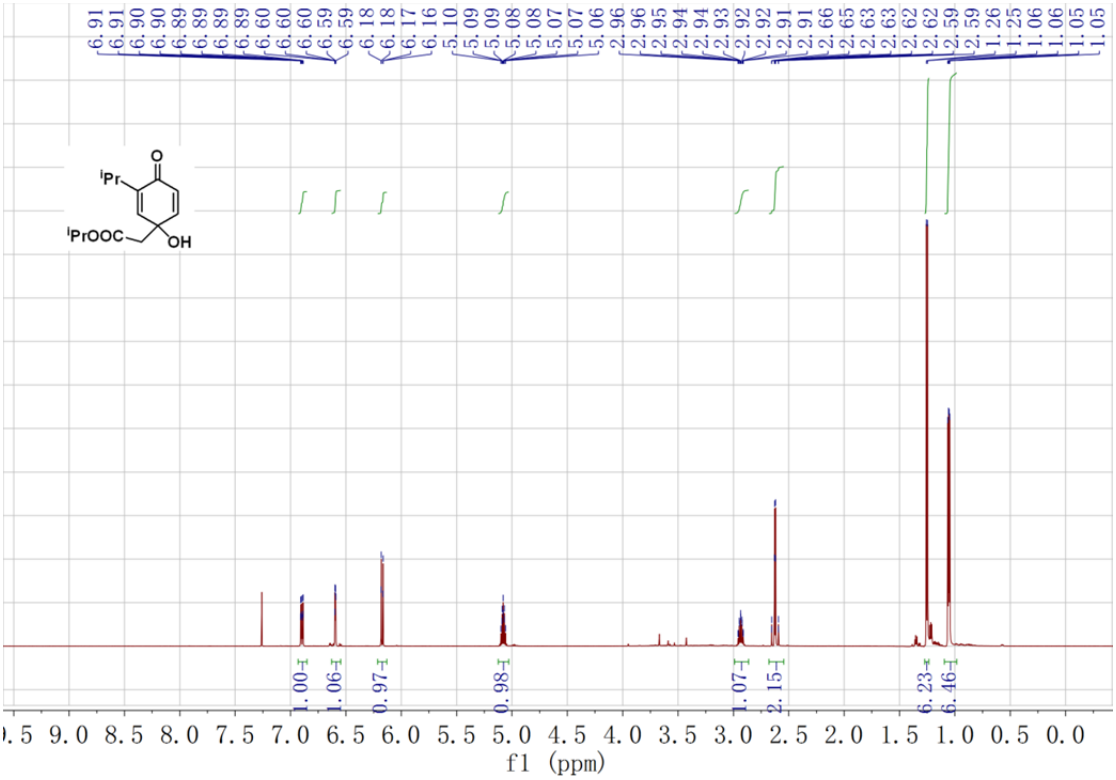
1i

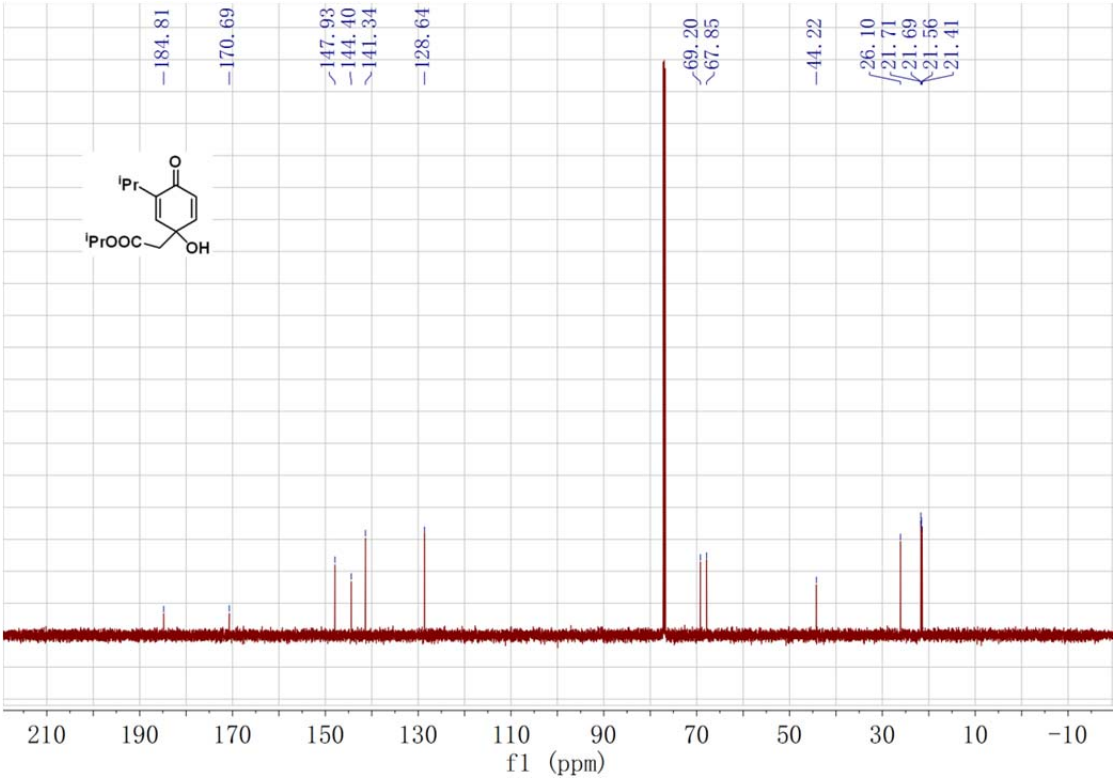

6.68
6.68
6.68
6.68
6.67
6.66
6.66
6.66
6.54
6.54
6.54
6.53
6.11
6.11
6.09
6.09
1.99
1.79
1.78
1.77
1.76
1.22
1.22
0.81
0.81
0.80
0.80
0.79
0.79
1.04
1.07
1.00
1.16
2.20
9.94
3.25
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

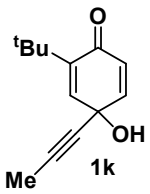

185.75
148.36
145.93
144.39
130.31
70.99
34.44
33.10
29.15
8.05
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

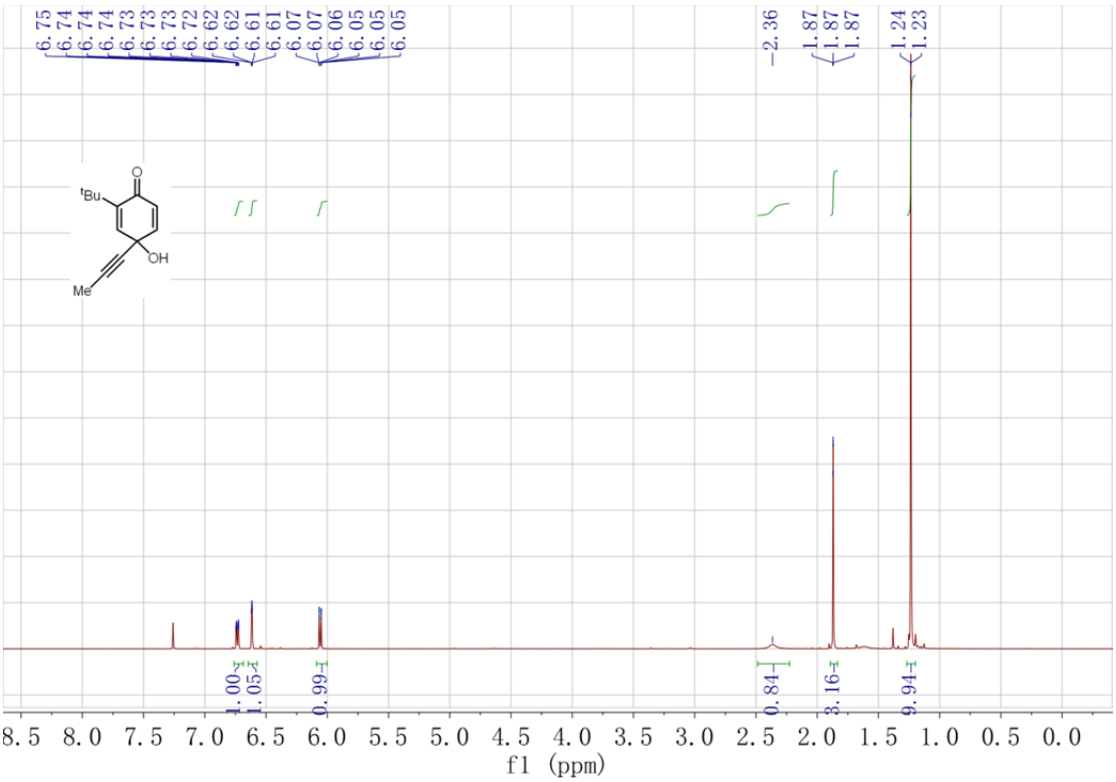

O
iPr
iPrOOC
OH

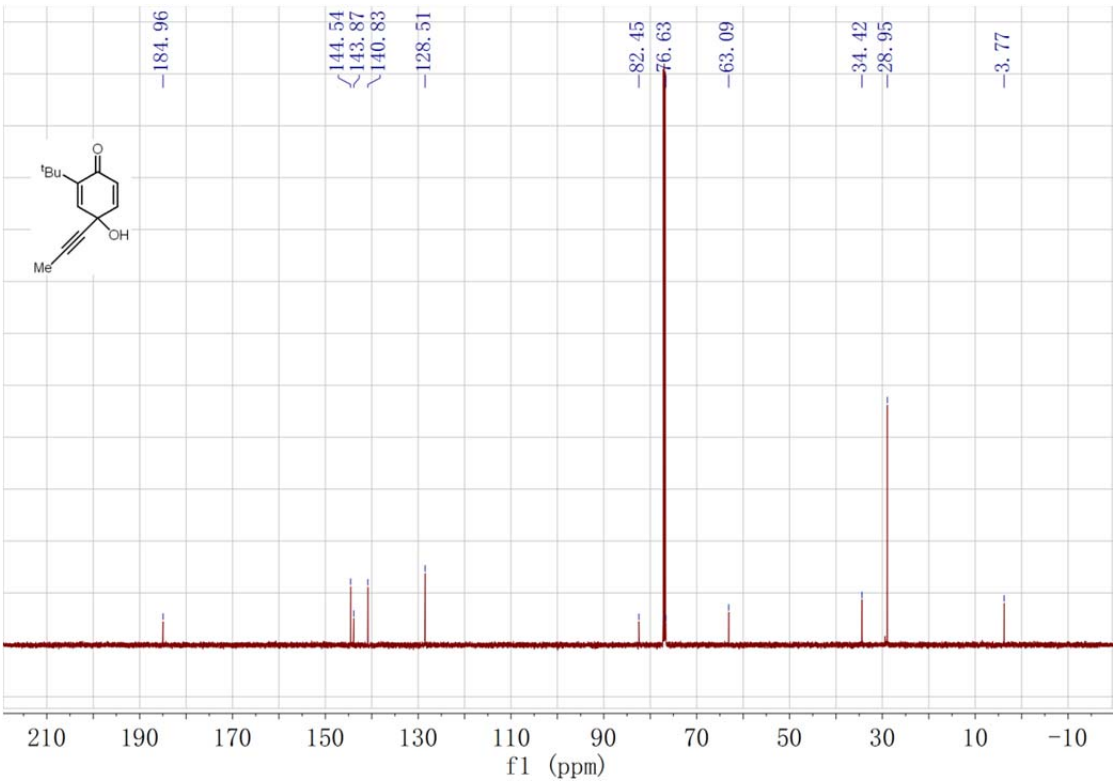
1j

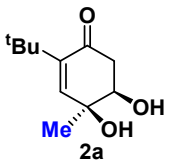

6.91 6.91 6.90 6.90 6.89 6.89 6.89 6.89 6.60 6.60 6.60 6.59 6.59 6.18 6.18 6.17 6.16 5.10 5.09 5.09 5.08 5.08 5.07 5.07 5.06 2.96 2.96 2.95 2.94 2.94 2.93 2.92 2.92 2.91 2.91 2.66 2.65 2.63 2.63 2.62 2.62 2.62 2.59 2.59 1.26 1.25 1.06 1.06 1.05 1.05
1.00 1.06 0.97 0.98 1.07 2.15 6.23 6.46
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


184.81 170.69 147.93 144.40 141.34 128.64 69.20 67.85 44.22 26.10 21.71 21.69 21.56 21.41
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)

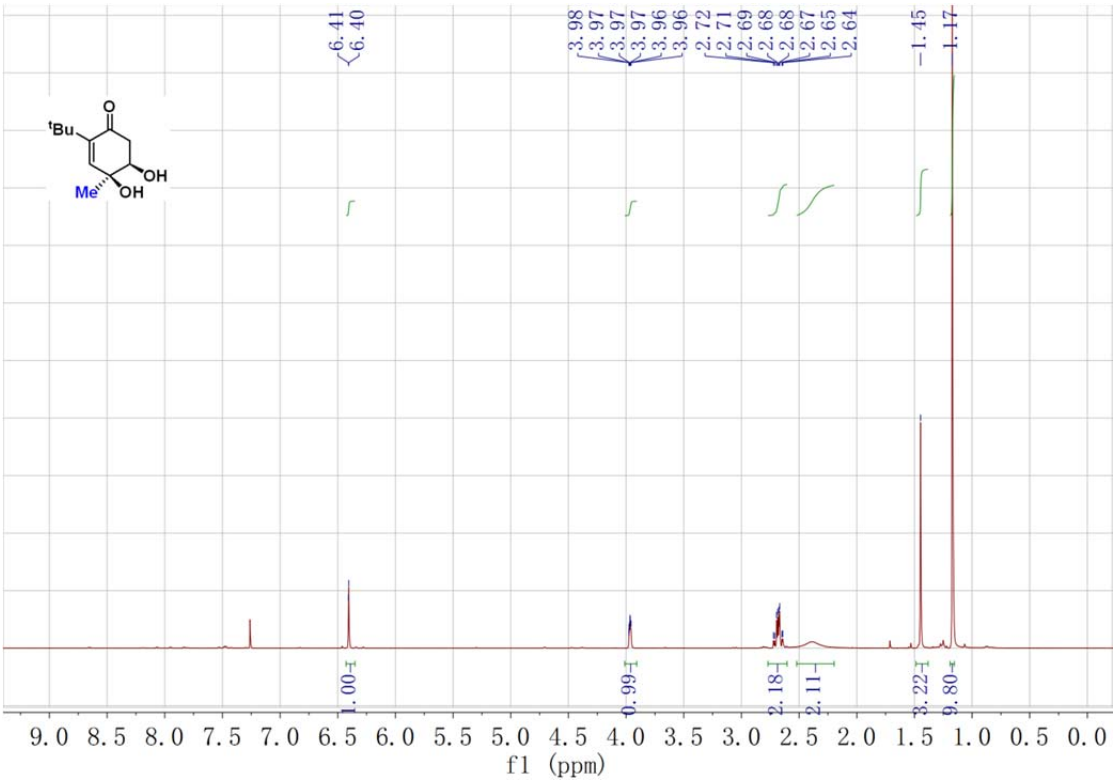

O
tBu
OH
Me
1k

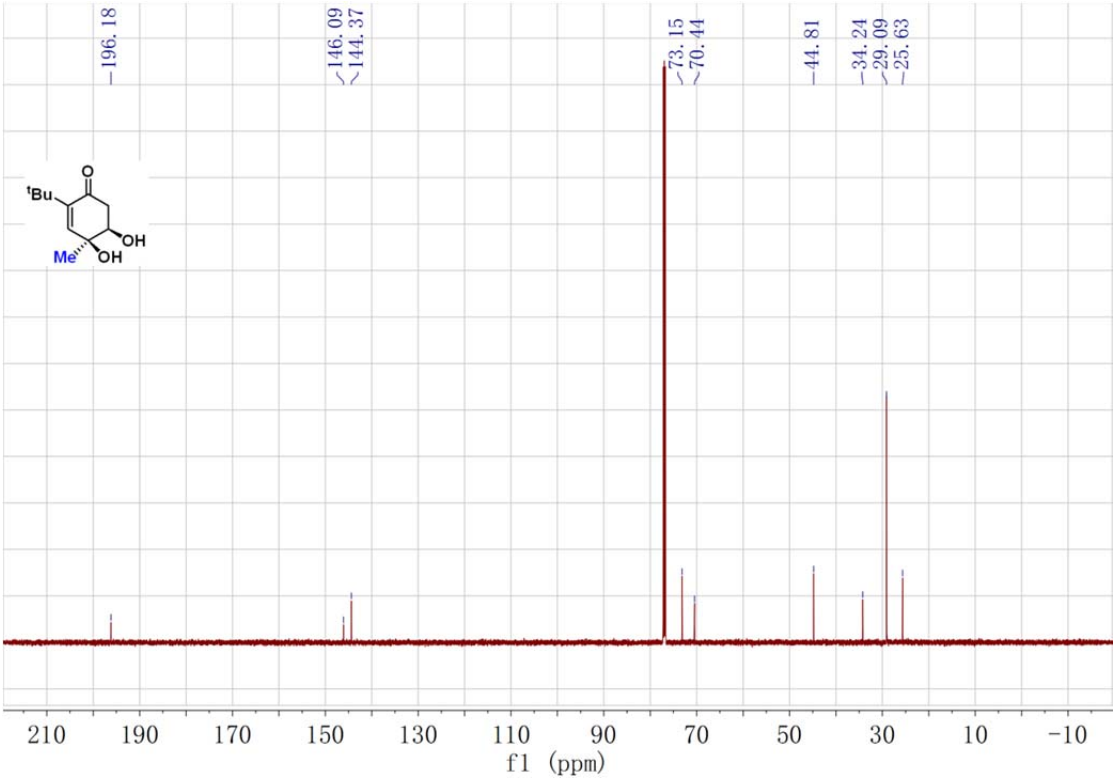

6.75
6.74
6.74
6.74
6.73
6.73
6.73
6.72
6.62
6.62
6.61
6.61
6.07
6.07
6.06
6.05
6.05
6.05
2.36
1.87
1.87
1.87
1.24
1.23
1.00
1.05
0.99
0.84
3.16
9.94
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

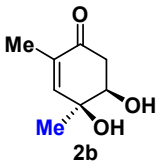

184.96
144.54
143.87
140.83
128.51
82.45
76.63
63.09
34.42
28.95
3.77
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


tBu
O
OH
Me
OH

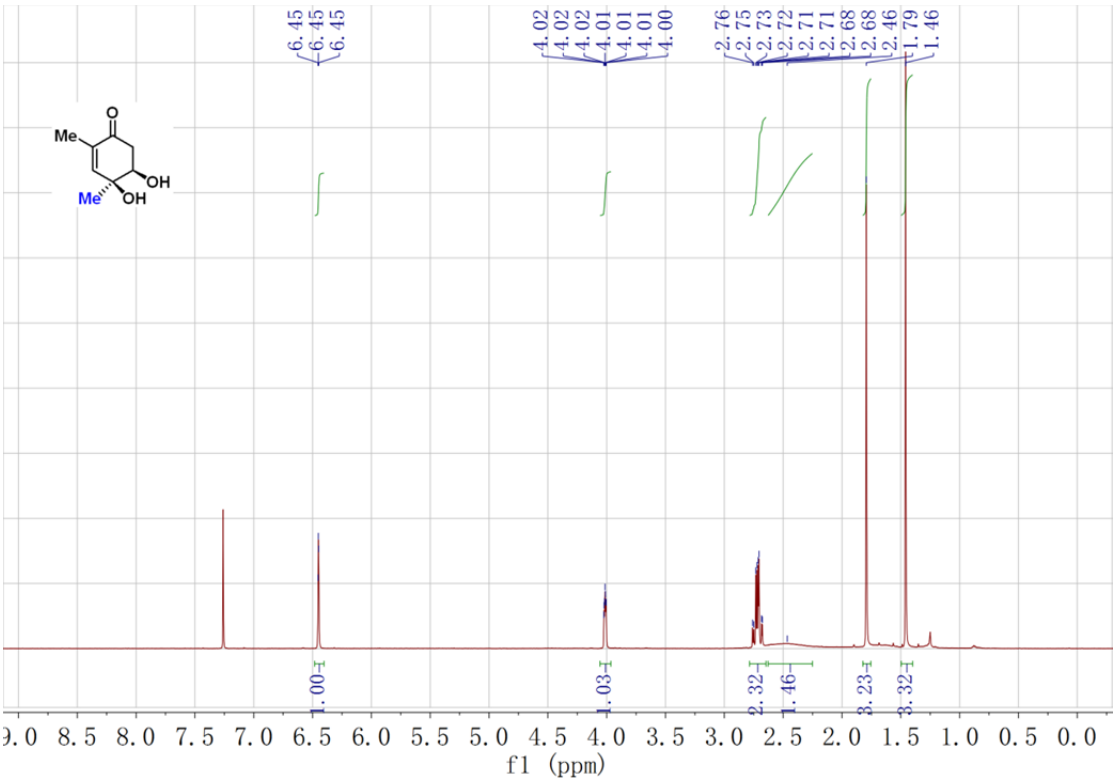
2a


6.41
6.40
3.98
3.97
3.97
3.97
3.96
3.96
2.72
2.71
2.69
2.68
2.68
2.67
2.65
2.64
1.45
1.17
1.00
0.99
2.18
2.11
3.22
9.80
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


196.18
146.09
144.37
73.15
70.44
44.81
34.24
29.09
25.63
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


O
Me
OH
Me
OH

2b


6.45
6.45
6.45
4.02
4.02
4.02
4.01
4.01
4.01
4.00
2.76
2.75
2.73
2.72
2.71
2.71
2.68
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1.79
1.46
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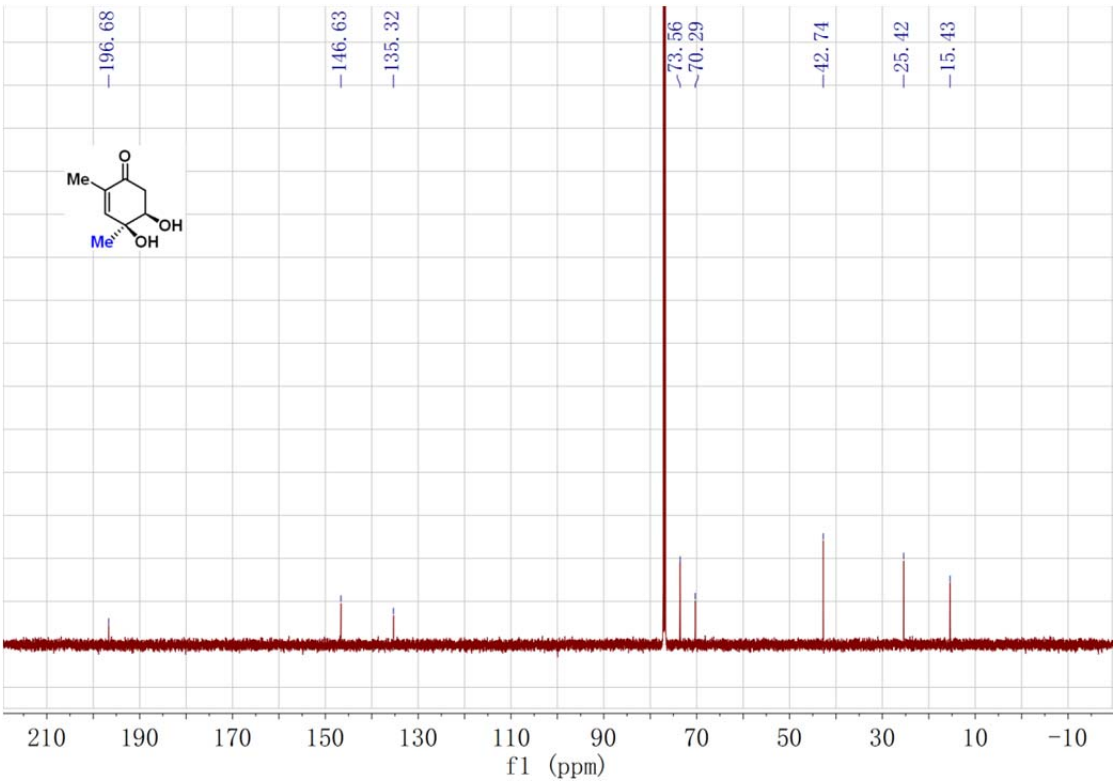
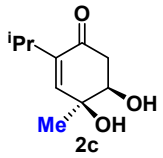
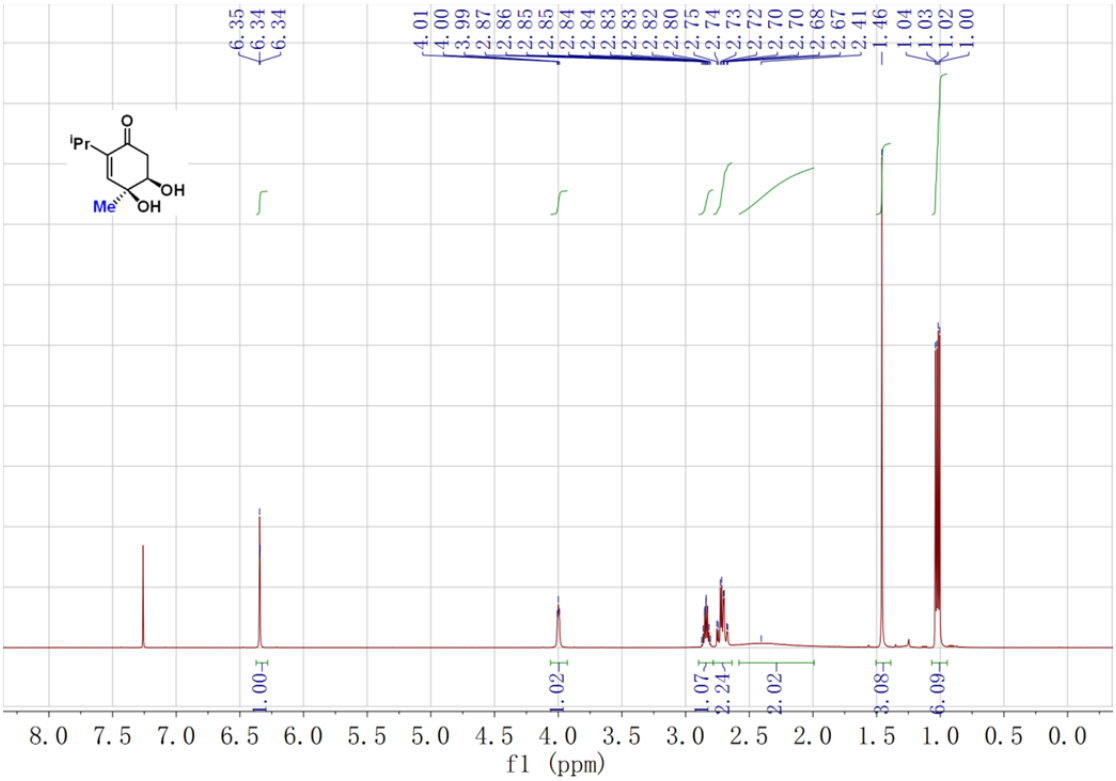
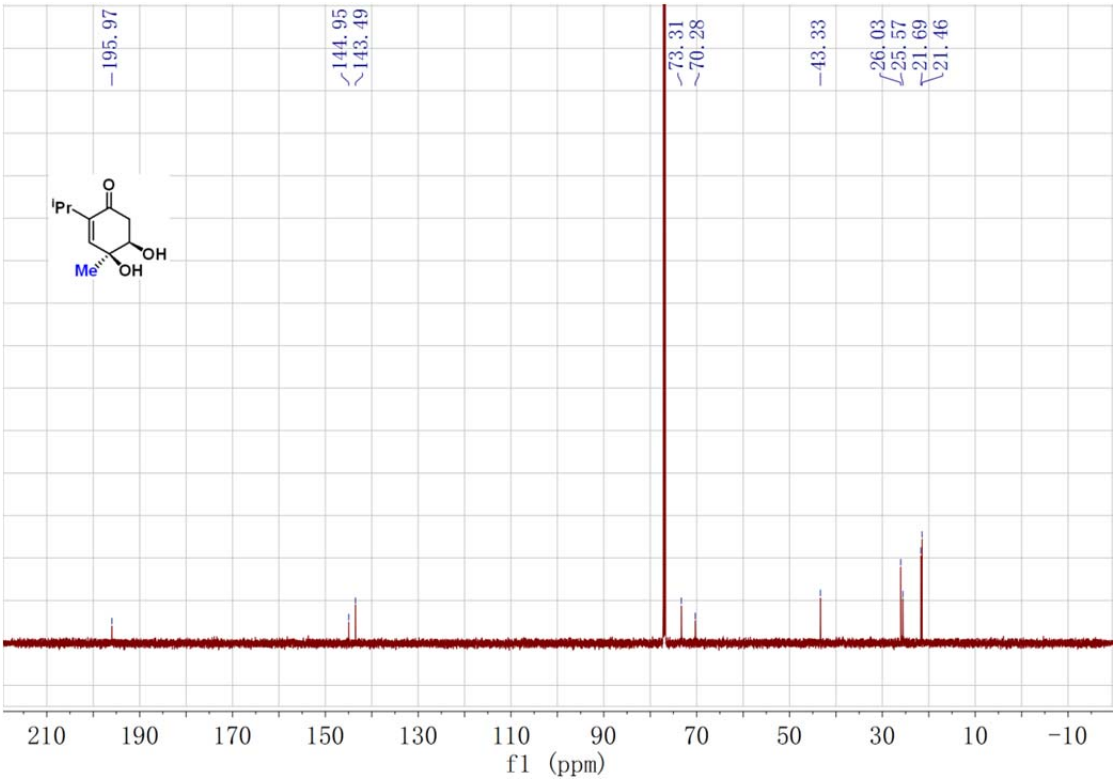
1.03
2.32
1.46
3.23
3.32
f1 (ppm)

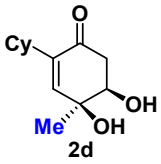

196.68
146.63
135.32
73.56
70.29
42.74
25.42
15.43
f1 (ppm)


O
iPr
OH
Me
OH

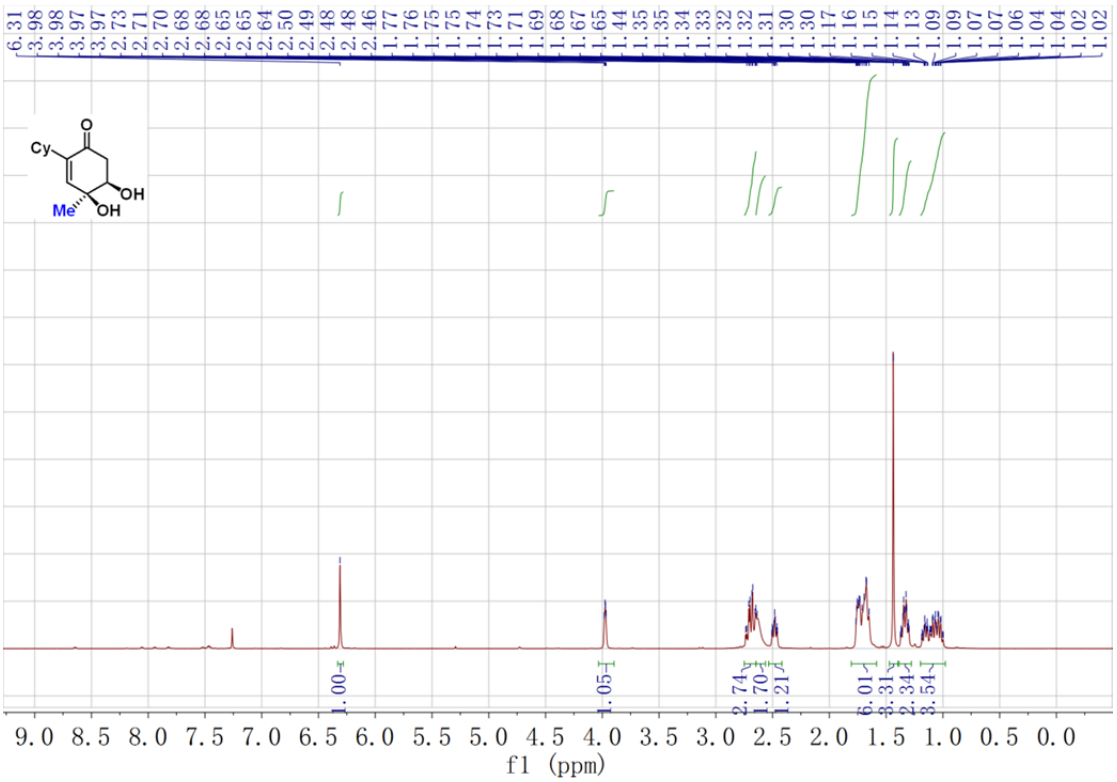
2c

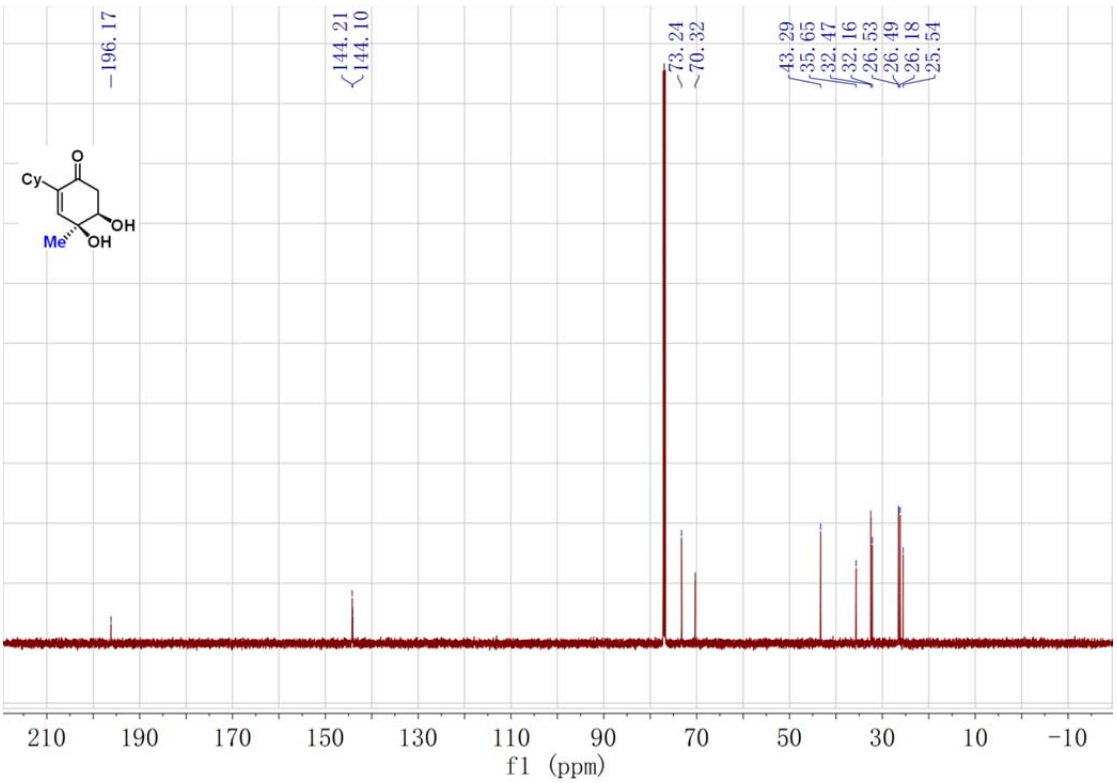

6.35
6.34
6.34
4.01
4.00
3.99
2.87
2.86
2.85
2.85
2.84
2.84
2.83
2.83
2.82
2.80
2.75
2.74
2.73
2.72
2.70
2.70
2.68
2.67
2.41
1.46
1.04
1.03
1.02
1.00
1.00
1.02
1.07
2.24
2.02
3.08
6.09
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

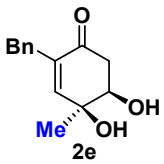

195.97
144.95
143.49
73.31
70.28
43.33
26.03
25.57
21.69
21.46
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


Cy
O
OH
Me
OH

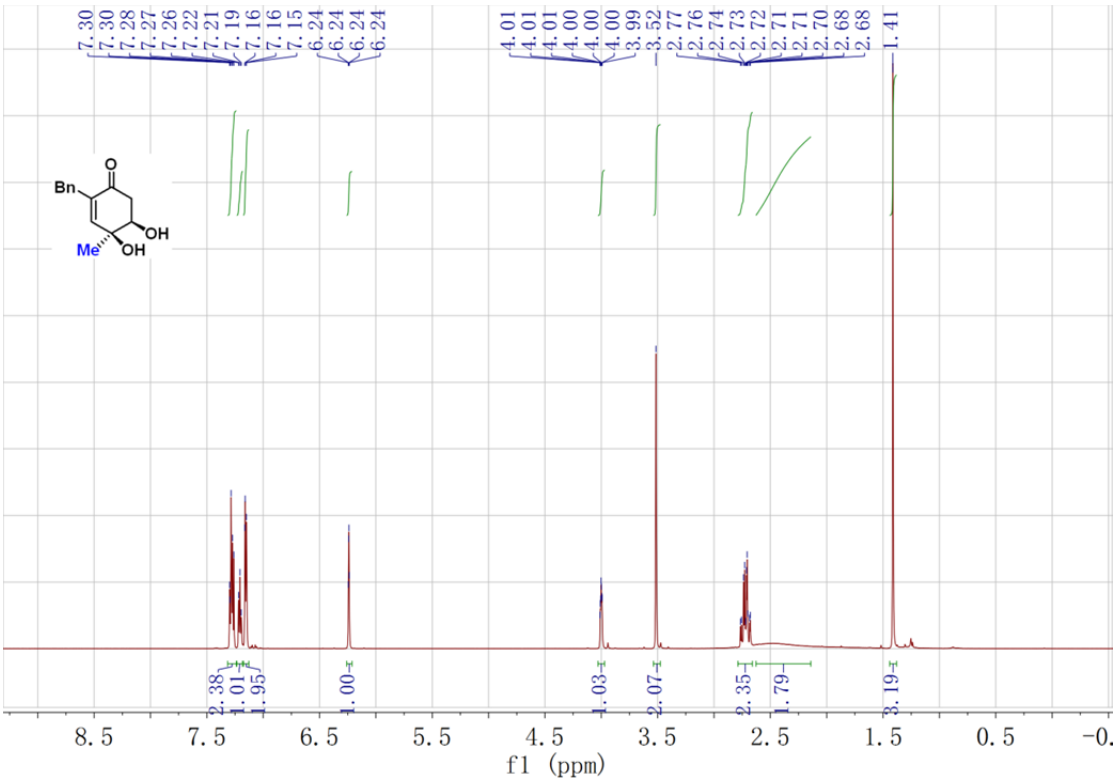
2d


6.31 3.98 3.98 3.97 3.97 2.73 2.71 2.70 2.68 2.68 2.65 2.65 2.64 2.50 2.49 2.48 2.48 2.46 1.77 1.76 1.75 1.75 1.74 1.73 1.71 1.69 1.68 1.67 1.65 1.44 1.35 1.35 1.34 1.33 1.32 1.32 1.31 1.30 1.30 1.17 1.16 1.15 1.14 1.13 1.09 1.09 1.07 1.07 1.06 1.04 1.04 1.02 1.02
1.00 1.05 2.74 1.70 1.21 6.01 3.31 2.34 3.54
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


196.17
144.21 144.10
73.24 70.32
43.29 35.65 32.47 32.16 26.53 26.49 26.18 25.54
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


O
Bn
OH
Me
OH

2e


7.30
7.30
7.28
7.27
7.26
7.22
7.21
7.19
7.16
7.16
7.15
6.24
6.24
6.24
6.24
4.01
4.01
4.01
4.00
4.00
4.00
3.99
3.52
2.77
2.76
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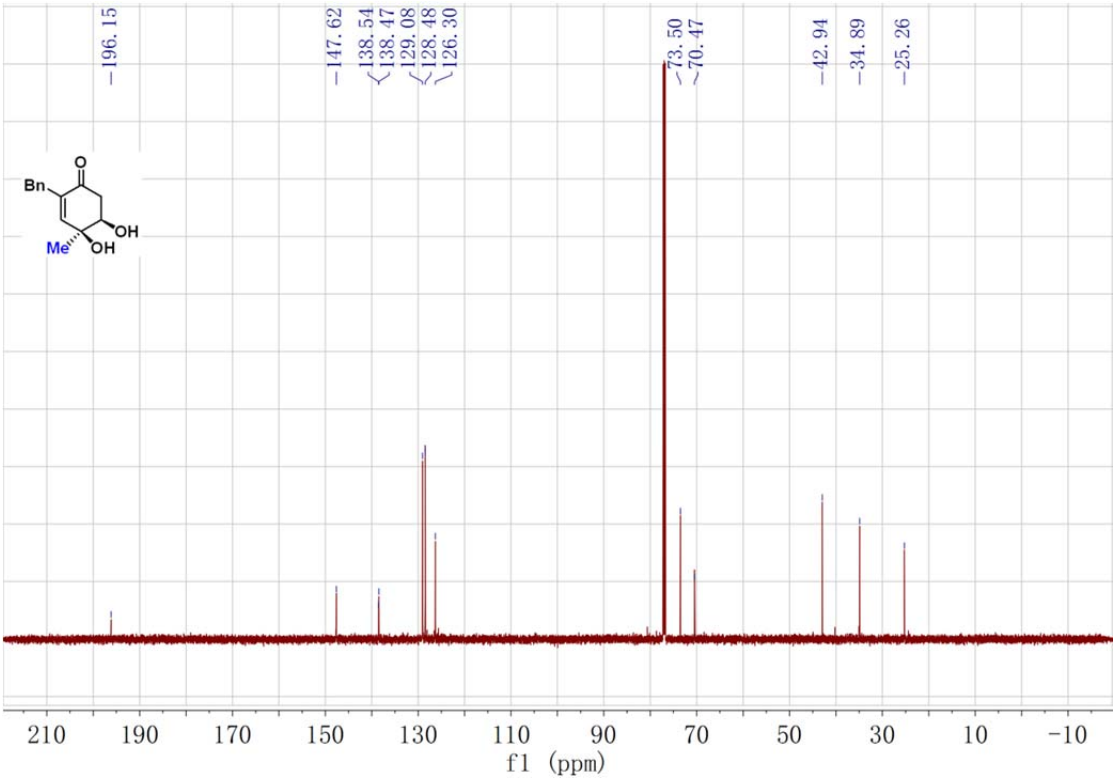
2.73
2.72
2.71
2.71
2.70
2.68
2.68
1.41
2.38
1.01
1.95
1.00
1.03
2.07
2.35
1.79
3.19
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


196.15
147.62
138.54
138.47
129.08
128.48
126.30
73.50
70.47
42.94
34.89
25.26
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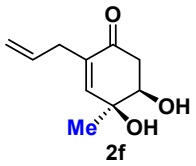
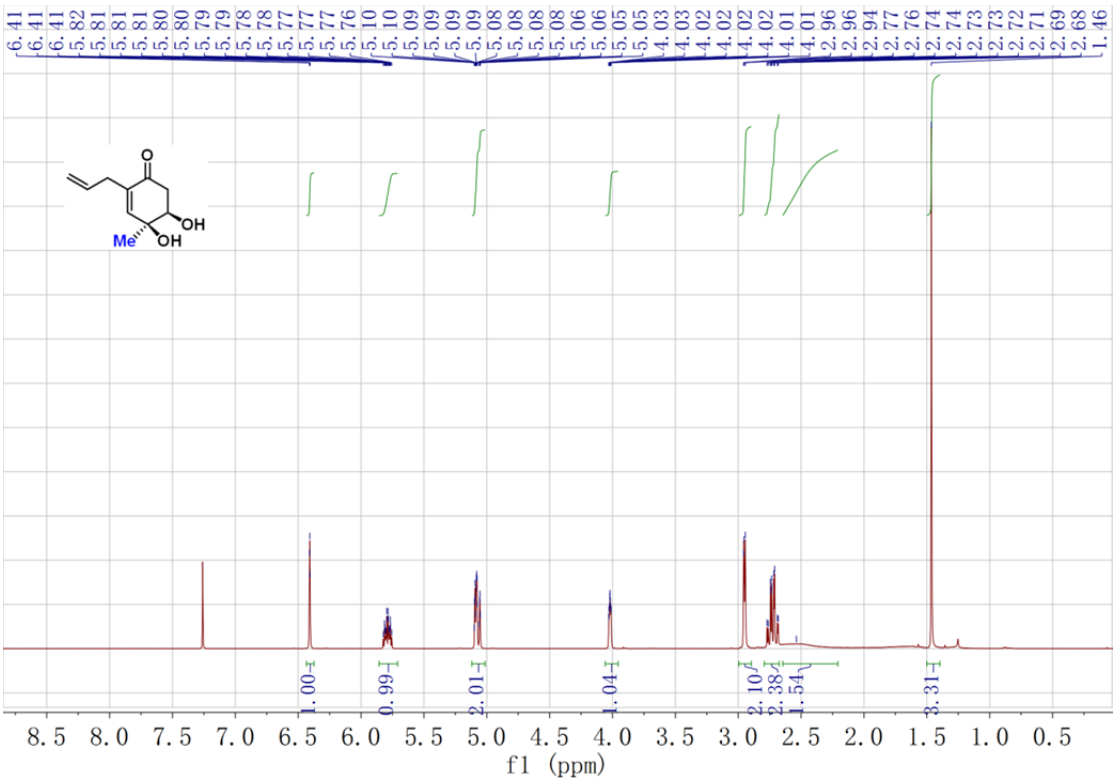
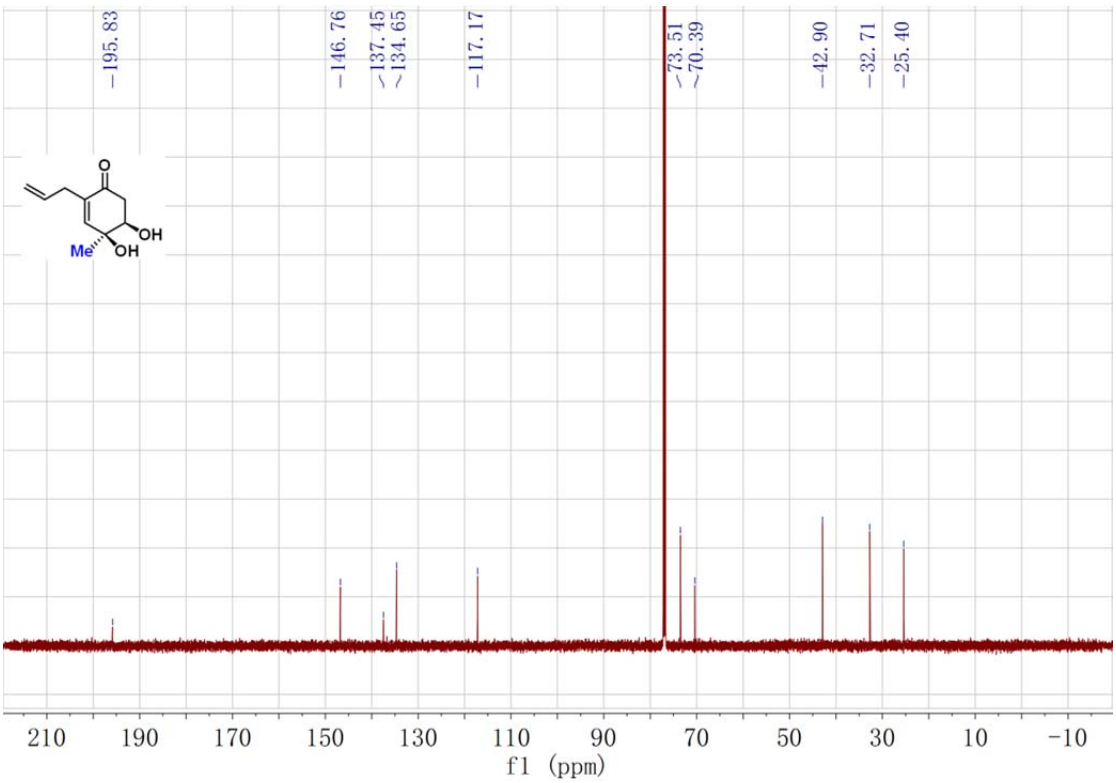
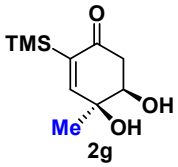
110
90
70
50
30
10
-10
f1 (ppm)


O
OH
Me
OH

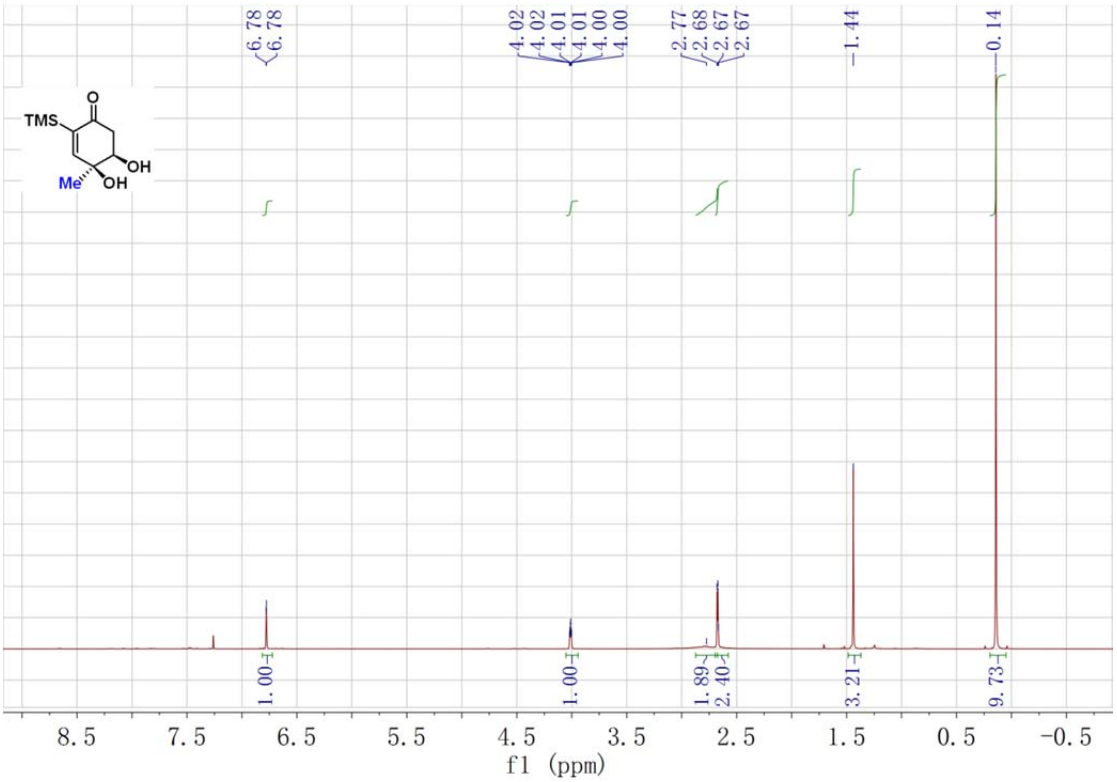
2f

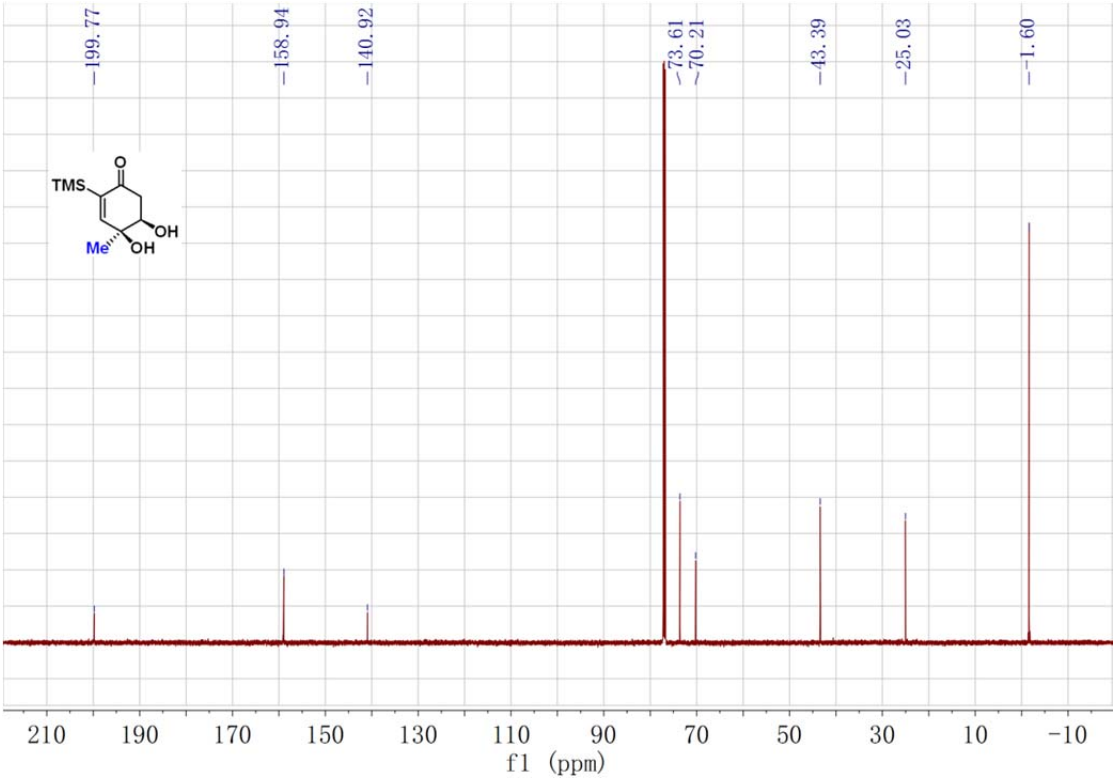

6.41 6.41 6.41 5.82 5.81 5.81 5.81 5.80 5.80 5.79 5.79 5.78 5.78 5.77 5.77 5.77 5.76 5.10 5.10 5.09 5.09 5.09 5.09 5.08 5.08 5.08 5.08 5.06 5.06 5.05 5.05 4.03 4.03 4.02 4.02 4.02 4.02 4.01 4.01 2.96 2.96 2.94 2.77 2.76 2.74 2.74 2.73 2.73 2.72 2.71 2.69 2.68 1.46
1.00 0.99 2.01 1.04 2.10 2.38 1.54 3.31
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
f1 (ppm)

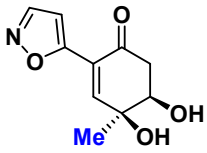

195.83
146.76
137.45
134.65
117.17
73.51
70.39
42.90
32.71
25.40
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


TMS
O
OH
Me
OH

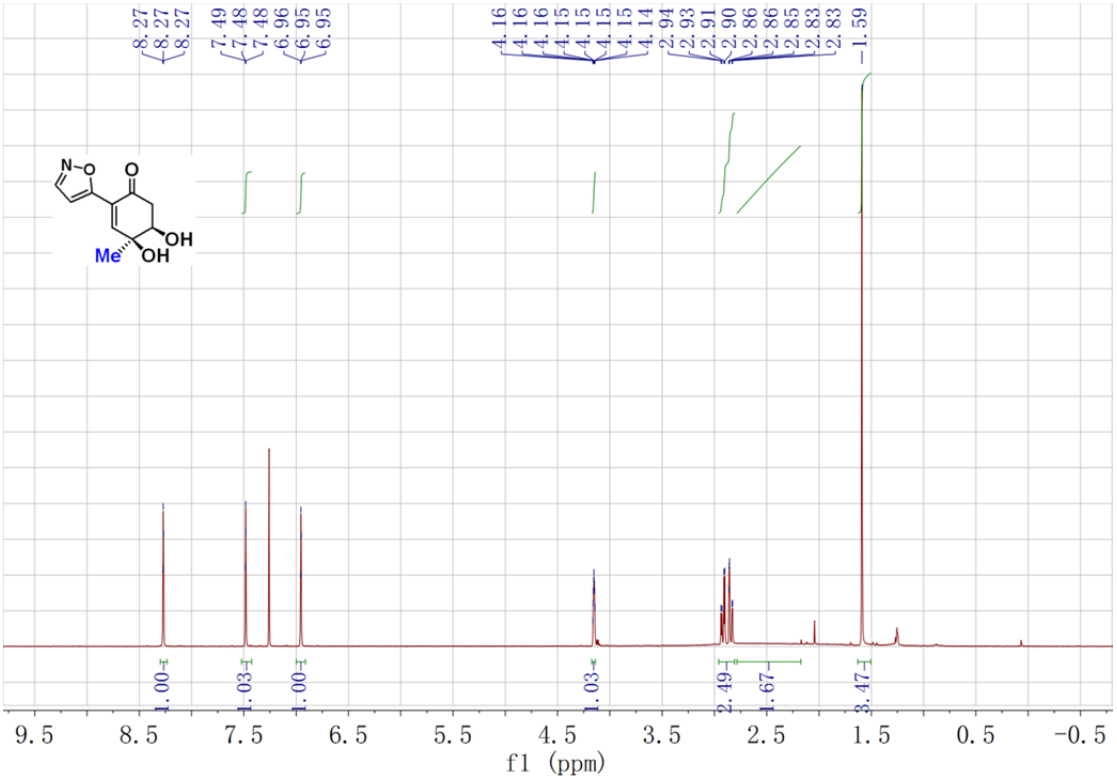
2g

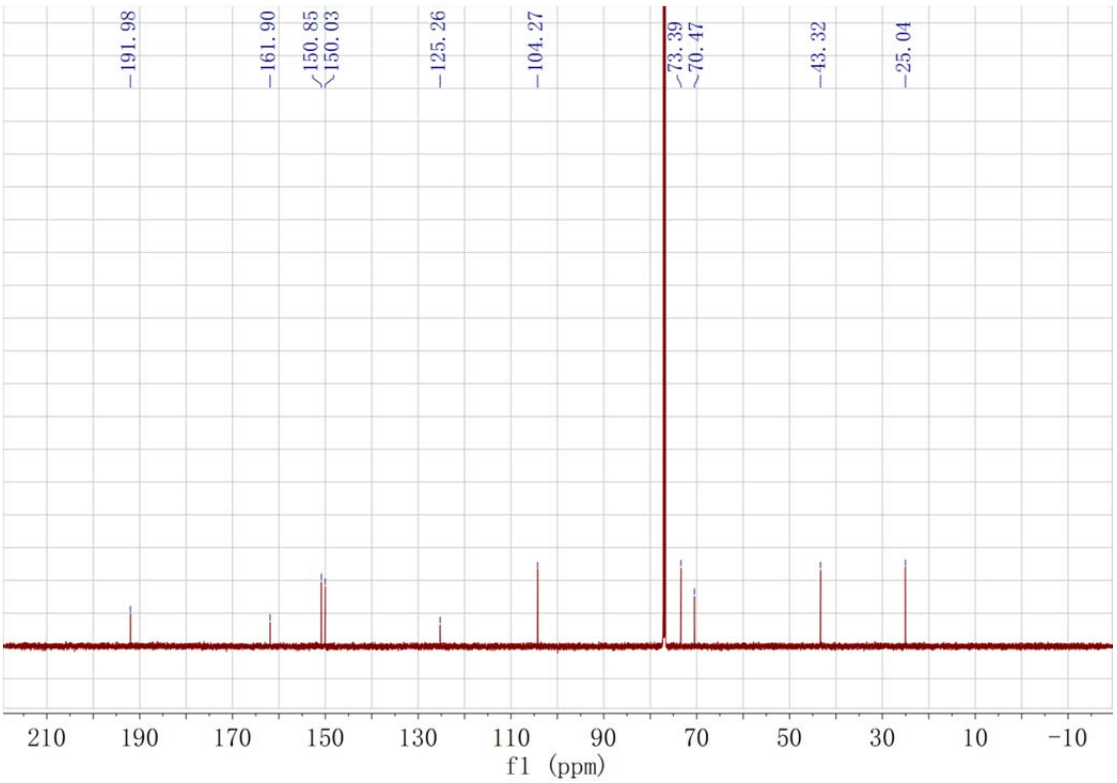

6.78
6.78
4.02
4.02
4.01
4.00
4.00
2.77
2.68
2.67
2.67
1.44
0.14
1.00
1.00
1.89
2.40
3.21
9.73
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

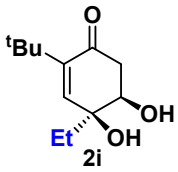

199.77
158.94
140.92
73.61
70.21
43.39
25.03
1.60
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


O
N
O
OH
Me
OH

2h

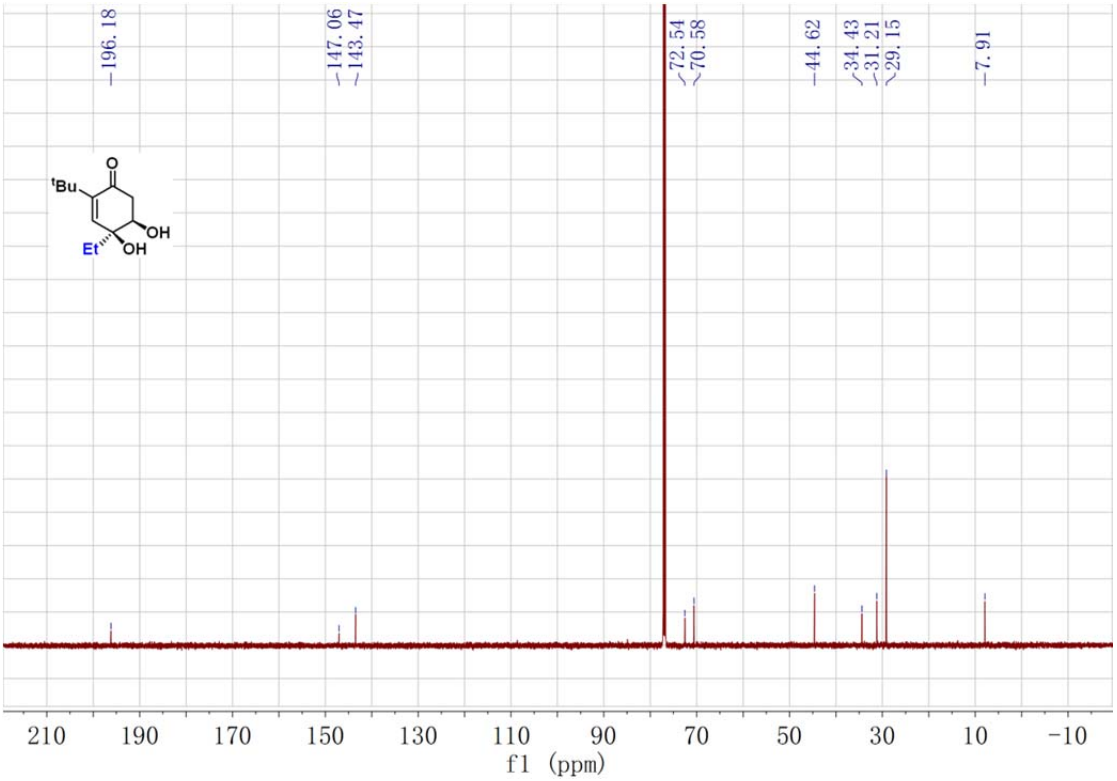

8.27
8.27
8.27
7.49
7.48
7.48
6.96
6.95
6.95
4.16
4.16
4.16
4.15
4.15
4.15
4.14
2.94
2.93
2.91
2.90
2.86
2.86
2.85
2.83
2.83
1.59
1.00
1.03
1.00
1.03
2.49
1.67
3.47
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

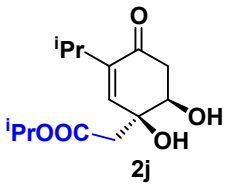

191.98
161.90
150.85
150.03
125.26
104.27
73.39
70.47
43.32
25.04
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


O
tBu
OH
Et
OH

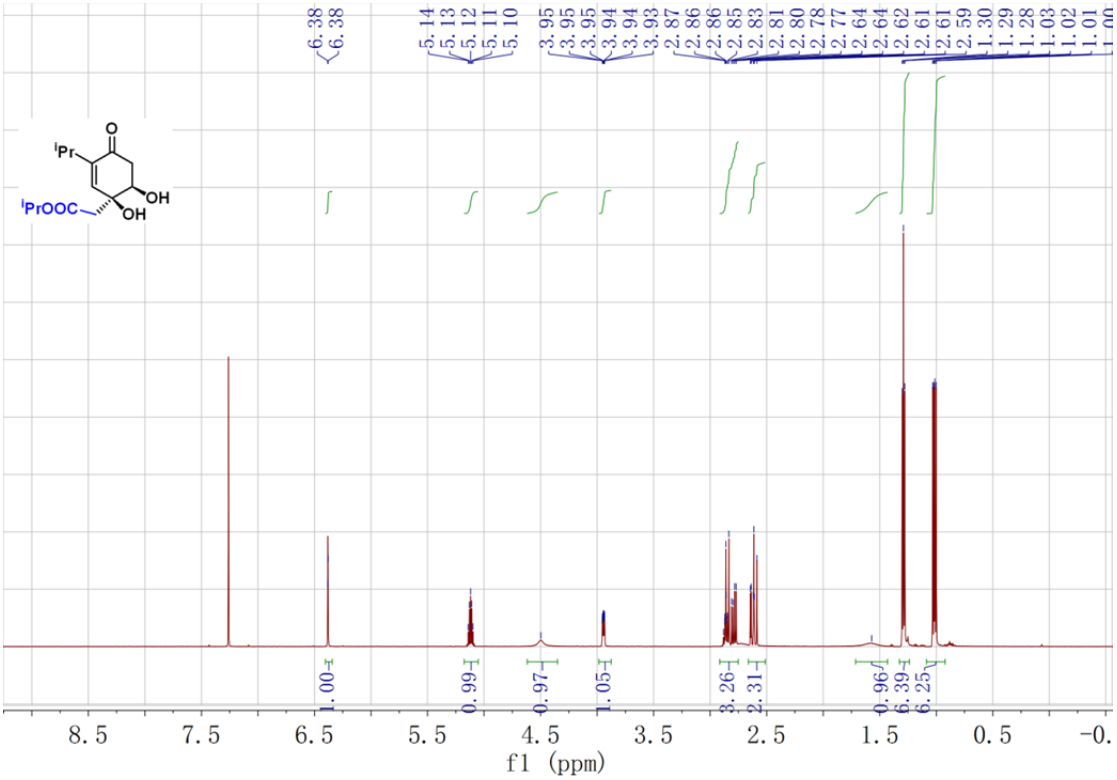
2i

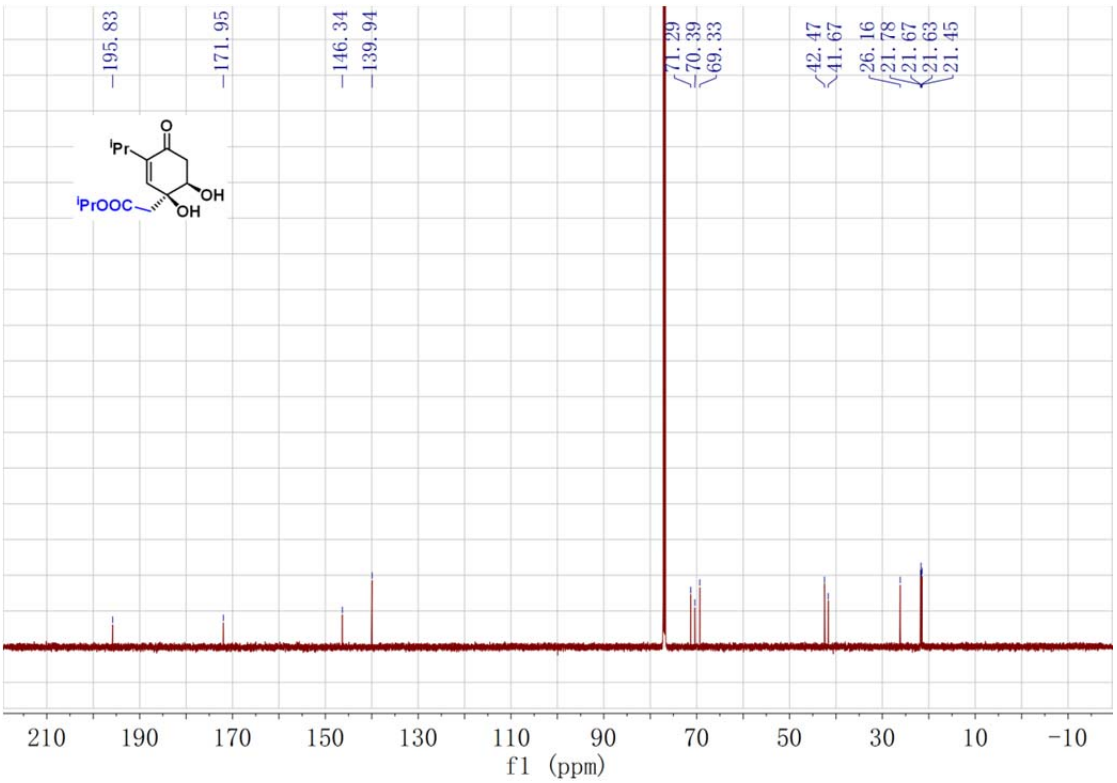

6.42
6.42
4.03
4.03
4.03
4.02
4.02
4.02
4.02
4.01
2.73
2.72
2.71
2.70
2.67
2.64
2.64
2.26
1.85
1.84
1.83
1.81
1.80
1.72
1.71
1.70
1.69
1.68
1.66
1.18
1.02
1.00
1.00
2.10
1.78
1.31
1.76
9.00
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

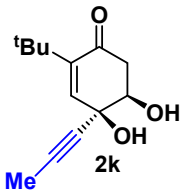

196.18
147.06
143.47
72.54
70.58
44.62
34.43
31.21
29.15
7.91
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


O
iPr
OH
iPrOOC
OH

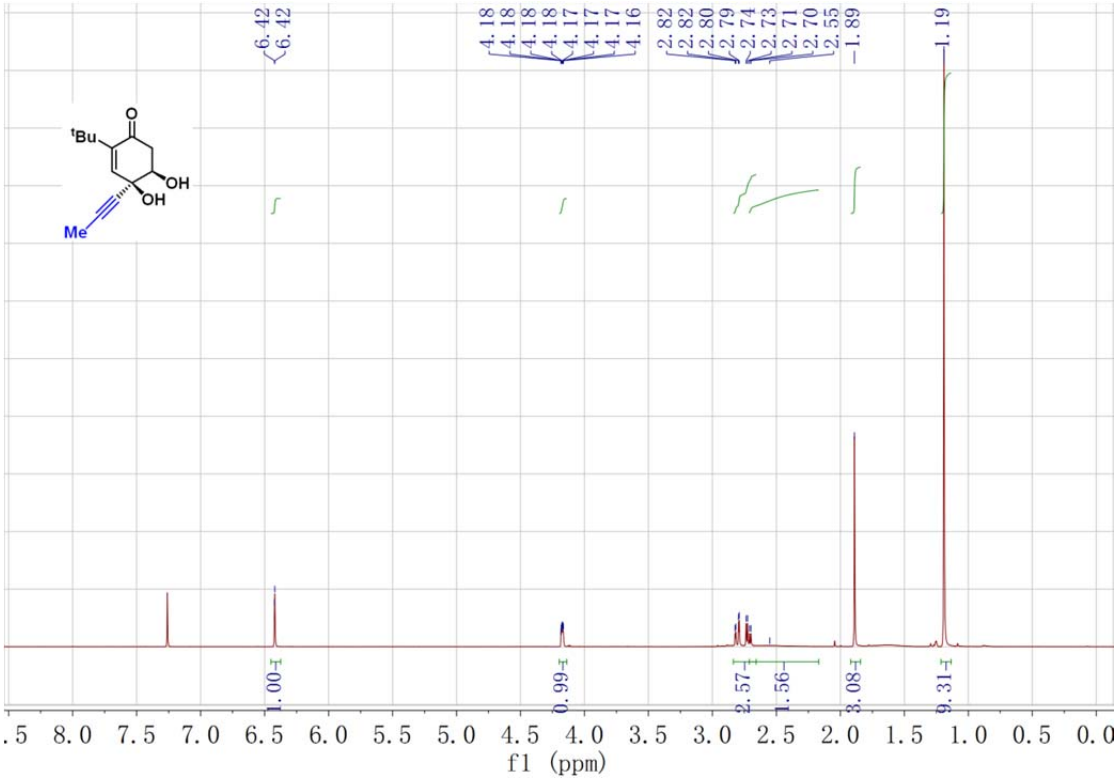
2j

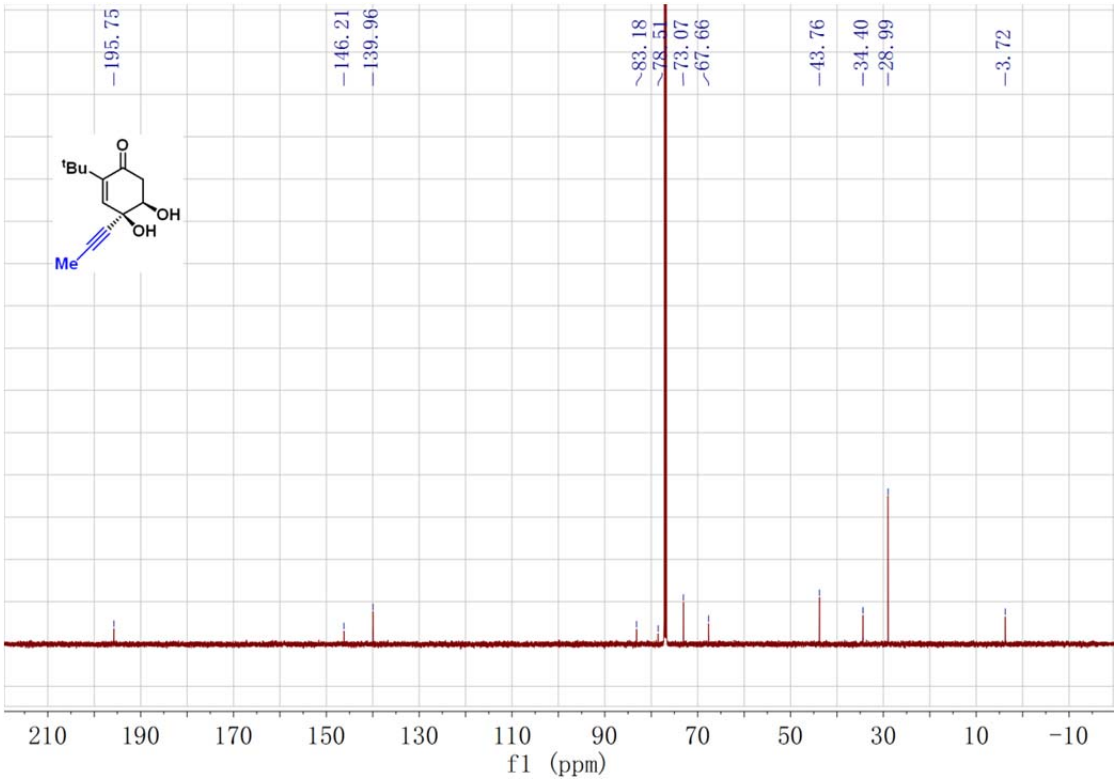

6.38
6.38
5.14
5.13
5.12
5.11
5.10
3.95
3.95
3.95
3.94
3.94
3.93
2.87
2.86
2.86
2.85
2.83
2.81
2.80
2.78
2.77
2.64
2.64
2.62
2.61
2.61
2.59
1.30
1.29
1.28
1.03
1.02
1.01
1.00
1.00
0.99
0.97
1.05
3.26
2.31
0.96
6.39
6.25
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

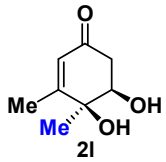

195.83
171.95
146.34
139.94
71.29
70.39
69.33
42.47
41.67
26.16
21.78
21.67
21.63
21.45
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


O
tBu
OH
OH
Me

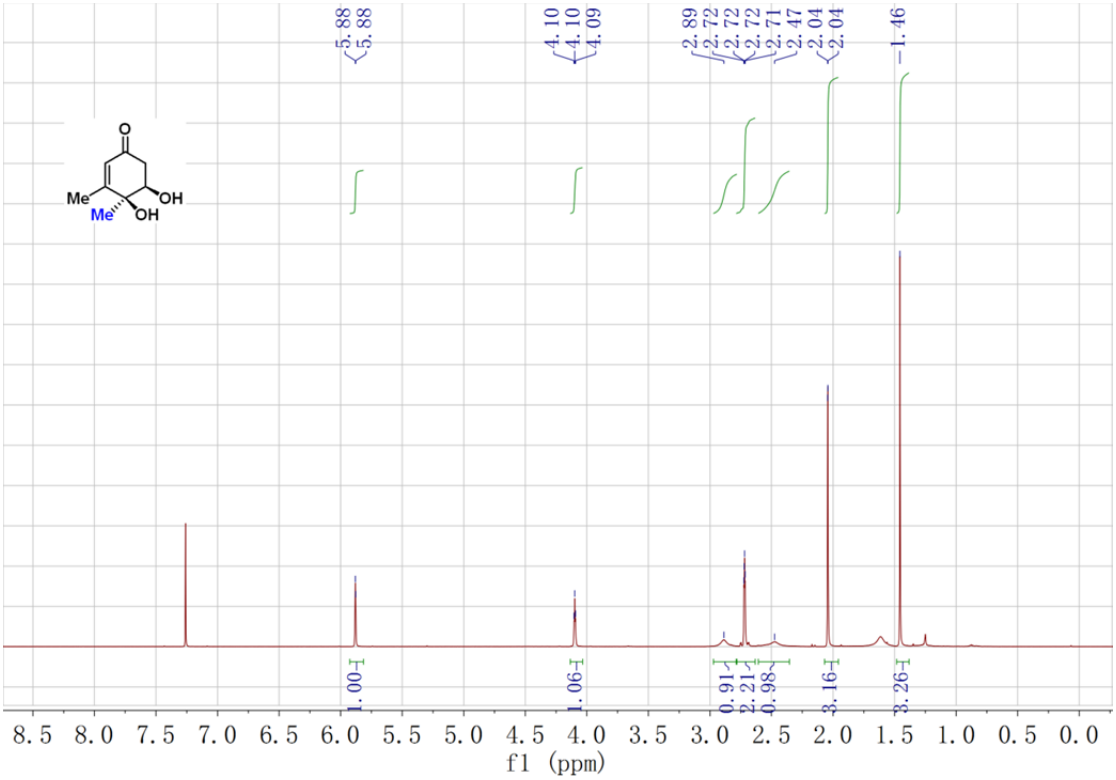
2k

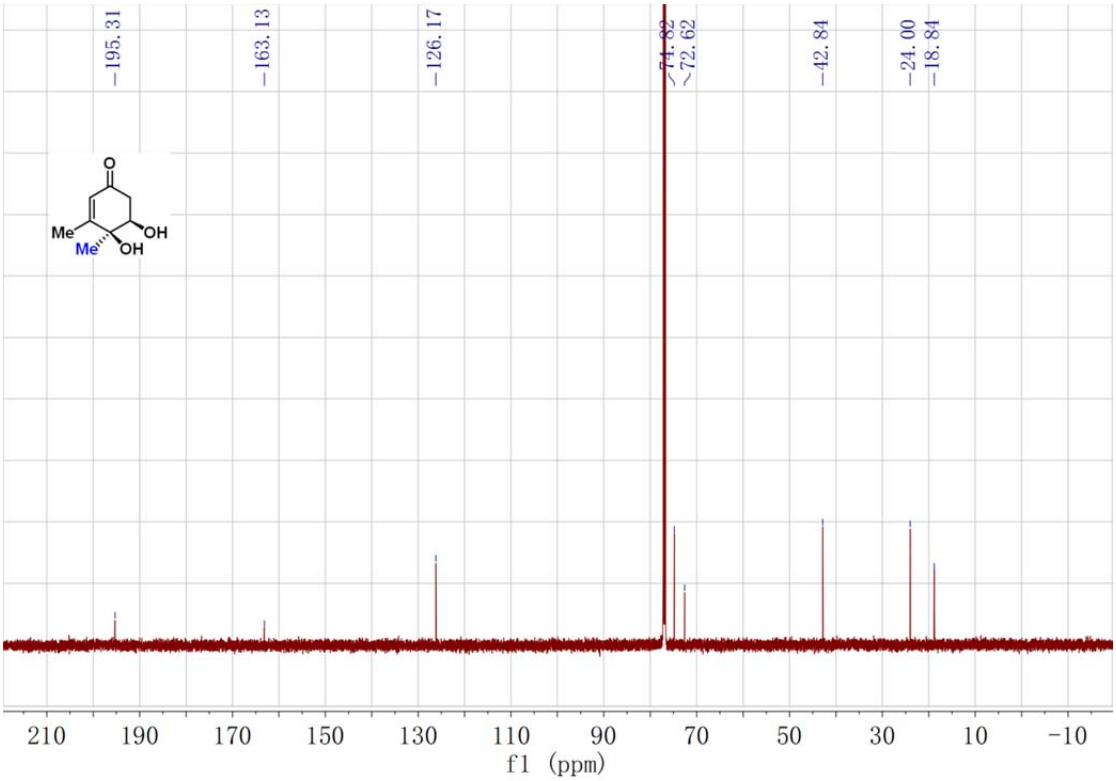

6.42
6.42
4.18
4.18
4.18
4.17
4.17
4.17
4.16
2.82
2.82
2.80
2.79
2.74
2.73
2.71
2.70
2.55
1.89
1.19
1.00
0.99
2.57
1.56
3.08
9.31
f1 (ppm)

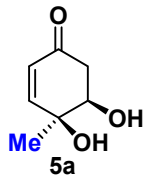

195.75
146.21
139.96
83.18
78.51
73.07
67.66
43.76
34.40
28.99
3.72
f1 (ppm)


O
Me
OH
Me
OH

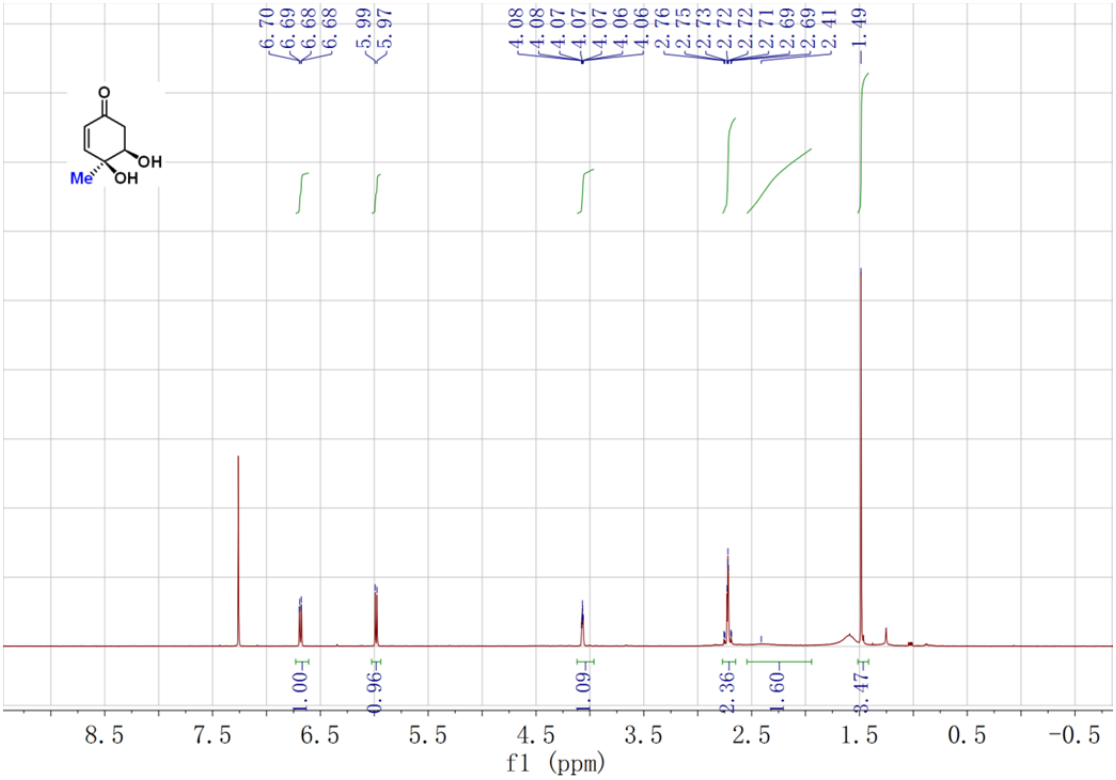
2l

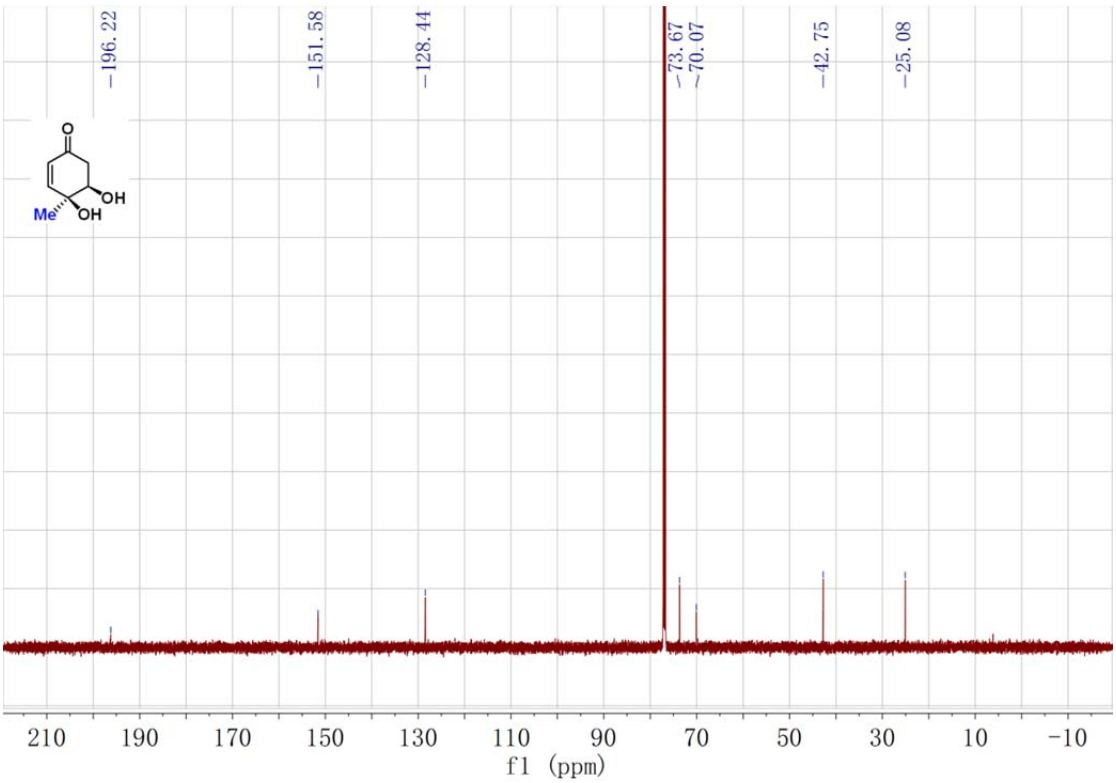

5.88
5.88
4.10
4.10
4.09
2.89
2.72
2.72
2.72
2.71
2.47
2.04
2.04
1.46
1.00
1.06
0.91
2.21
0.98
3.16
3.26
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

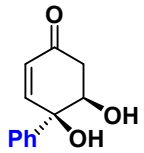

195.31
163.13
126.17
74.82
72.62
42.84
24.00
18.84
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)


O
OH
Me
OH

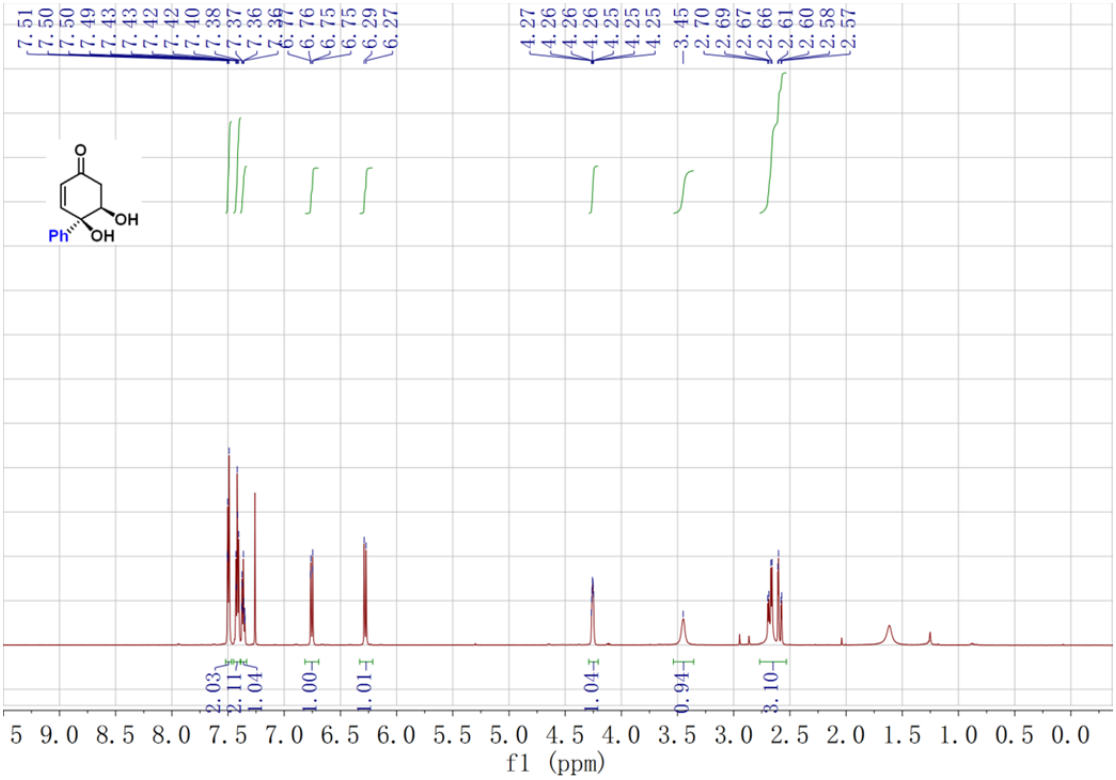
5a

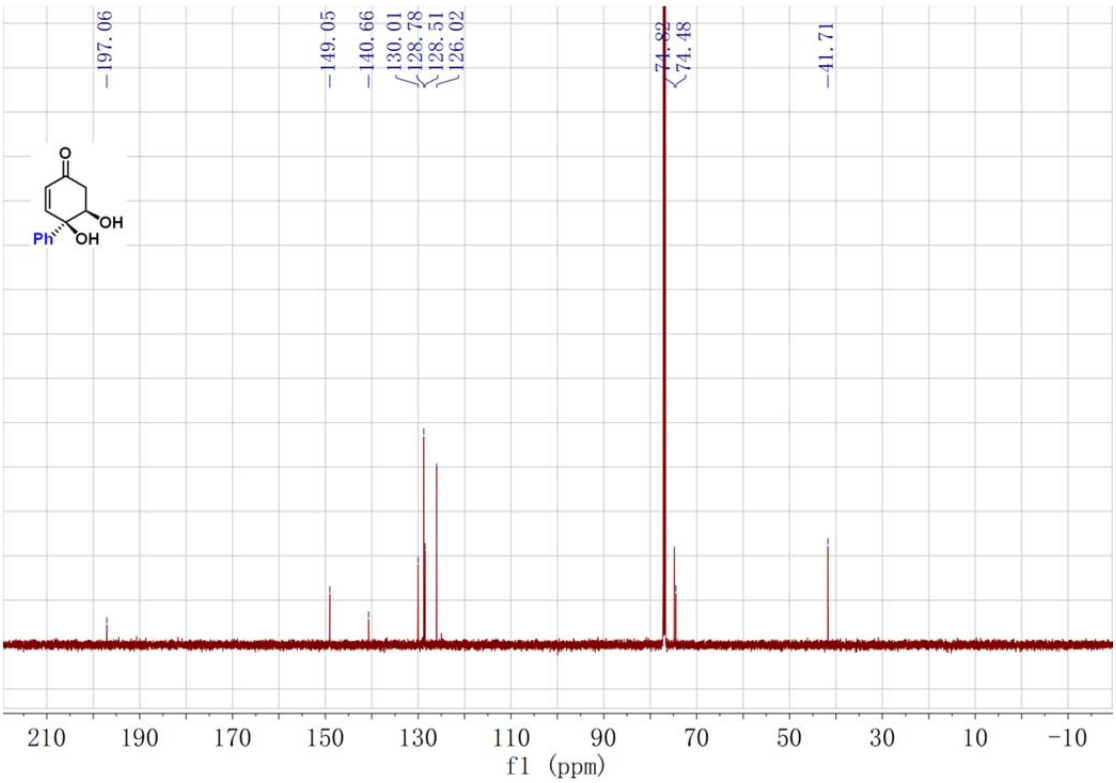

6.70
6.69
6.68
6.68
5.99
5.97
4.08
4.08
4.07
4.07
4.07
4.06
4.06
2.76
2.75
2.73
2.72
2.72
2.71
2.69
2.69
2.41
1.49
1.00
0.96
1.09
2.36
1.60
3.47
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

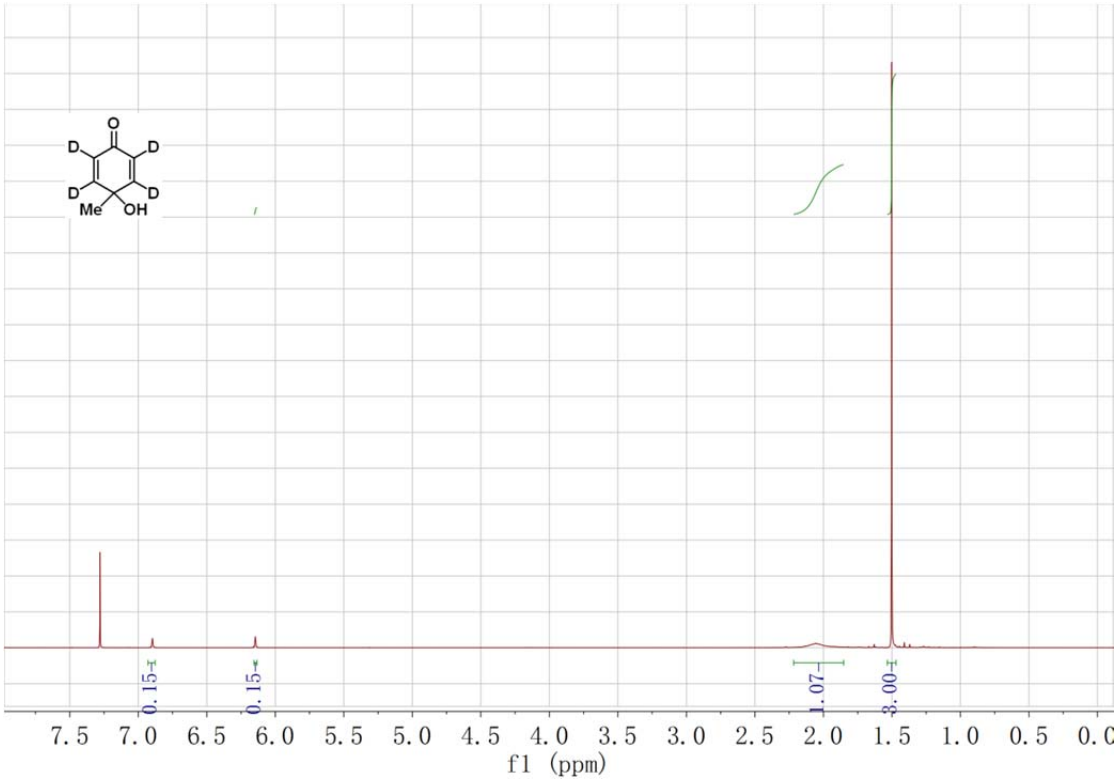

196.22
151.58
128.44
73.67
70.07
42.75
25.08
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


O
OH
Ph
OH

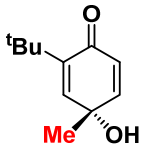
5b


7.51
7.50
7.50
7.49
7.43
7.42
7.42
7.40
7.38
7.37
7.36
6.77
6.76
6.75
6.75
6.29
6.27
4.27
4.26
4.26
4.26
4.25
4.25
4.25
3.45
2.70
2.69
2.67
2.66
2.61
2.60
2.58
2.57
2.03
2.11
1.04
1.00
1.01
1.04
0.94
3.10
f1 (ppm)

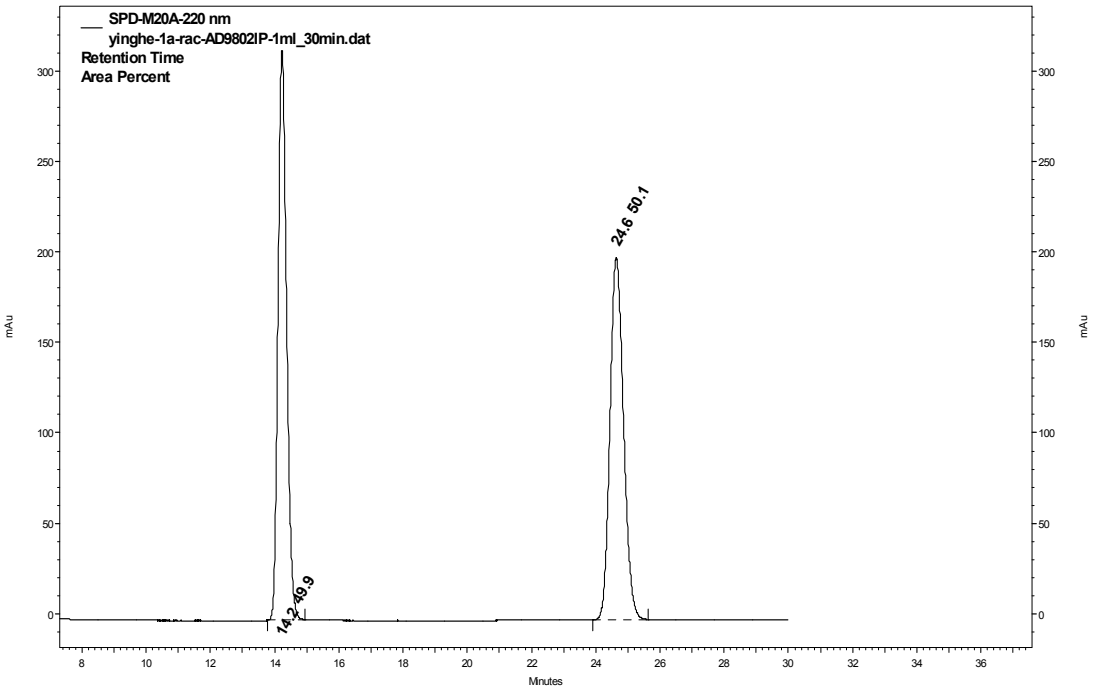

197.06
149.05
140.66
130.01
128.78
128.51
126.02
74.92
74.48
41.71
f1 (ppm)

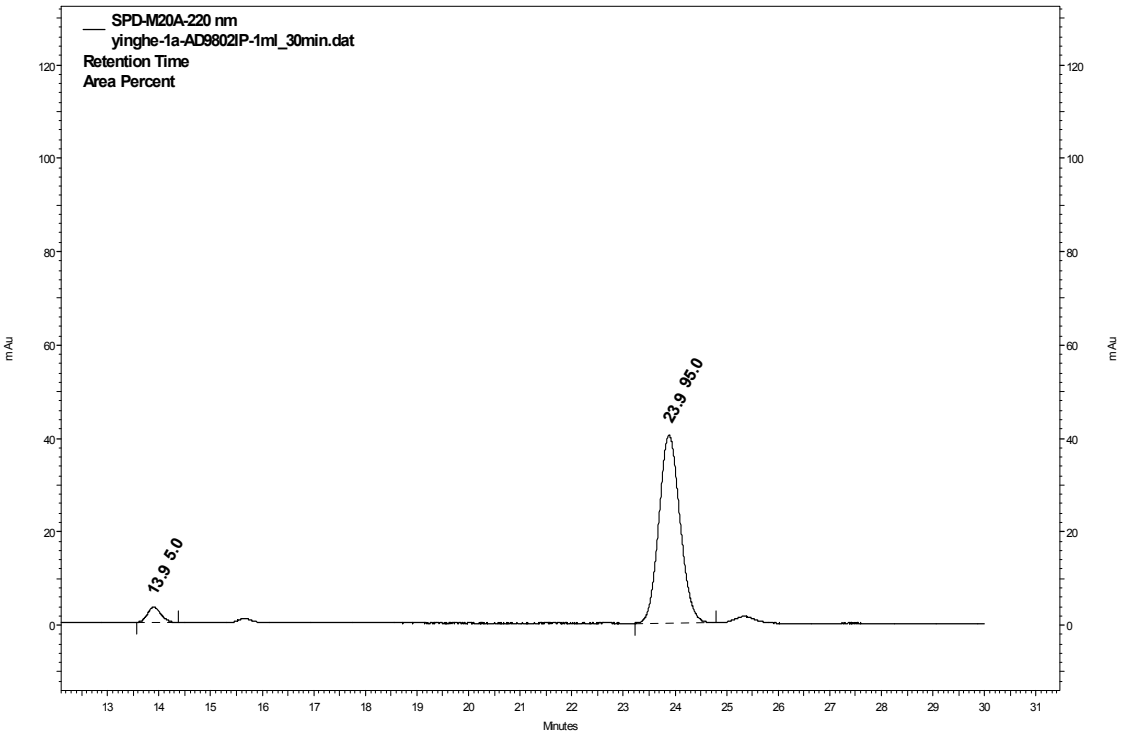

O
D
D
D
D
Me
OH
0.15
0.15
1.07
3.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

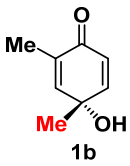
HPLC Data


O
tBu
Me
OH

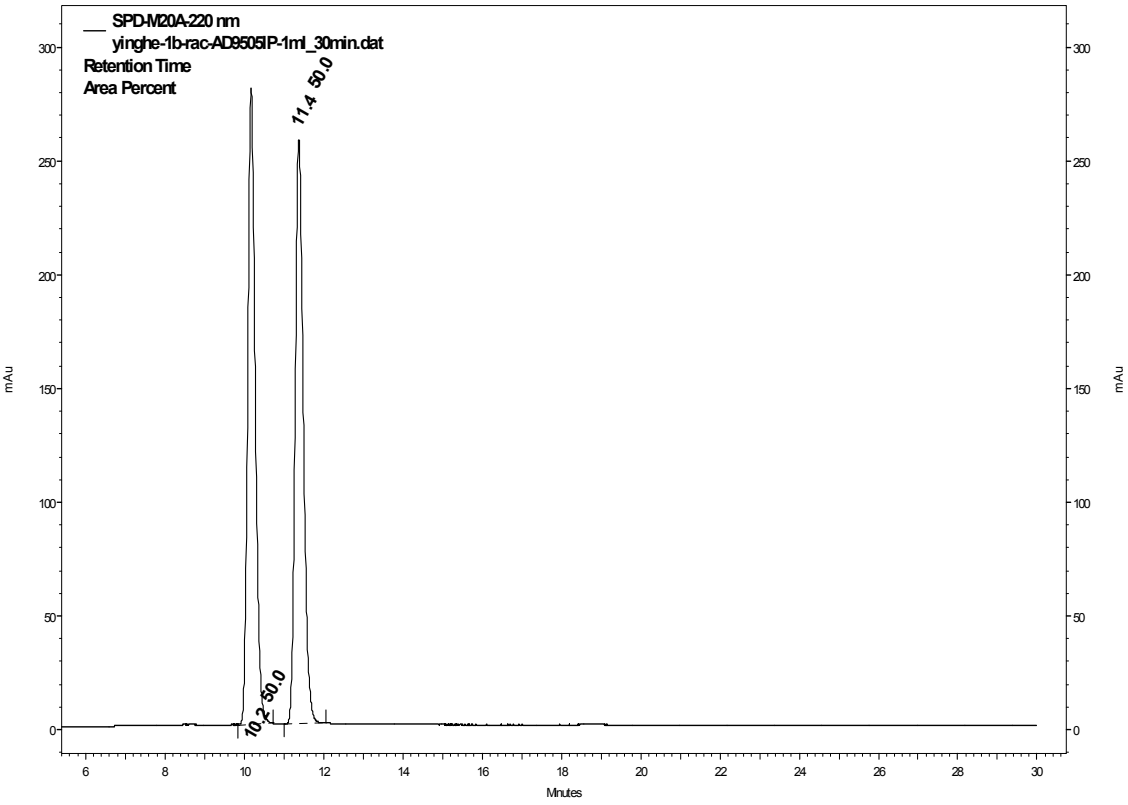
1a

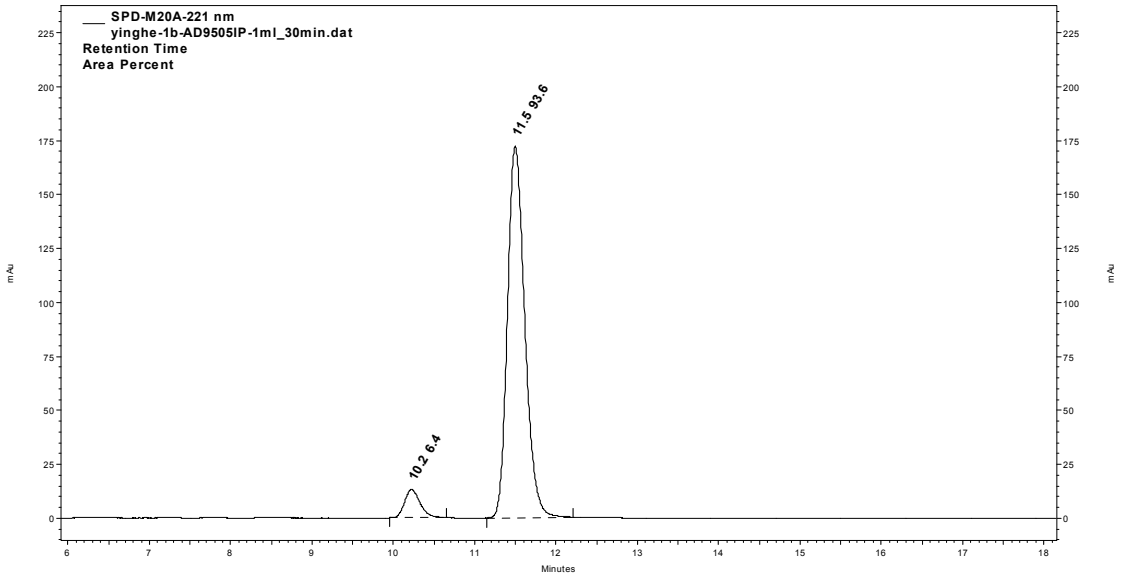

SPD-M20A-220 nm
yinghe-1a-rac-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
14.2 49.9
24.6 50.1
mAu
Minutes

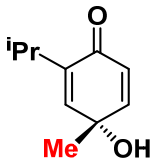

SPD-M20A-220 nm
yinghe-1a-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
13.9 5.0
23.9 95.0
mAu
Minutes


O
Me
Me
OH

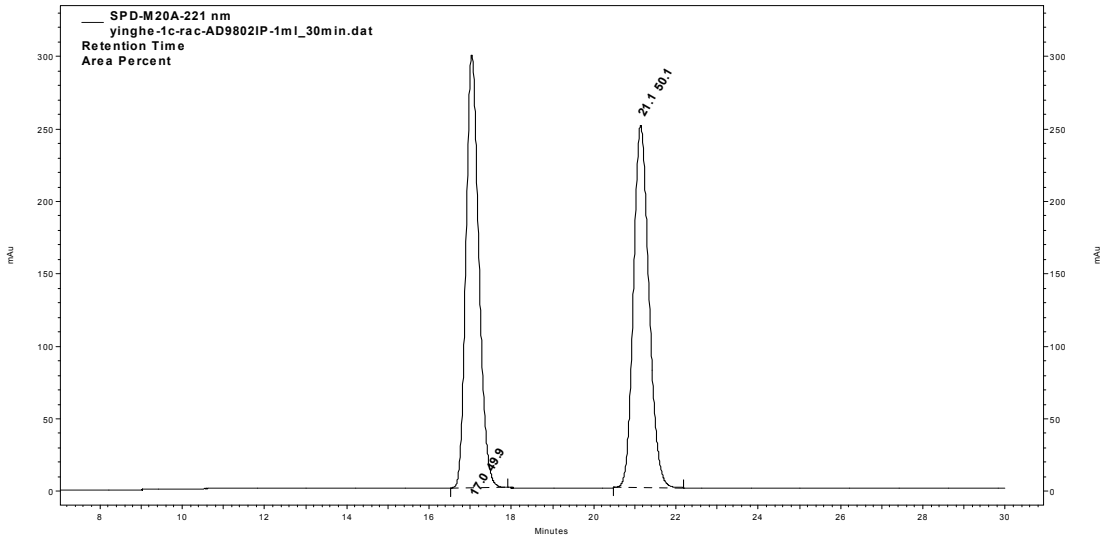
1b

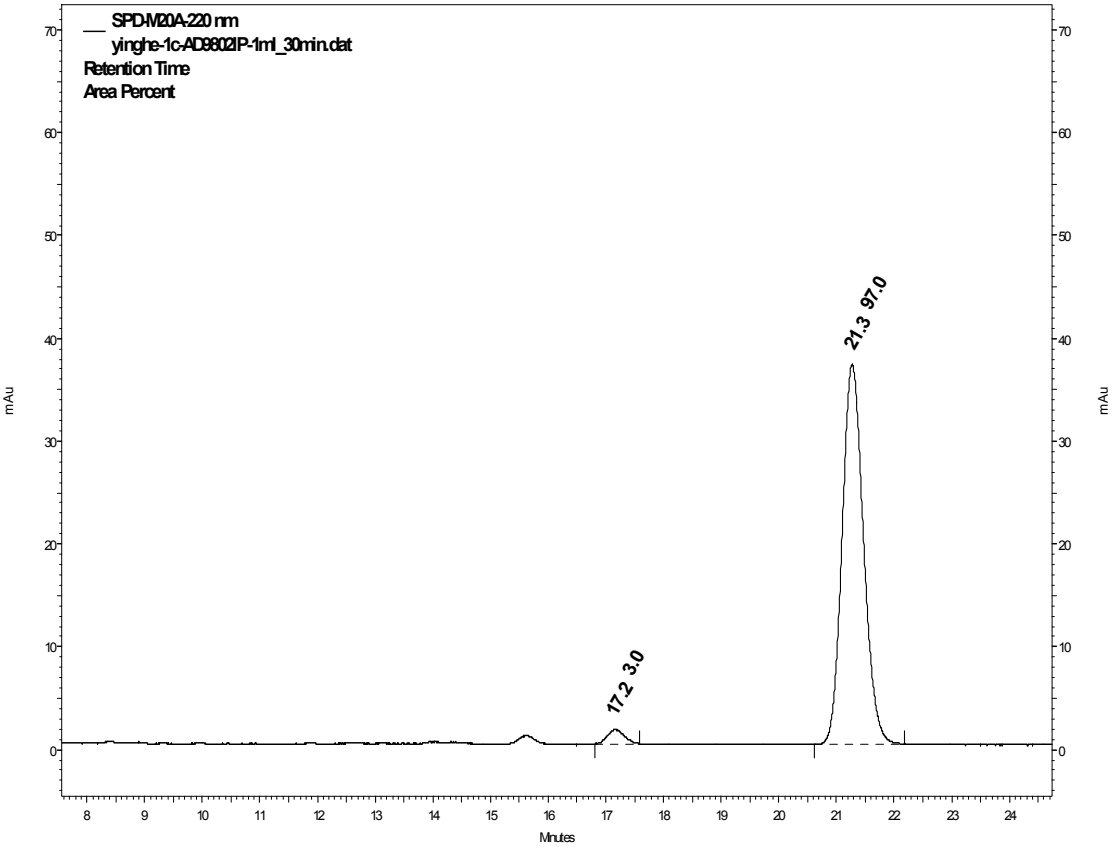

SPD-M20A-220 nm
yinghe-1b-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
11.4 50.0
10.2 50.0
mAu
Minutes

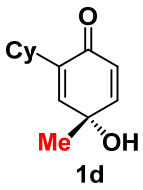

SPD-M20A-221 nm
yinghe-1b-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
11.5 93.6
10.2 6.4
mAu
Minutes


O
iPr
Me
OH

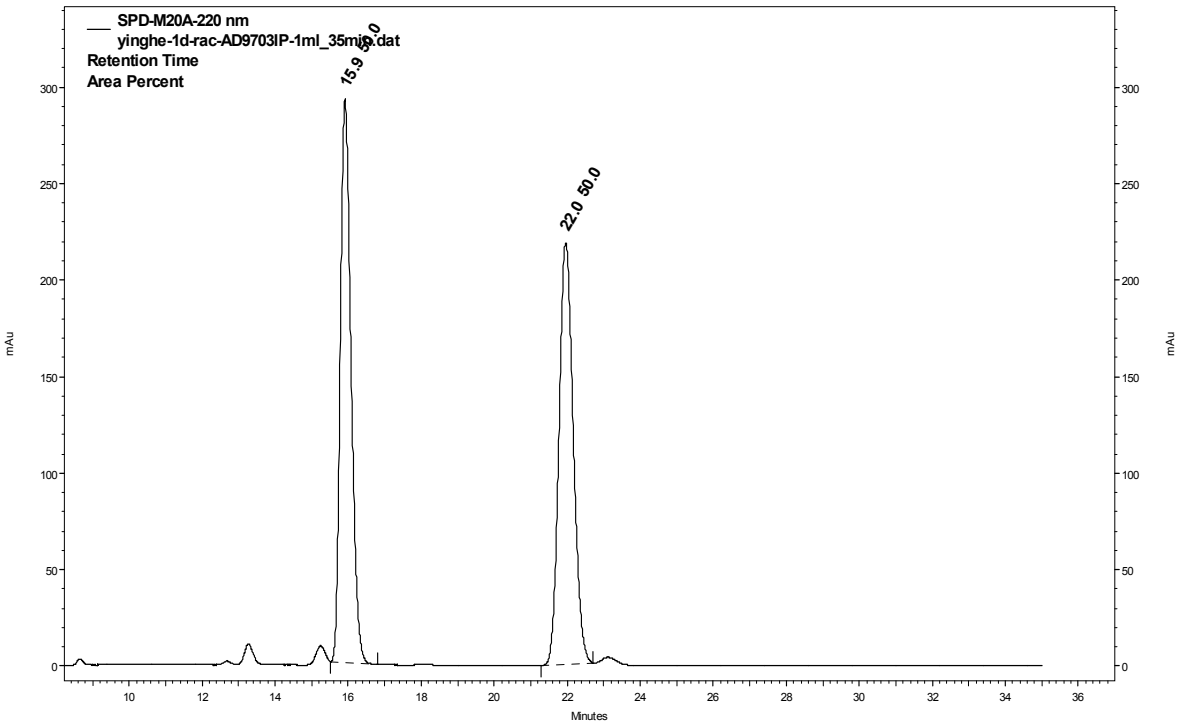
1c

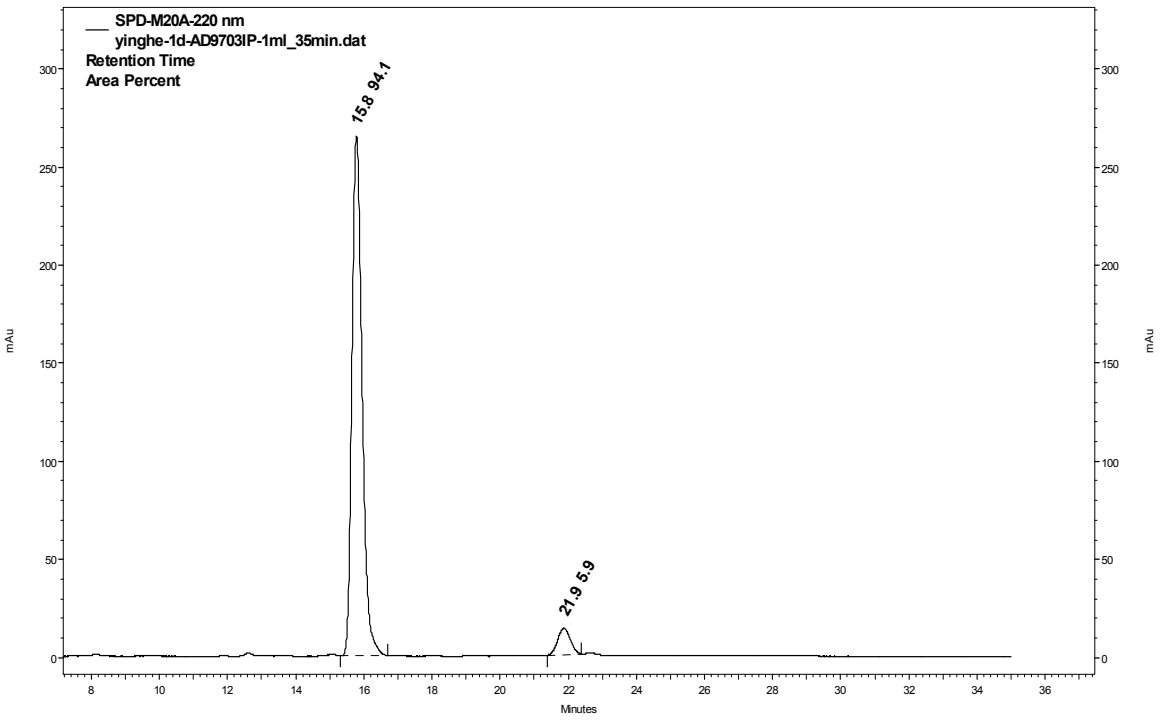

SPD-M20A-221 nm
yinghe-1c-rac-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
17.0 49.9
21.1 50.1
mAu
Minutes

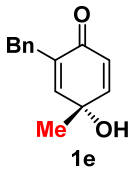

SPD-M20A-220 nm
yinghe-1c-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
17.2 3.0
21.3 97.0
mAu
Minutes


O
Cy
Me
OH

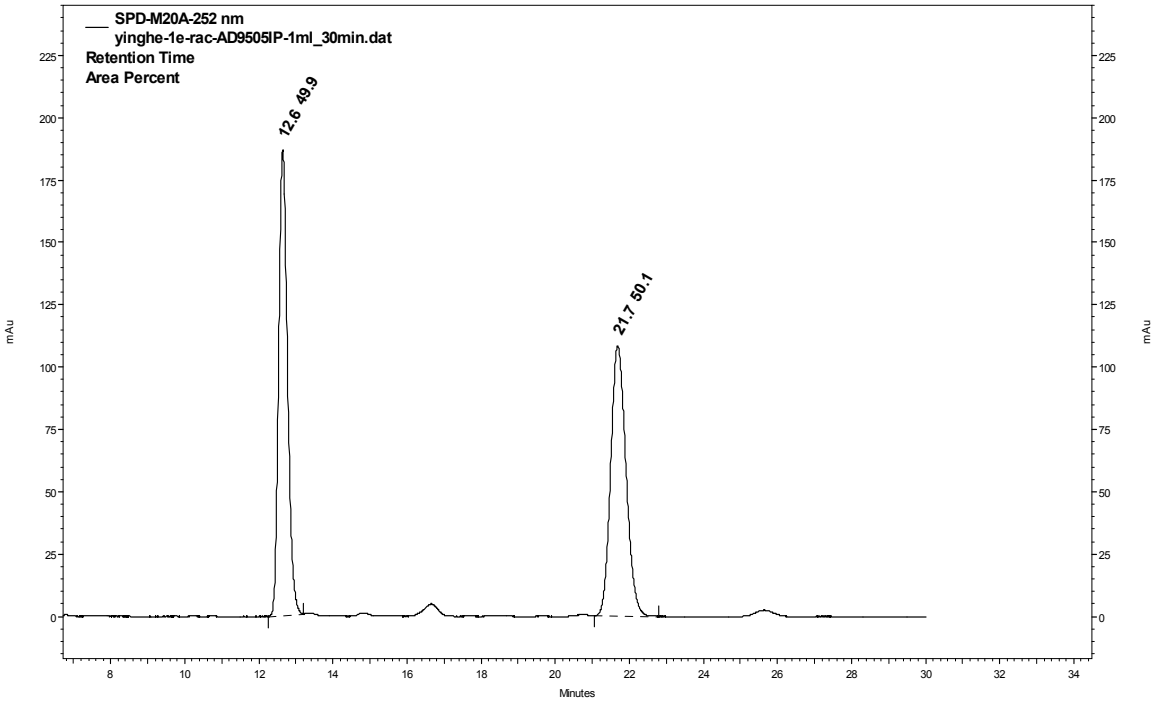
1d

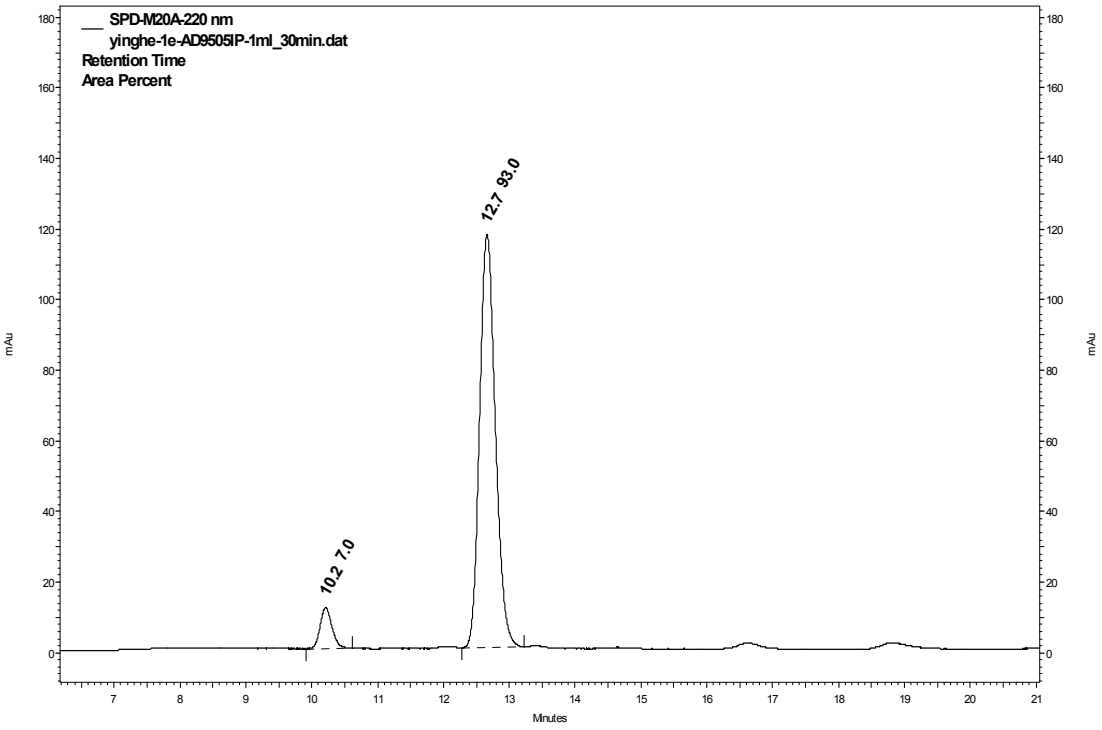

SPD-M20A-220 nm
yinghe-1d-rac-AD9703IP-1ml_35min.dat
Retention Time
Area Percent
15.9 50.0
22.0 50.0
mAu
Minutes

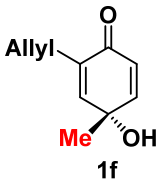

SPD-M20A-220 nm
yinghe-1d-AD9703IP-1ml_35min.dat
Retention Time
Area Percent
15.8 94.1
21.9 5.9
mAu
Minutes


O
Bn
Me
OH

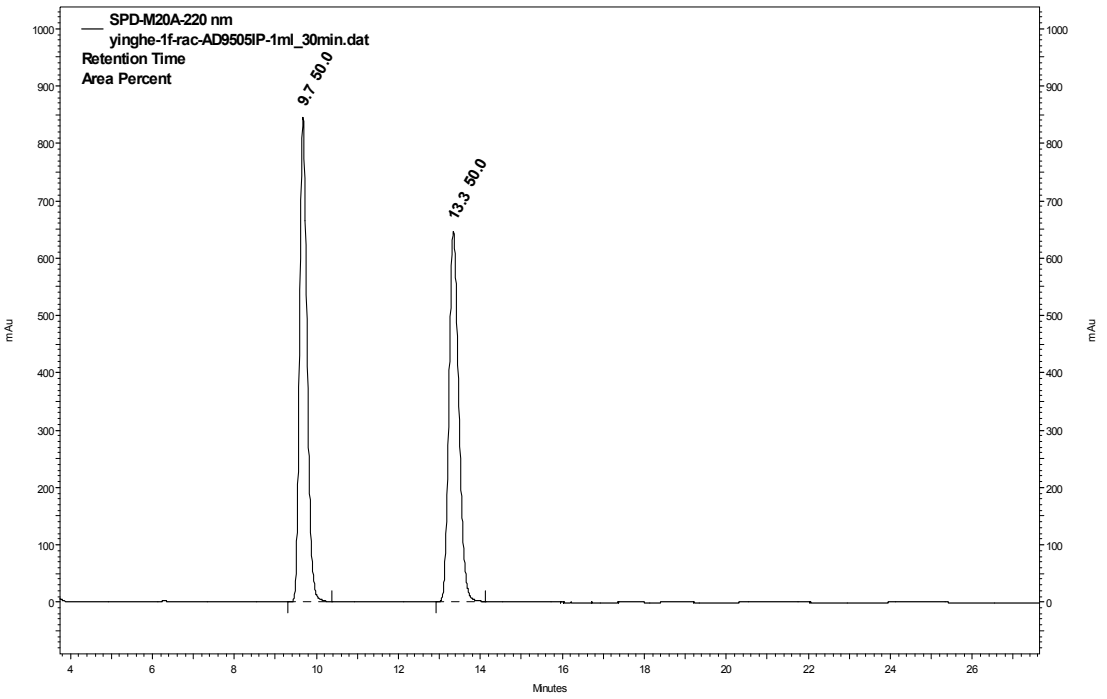
1e

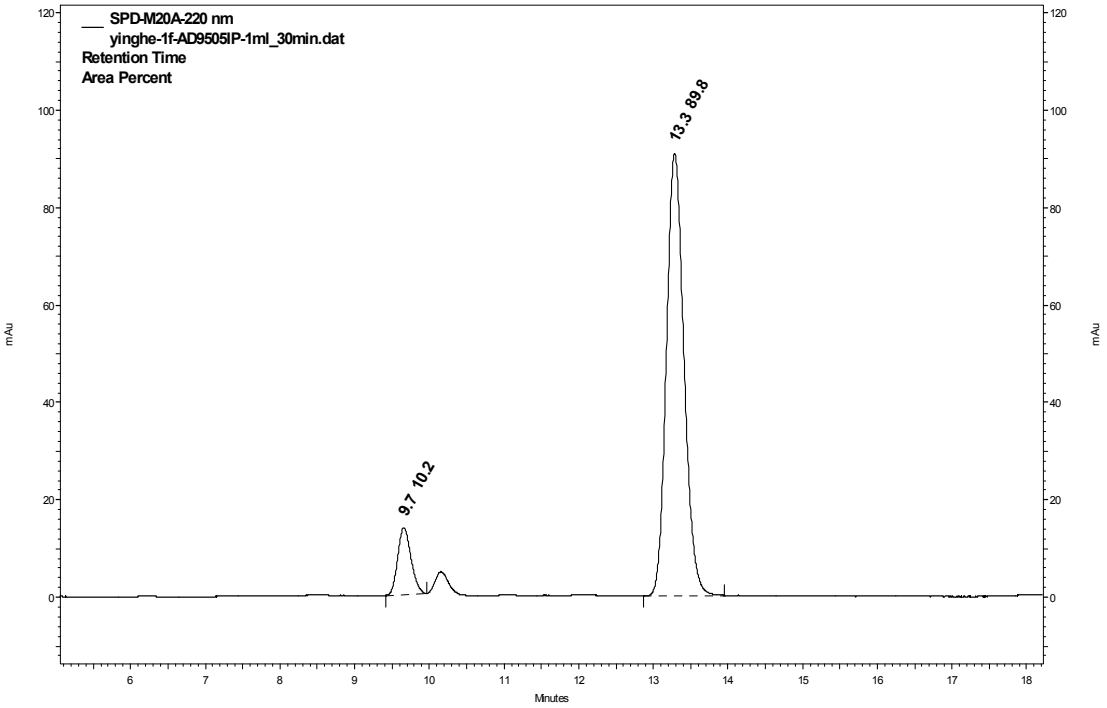

SPD-M20A-252 nm
yinghe-1e-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
12.6 49.9
21.7 50.1
mAu
Minutes

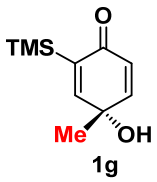

SPD-M20A-220 nm
yinghe-1e-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
12.7 93.0
10.2 7.0
mAu
Minutes


O
Allyl
Me
OH

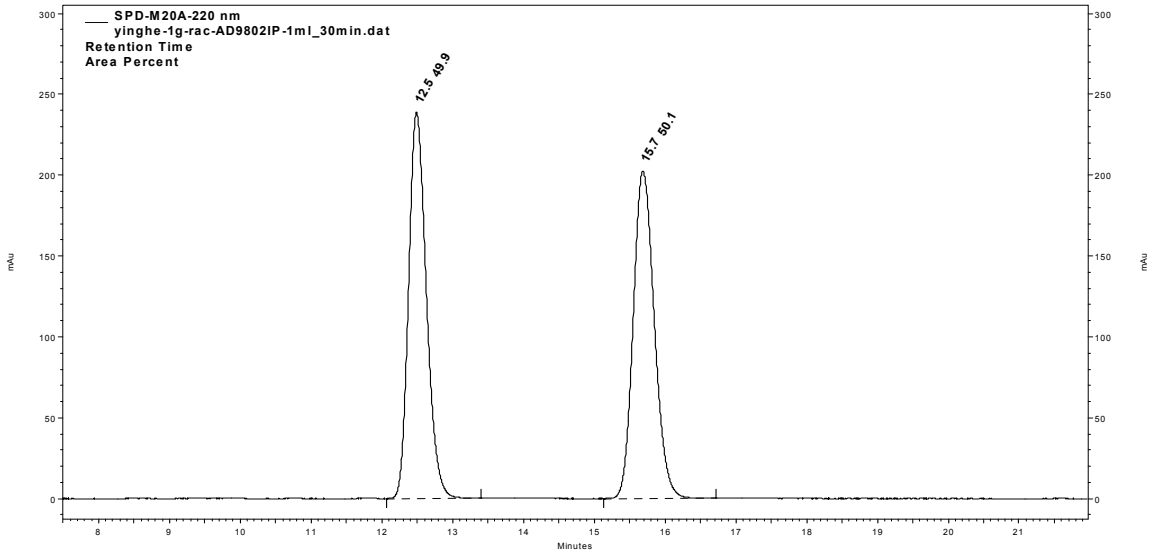
1f

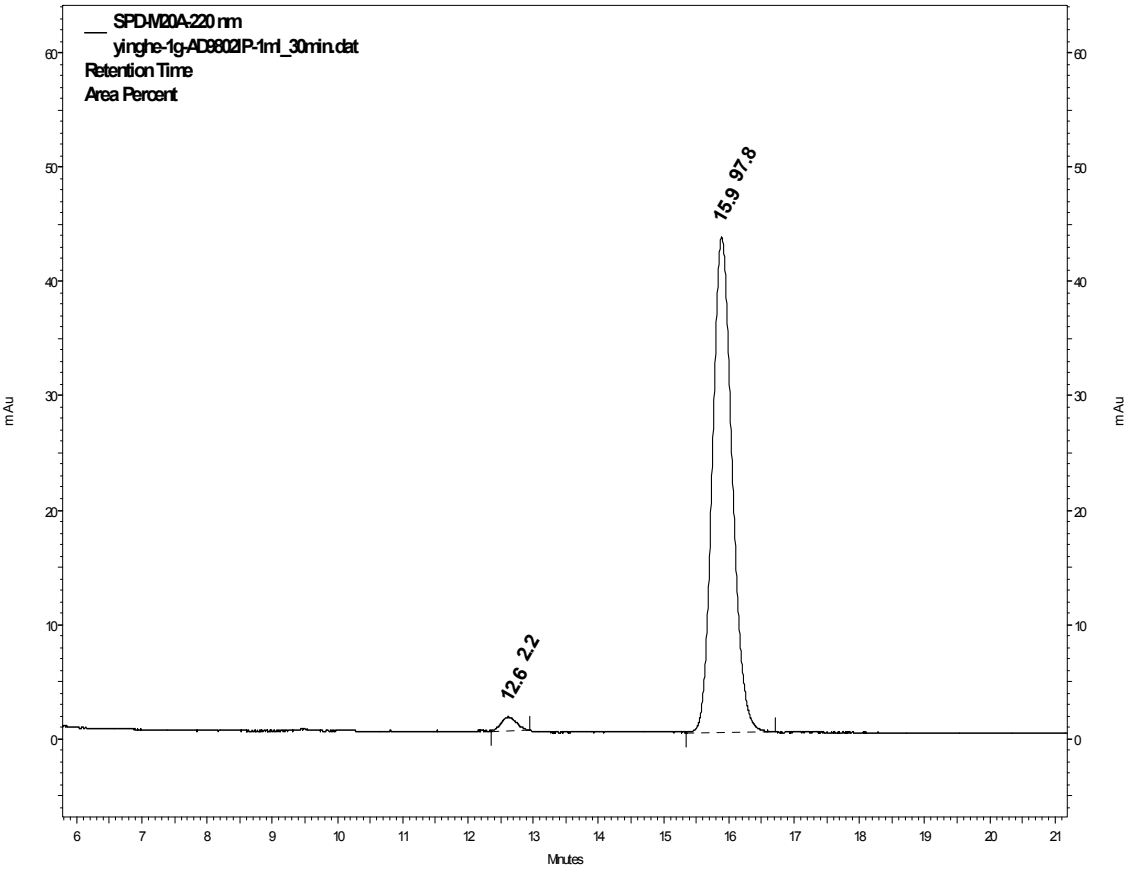

SPD-M20A-220 nm
yinghe-1f-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
9.7 50.0
13.3 50.0
mAu
Minutes

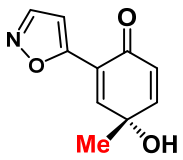

SPD-M20A-220 nm
yinghe-1f-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
9.7 10.2
13.3 89.8
mAu
Minutes


O
TMS
Me
OH

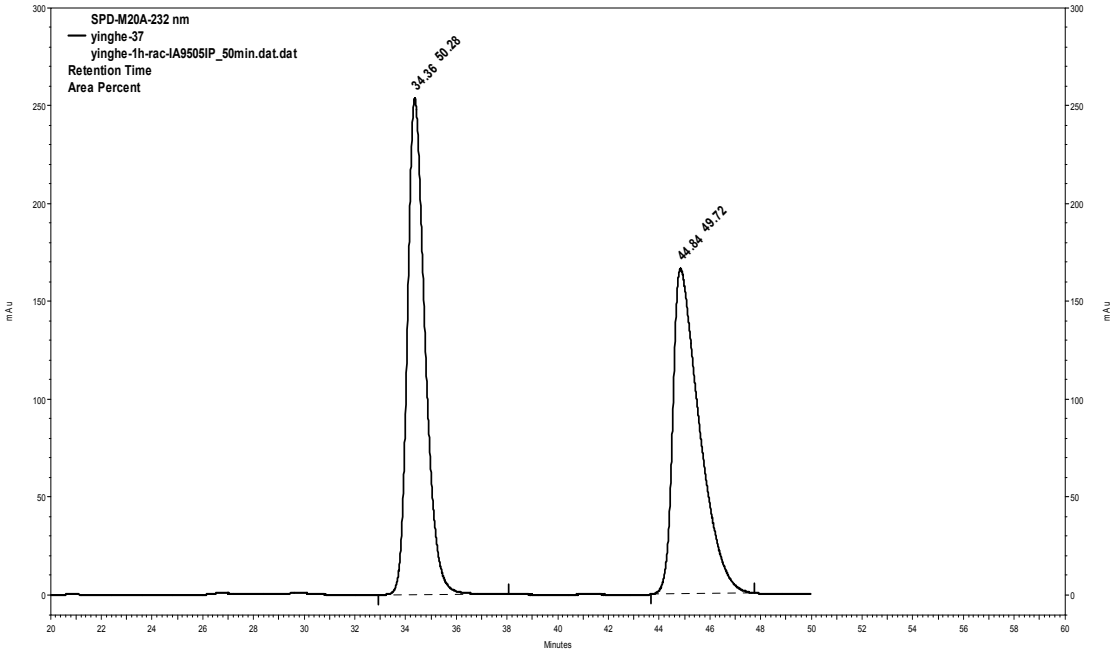
1g

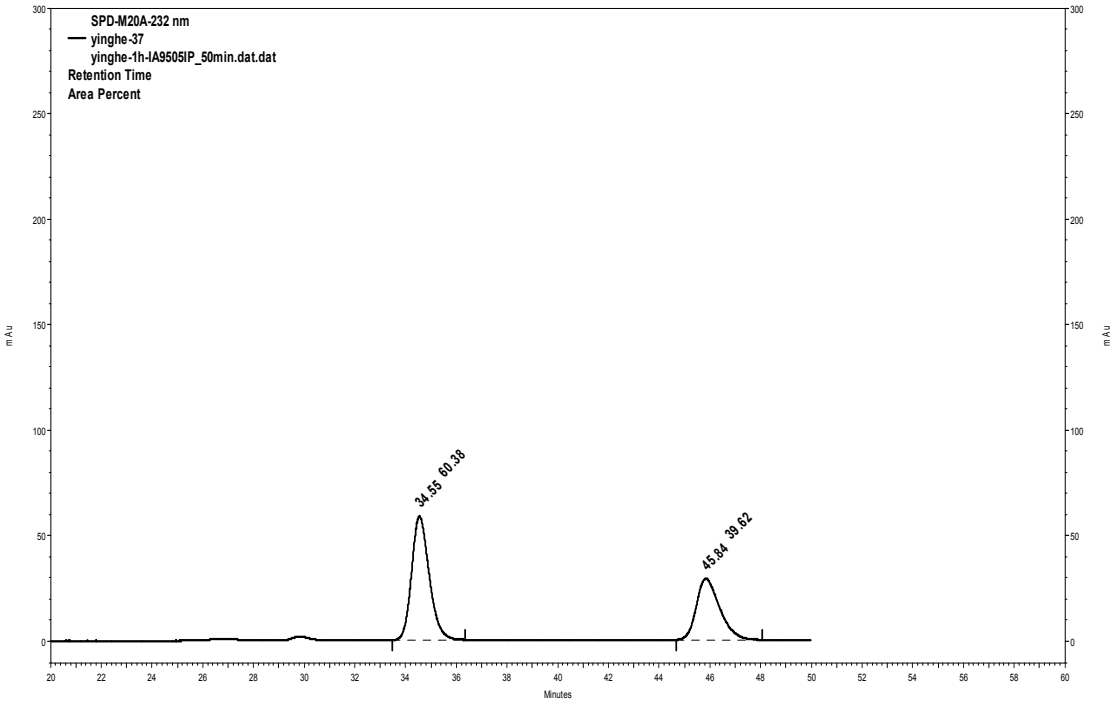

SPD-M20A-220 nm
yinghe-1g-rac-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
12.5 49.9
15.7 50.1
mAu
Minutes

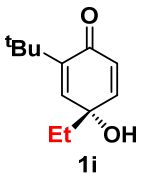

SPD-M20A-220 nm
yinghe-1g-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
15.9 97.8
12.6 2.2
mAu
Minutes


O
N
O
Me
OH

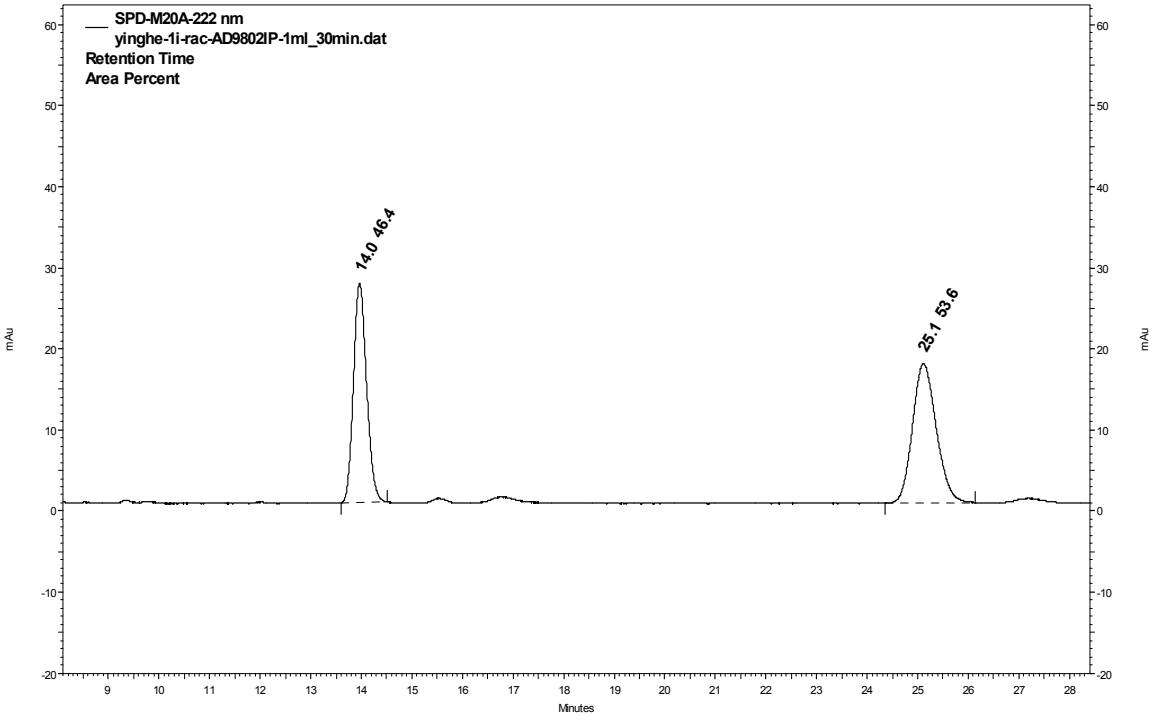
1h

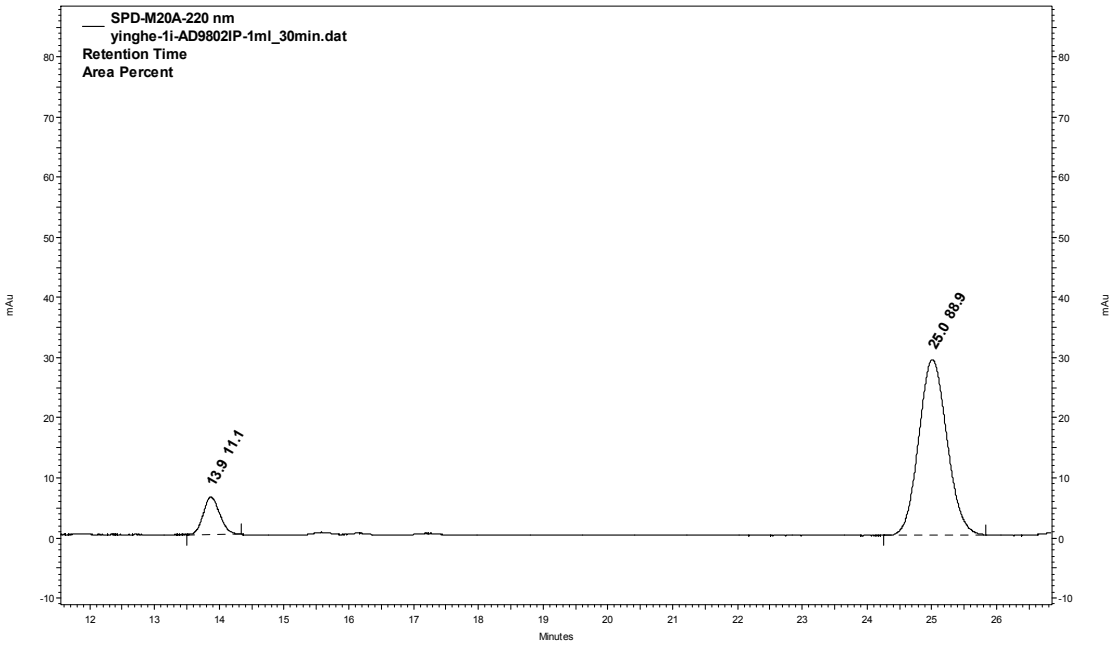

SPD-M20A-232 nm
yinghe-37
yinghe-1h-rac-IA9505IP_50min.dat.dat
Retention Time
Area Percent
34.36 50.28
44.84 49.72
mAu
Minutes

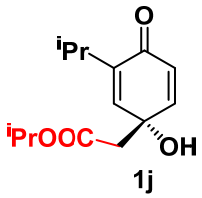

SPD-M20A-232 nm
yinghe-37
yinghe-1h-IA9505IP_50min.dat.dat
Retention Time
Area Percent
34.55 60.38
45.84 39.62
mAu
Minutes


O
tBu
Et
OH

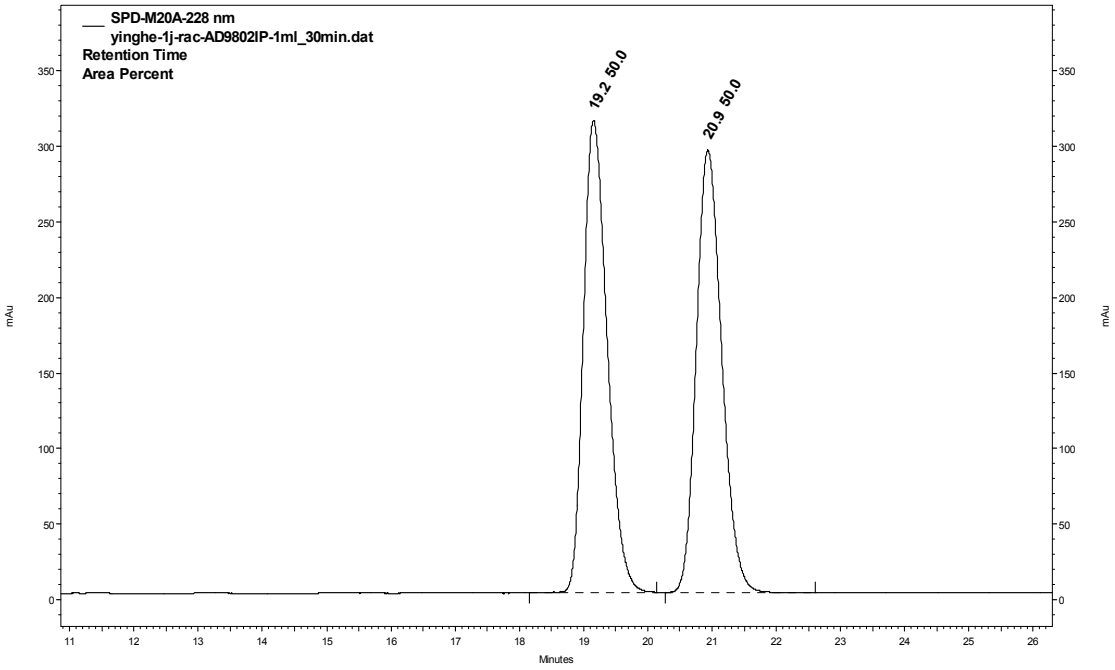
1i

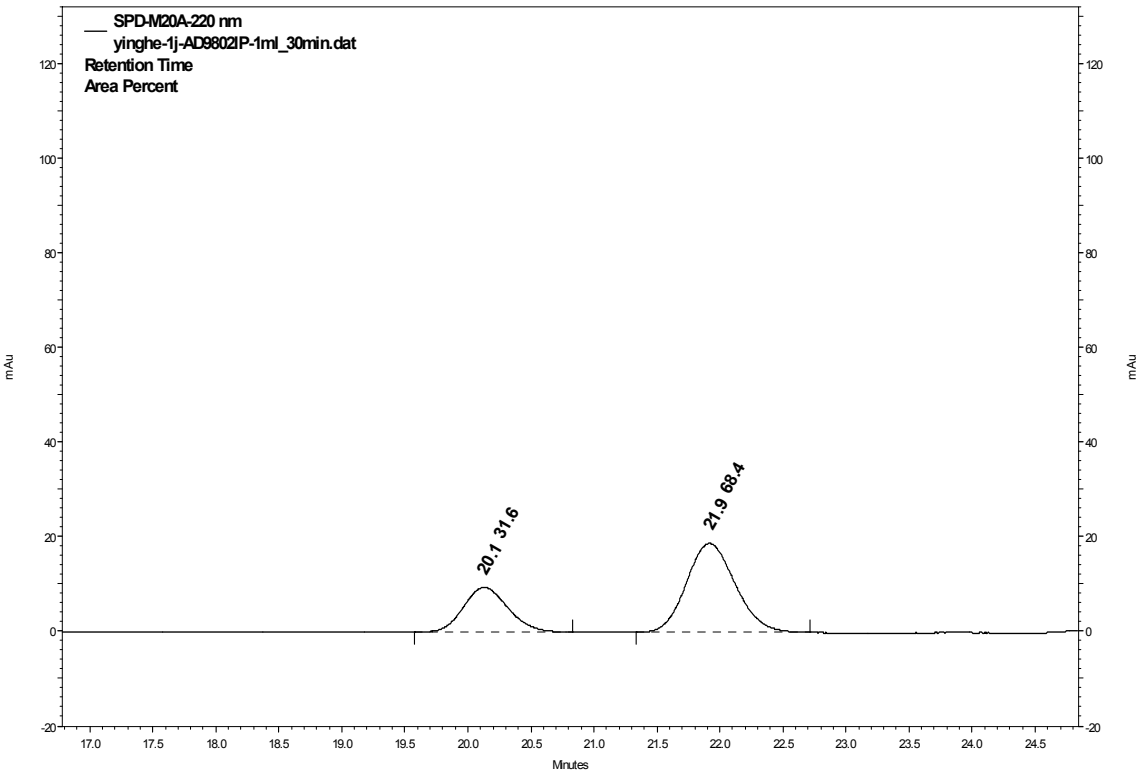

SPD-M20A-222 nm
yinghe-1i-rac-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
14.0 46.4
25.1 53.6
mAu
Minutes

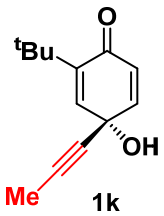

SPD-M20A-220 nm
yinghe-1i-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
13.9 11.1
25.0 88.9
mAu
Minutes


O
iPr
iPrOOC
OH

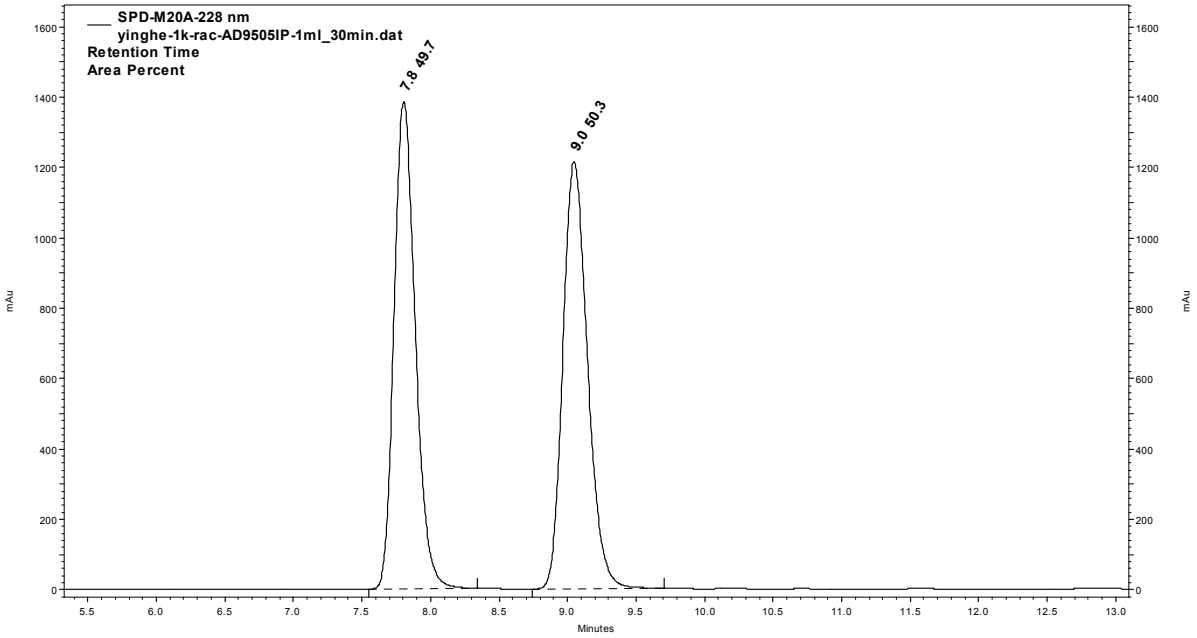
1j

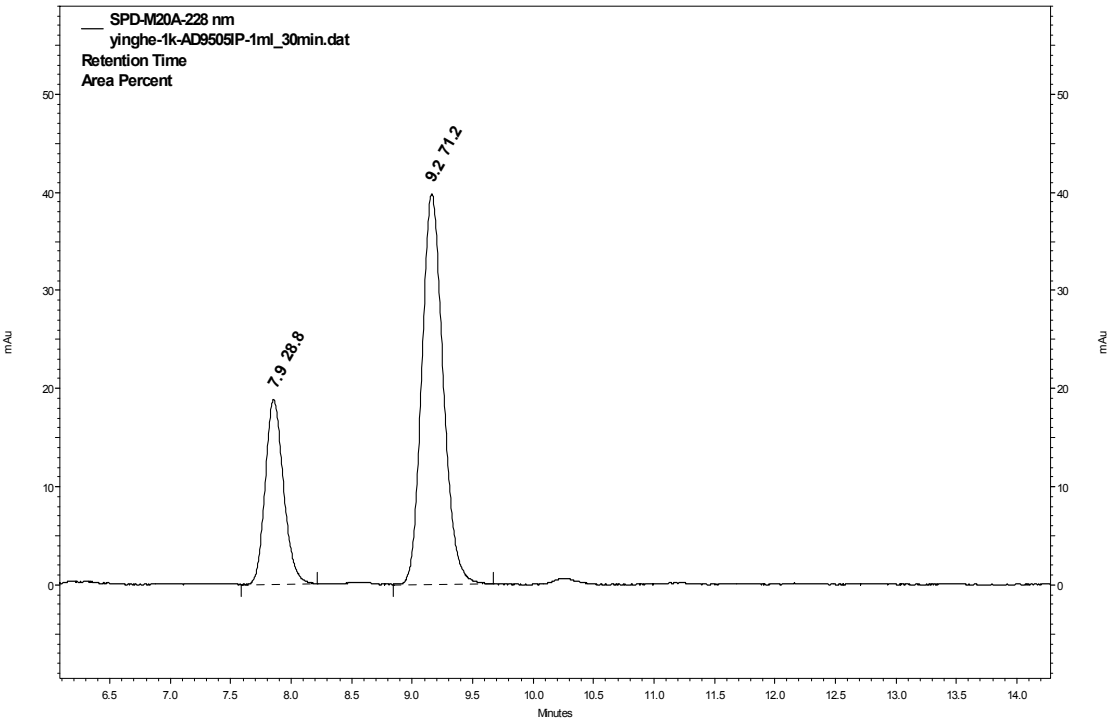

SPD-M20A-228 nm
yinghe-1j-rac-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
19.2 50.0
20.9 50.0
mAu
Minutes

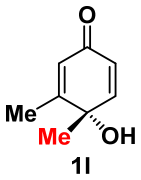

SPD-M20A-220 nm
yinghe-1j-AD9802IP-1ml_30min.dat
Retention Time
Area Percent
20.1 31.6
21.9 68.4
mAu
Minutes


O
tBu
OH
Me

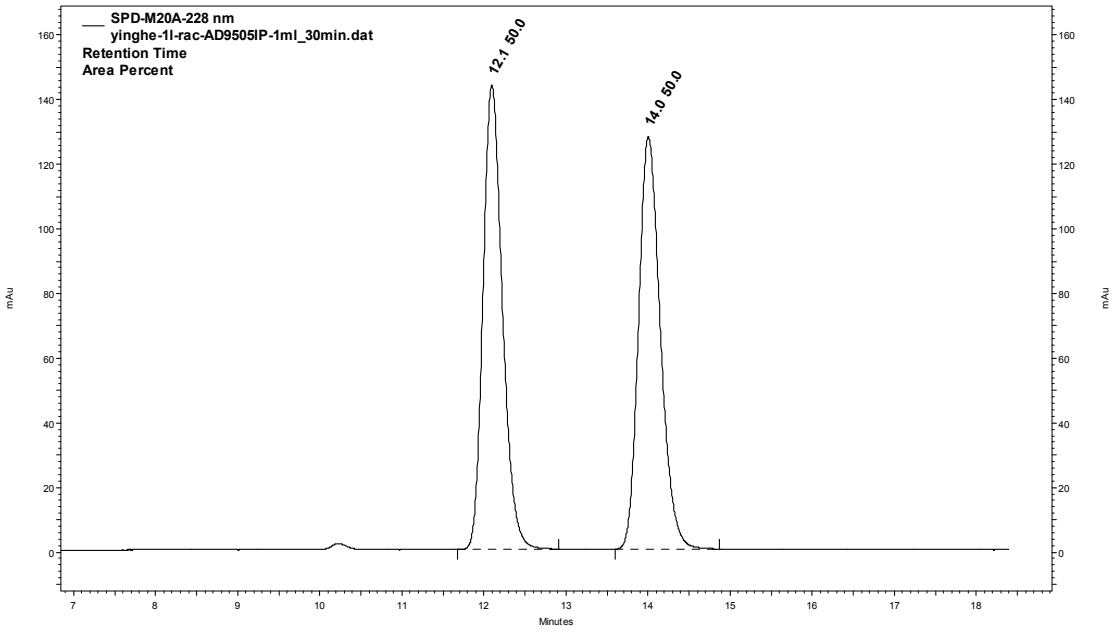
1k

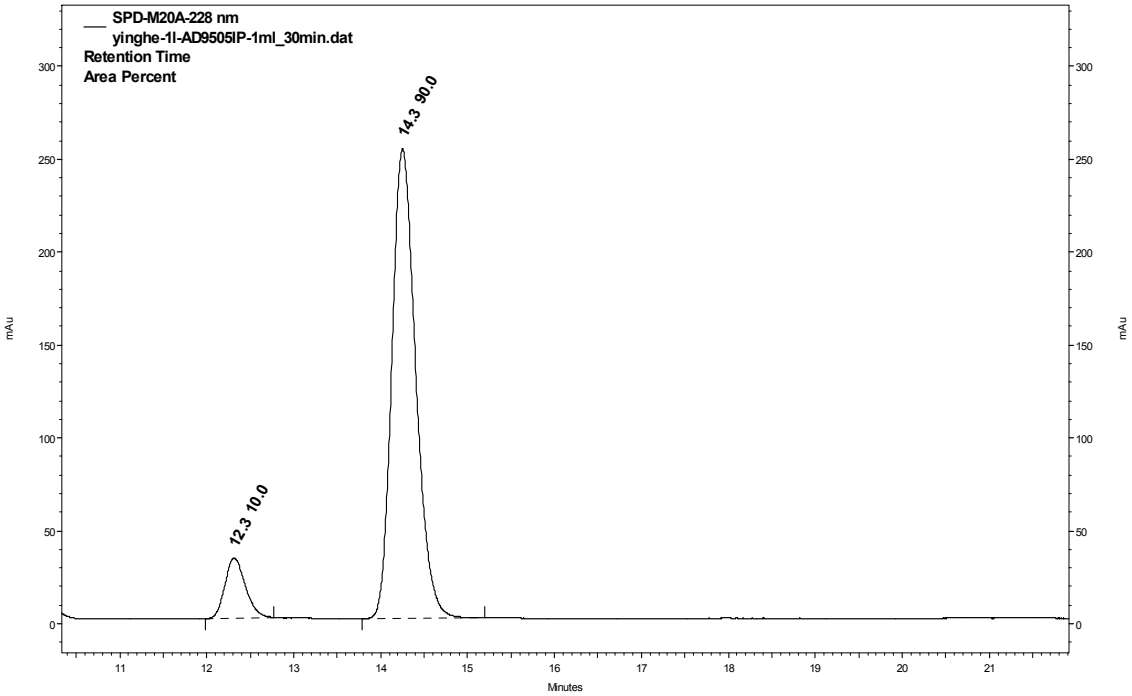

SPD-M20A-228 nm
yinghe-1k-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
7.8 49.7
9.0 50.3
mAu
Minutes

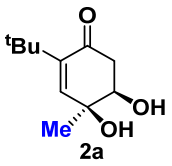

SPD-M20A-228 nm
yinghe-1k-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
7.9 28.8
9.2 71.2
mAu
Minutes


O
Me
Me
OH

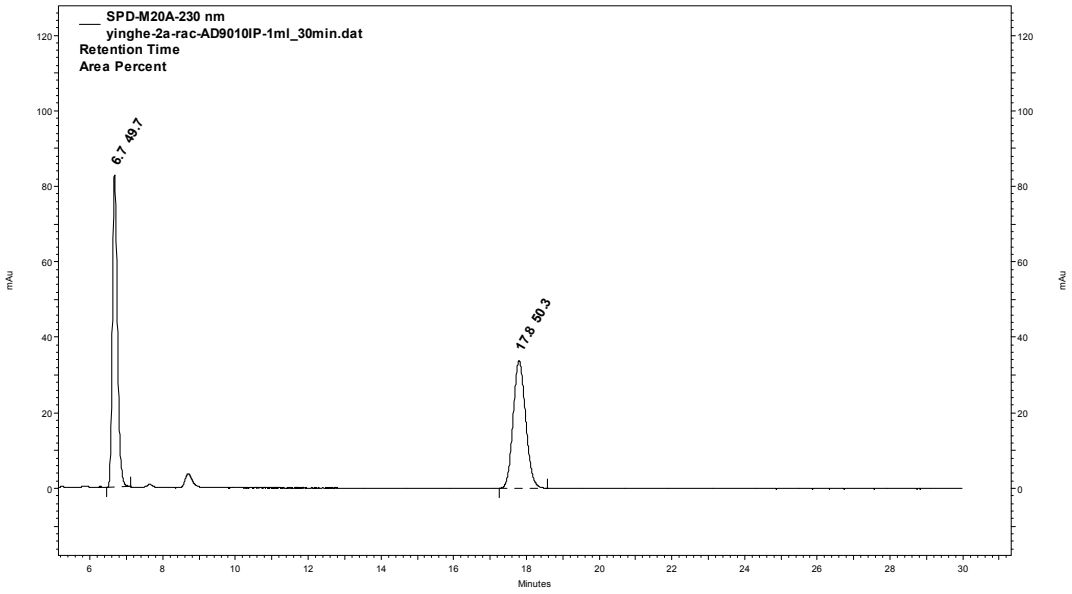
1l

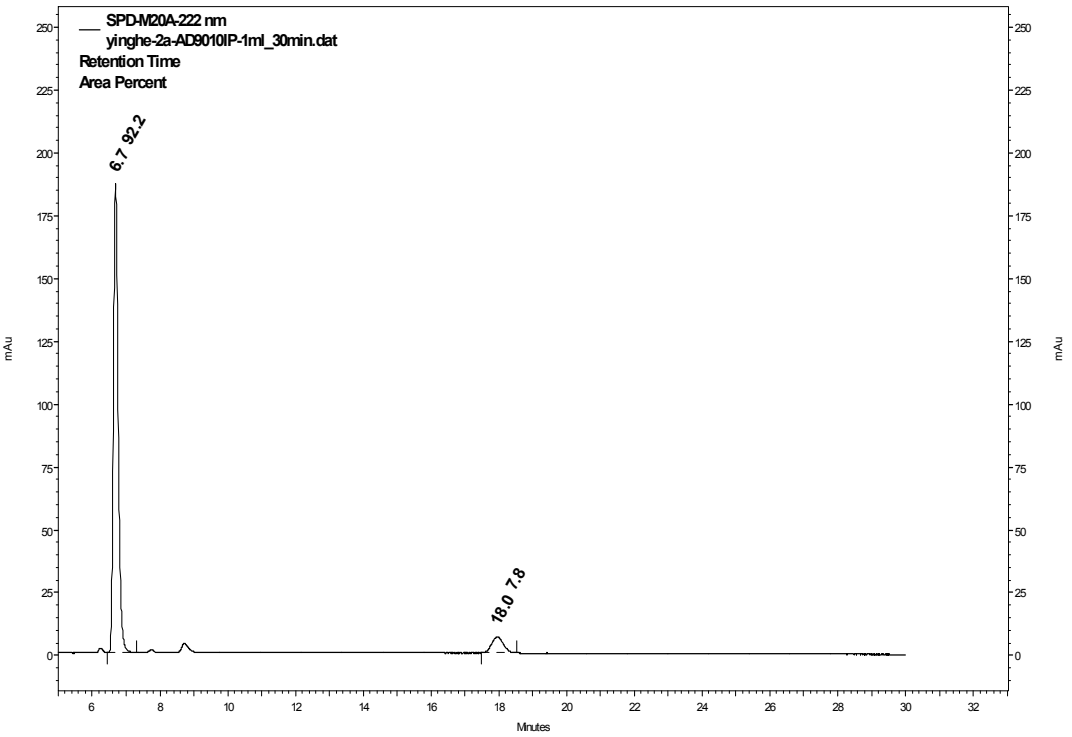

SPD-M20A-228 nm
yinghe-1l-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
12.1 50.0
14.0 50.0
mAu
Minutes

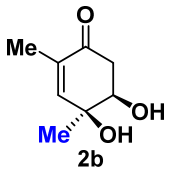

SPD-M20A-228 nm
yinghe-1l-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
14.3 90.0
12.3 10.0
mAu
Minutes


O
tBu
OH
Me
OH

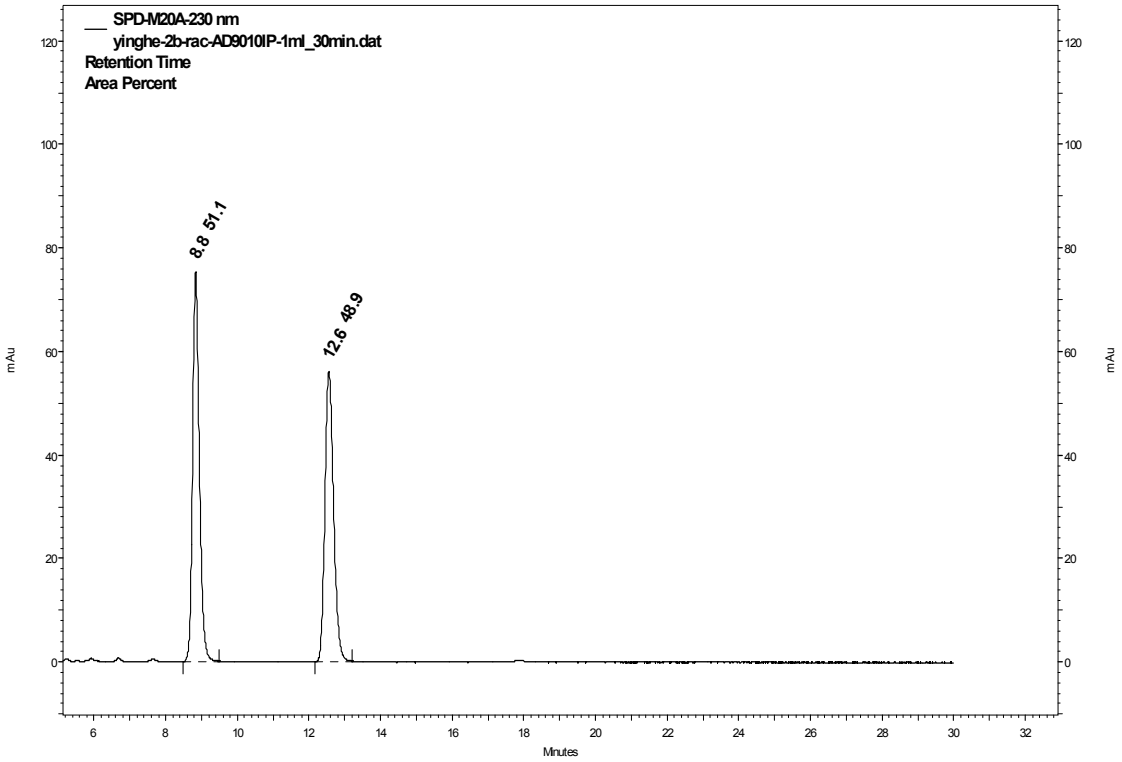
2a

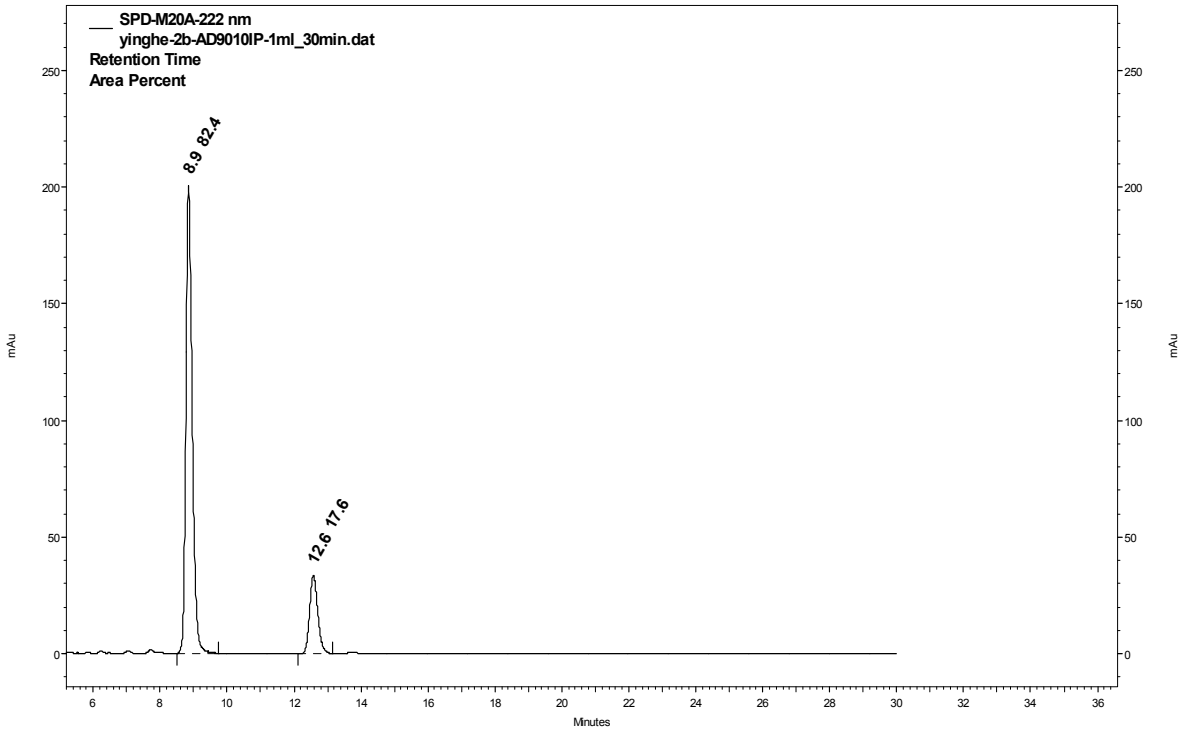

SPD-M20A-230 nm
yinghe-2a-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.7 49.7
17.8 50.3
mAu
Minutes

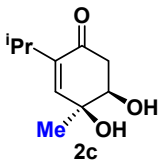

SPD-M20A-222 nm
yinghe-2a-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.7 92.2
18.0 7.8
mAu
Minutes


O
Me
OH
Me
OH

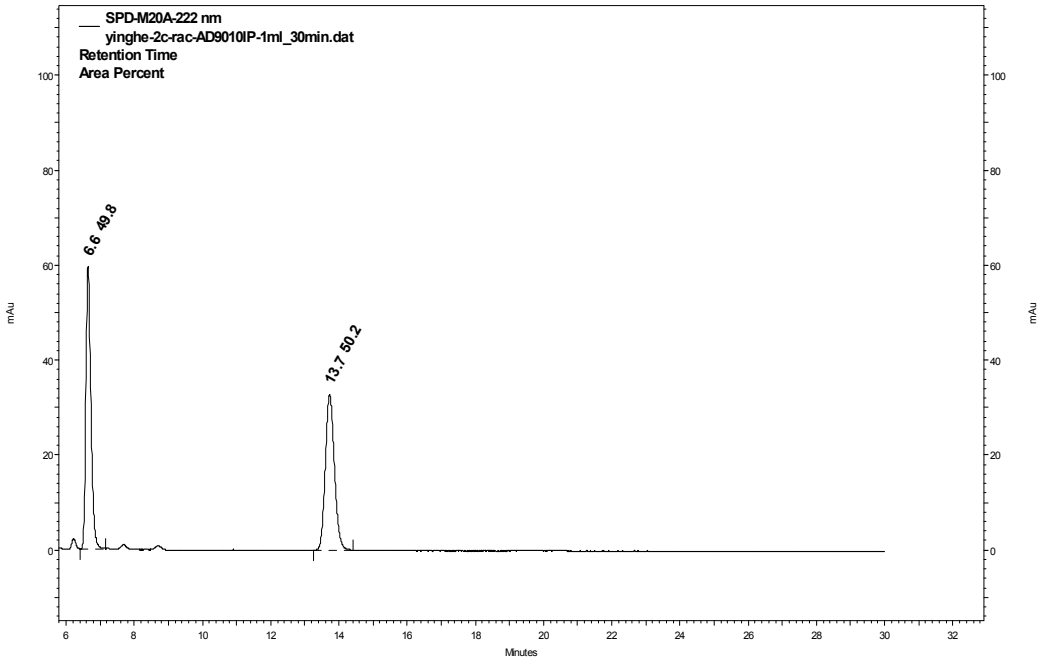
2b

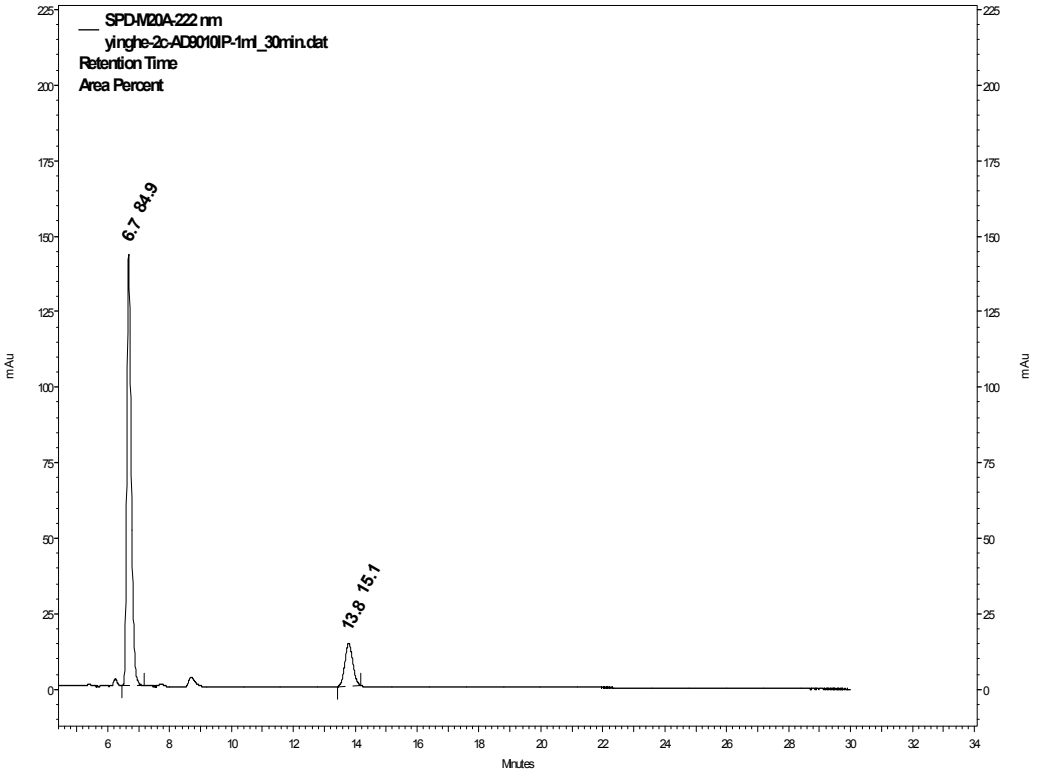

SPD-M20A-230 nm
yinghe-2b-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
8.8 51.1
12.6 48.9
mAu
Minutes

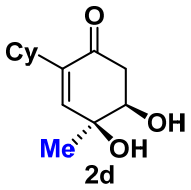

SPD-M20A-222 nm
yinghe-2b-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
8.9 82.4
12.6 17.6
mAu
Minutes


O
iPr
OH
Me
OH

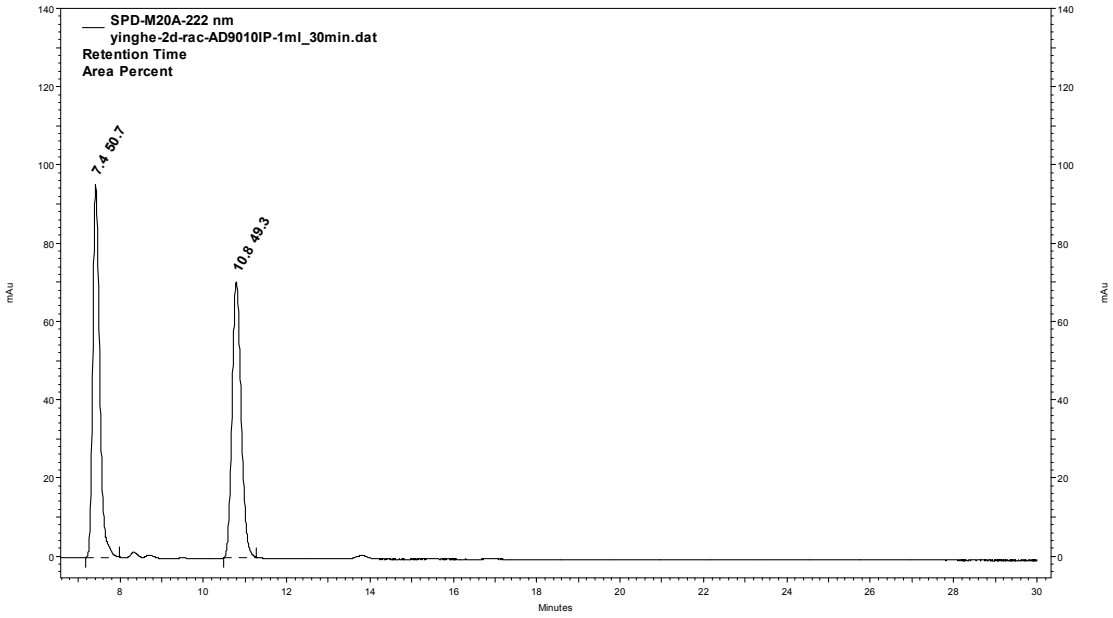
2c

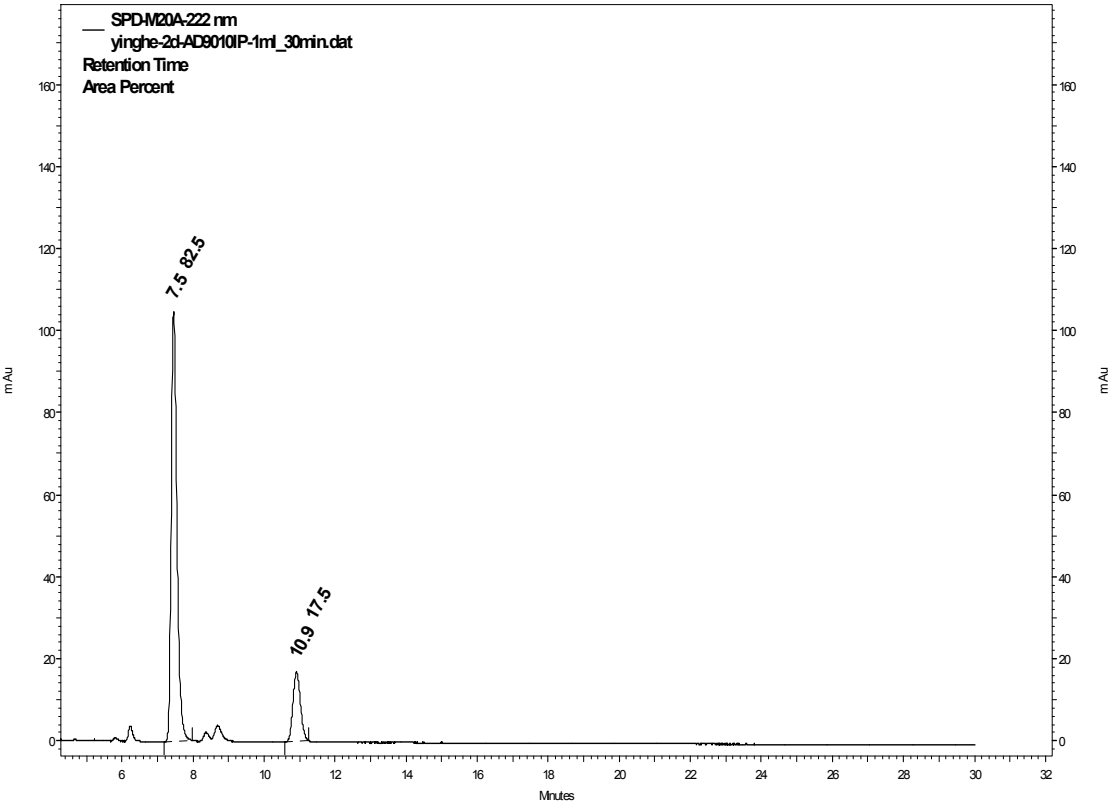

SPD-M20A-222 nm
yinghe-2c-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.6 49.8
13.7 50.2
mAu
Minutes

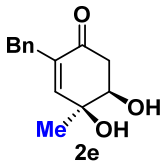

SPD-M20A-222 nm
yinghe-2c-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.7 84.9
13.8 15.1
mAu
Minutes


O
Cy
OH
Me
OH

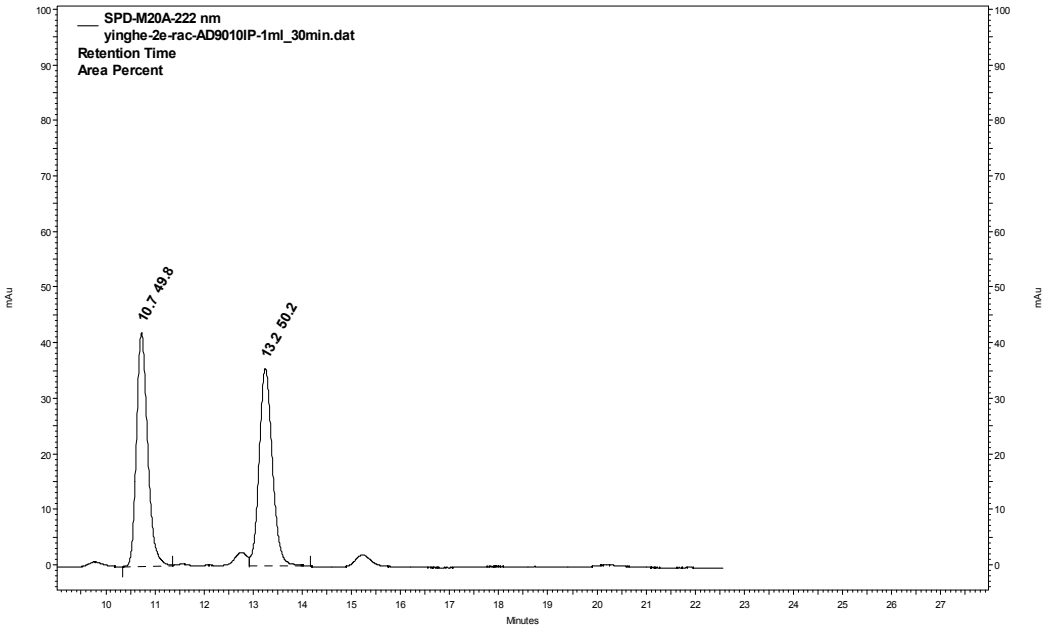
2d

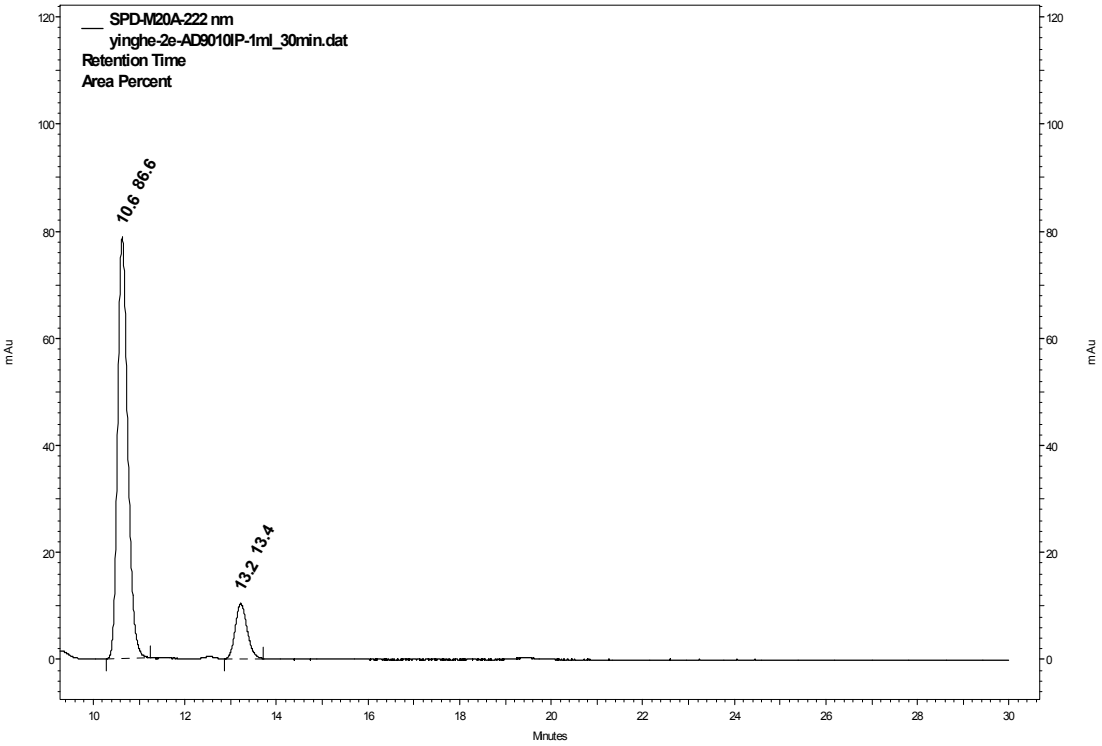

SPD-M20A-222 nm
yinghe-2d-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
7.4 50.7
10.8 49.3
mAu
Minutes

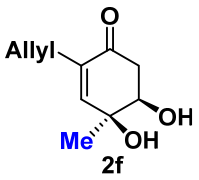

SPD-M20A-222 nm
yinghe-2d-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
7.5 82.5
10.9 17.5
mAu
Minutes


O
Bn
OH
Me
OH

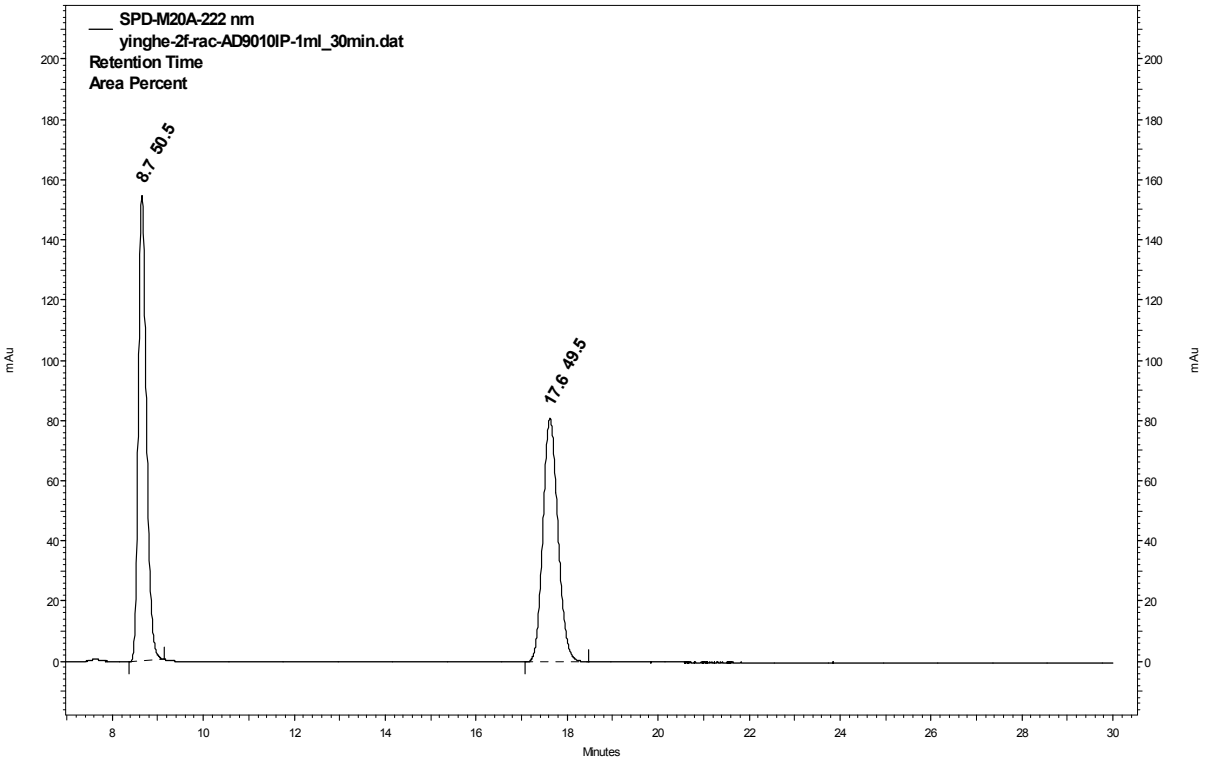
2e

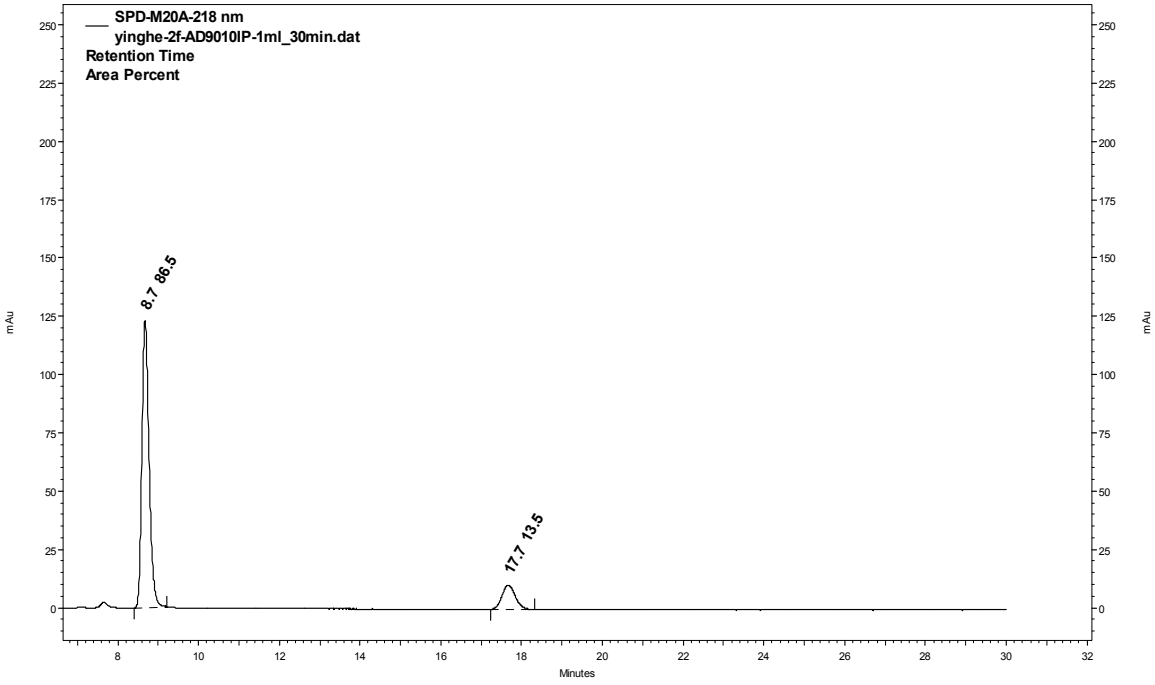

SPD-M20A-222 nm
yinghe-2e-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
10.7 49.8
13.2 50.2
mAu
Minutes

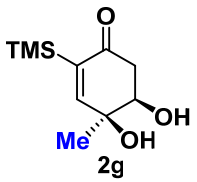

SPD-M20A-222 nm
yinghe-2e-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
10.6 86.6
13.2 13.4
mAu
Mnutes


O
Allyl
OH
Me
OH

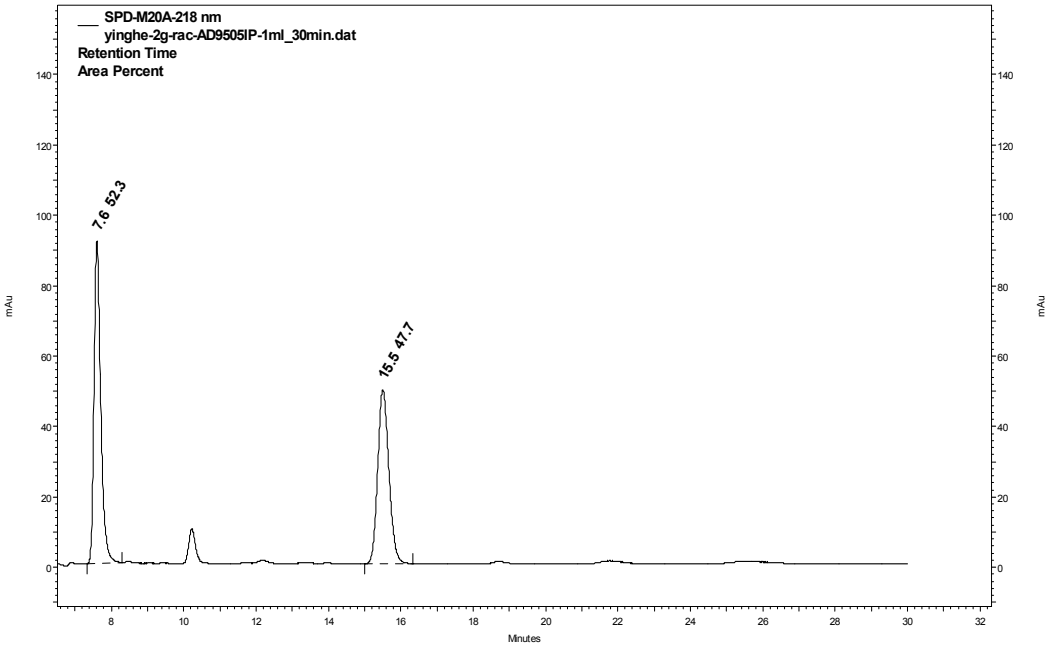
2f

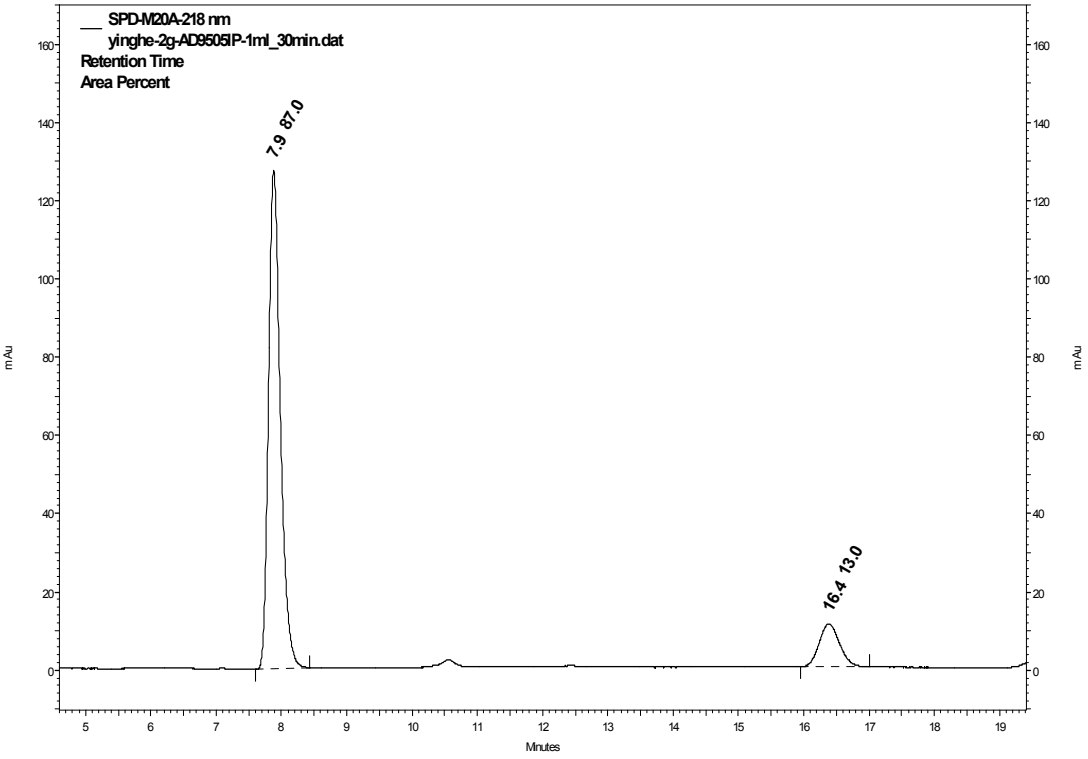

SPD-M20A-222 nm
yinghe-2f-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
8.7 50.5
17.6 49.5
mAu
Minutes

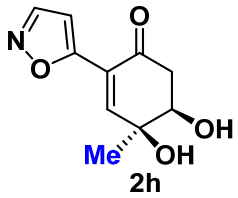

SPD-M20A-218 nm
yinghe-2f-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
8.7 86.5
17.7 13.5
mAu
Minutes


O
TMS
OH
Me
OH

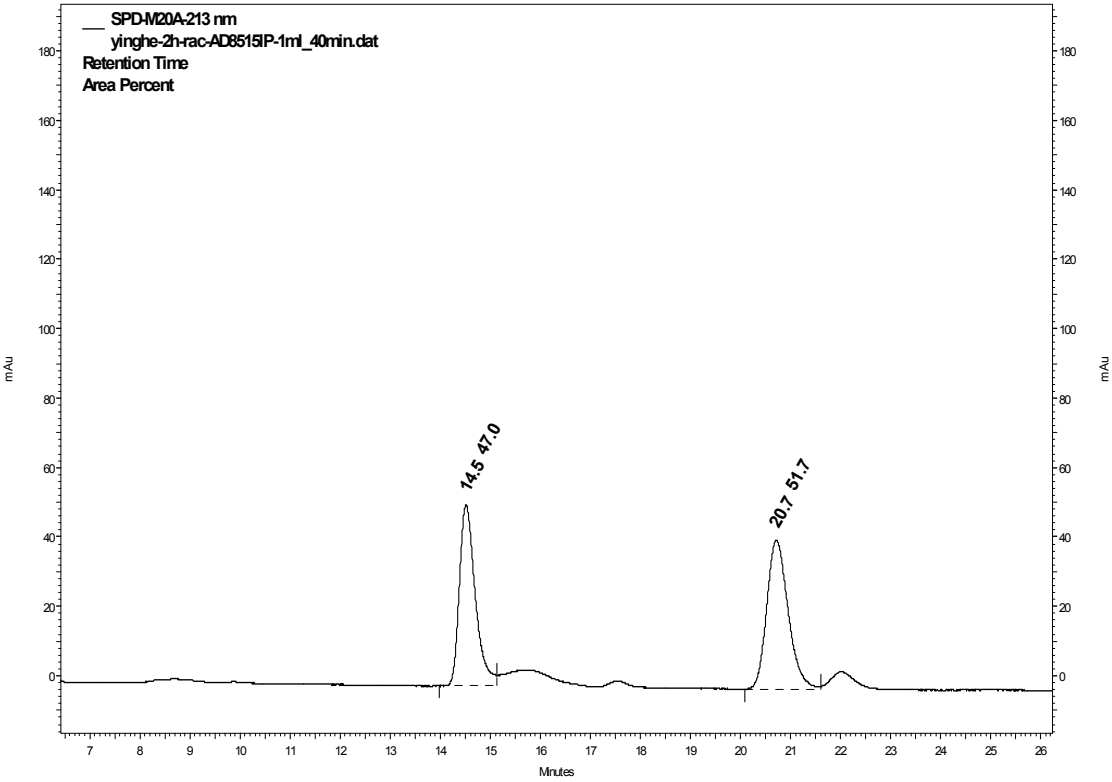
2g

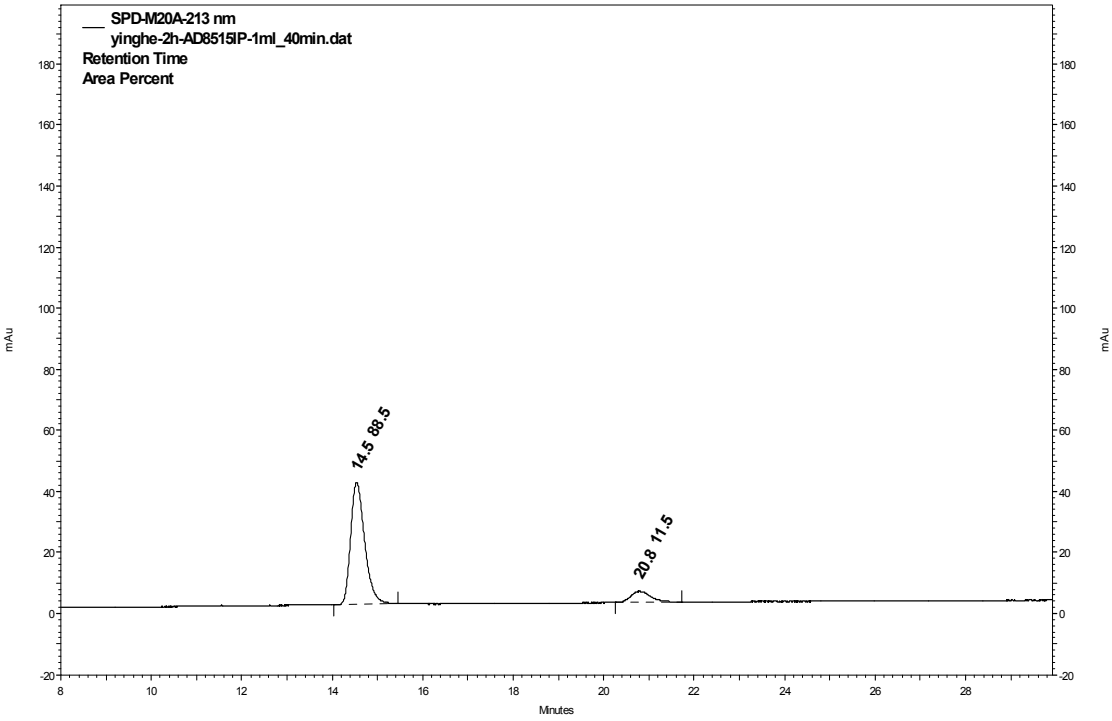

SPD-M20A-218 nm
yinghe-2g-rac-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
7.6 52.3
15.5 47.7
mAu
Minutes

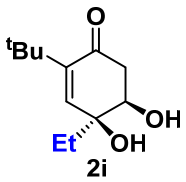

SPD-M20A-218 nm
yinghe-2g-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
7.9 87.0
16.4 13.0
mAu
Minutes


O
N
O
OH
Me
OH

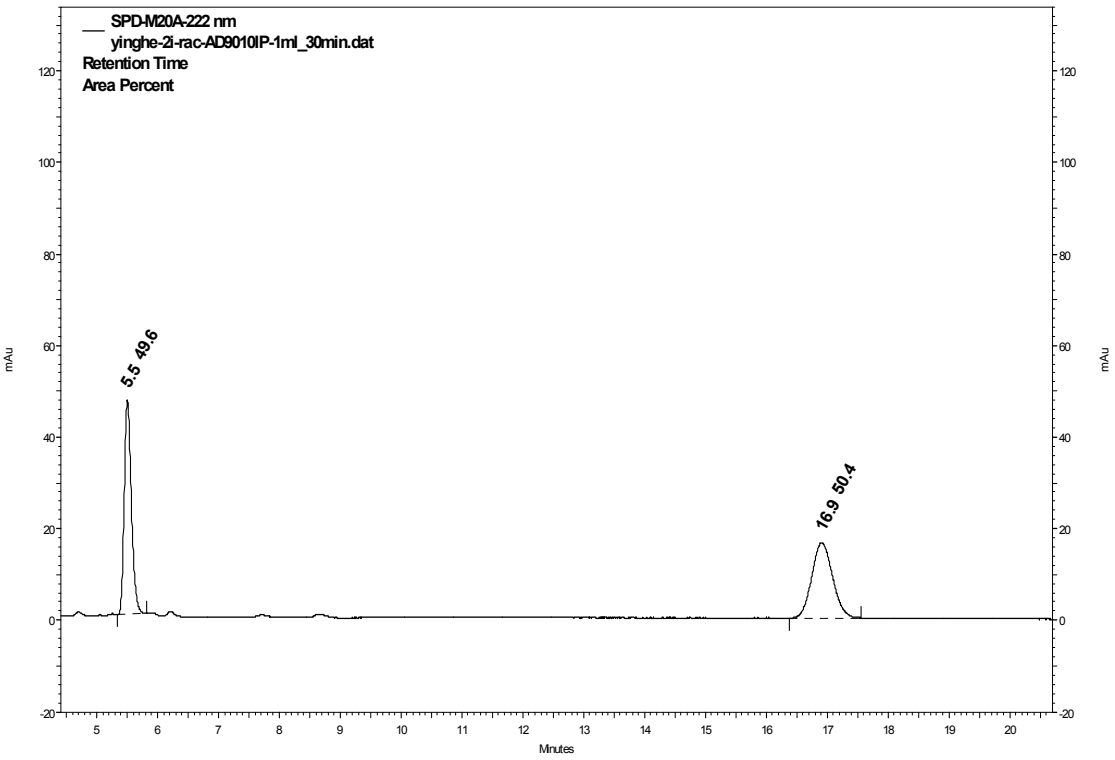
2h

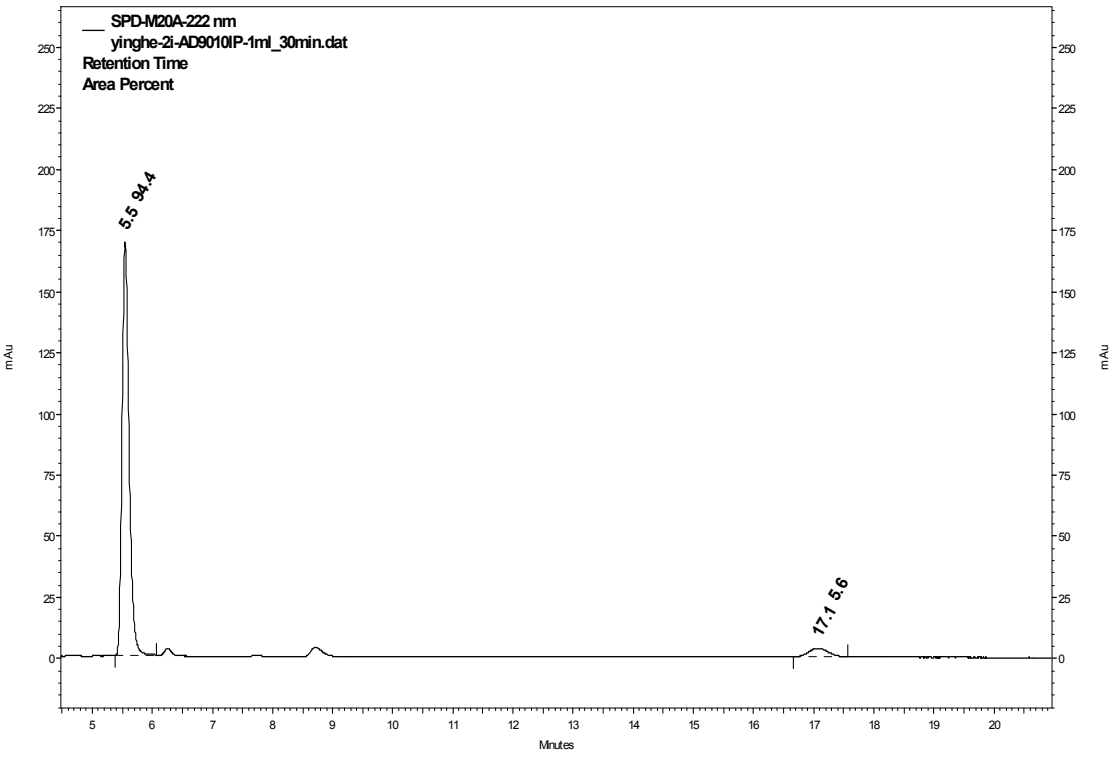

SPD-M20A-213 nm
yinghe-2h-rac-AD8515IP-1ml_40min.dat
Retention Time
Area Percent
14.5 47.0
20.7 51.7
mAu
Minutes

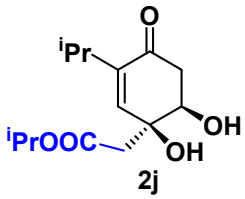

SPD-M20A-213 nm
yinghe-2h-AD8515IP-1ml_40min.dat
Retention Time
Area Percent
14.5 88.5
20.8 11.5
mAu
Minutes


O
tBu
OH
Et
OH

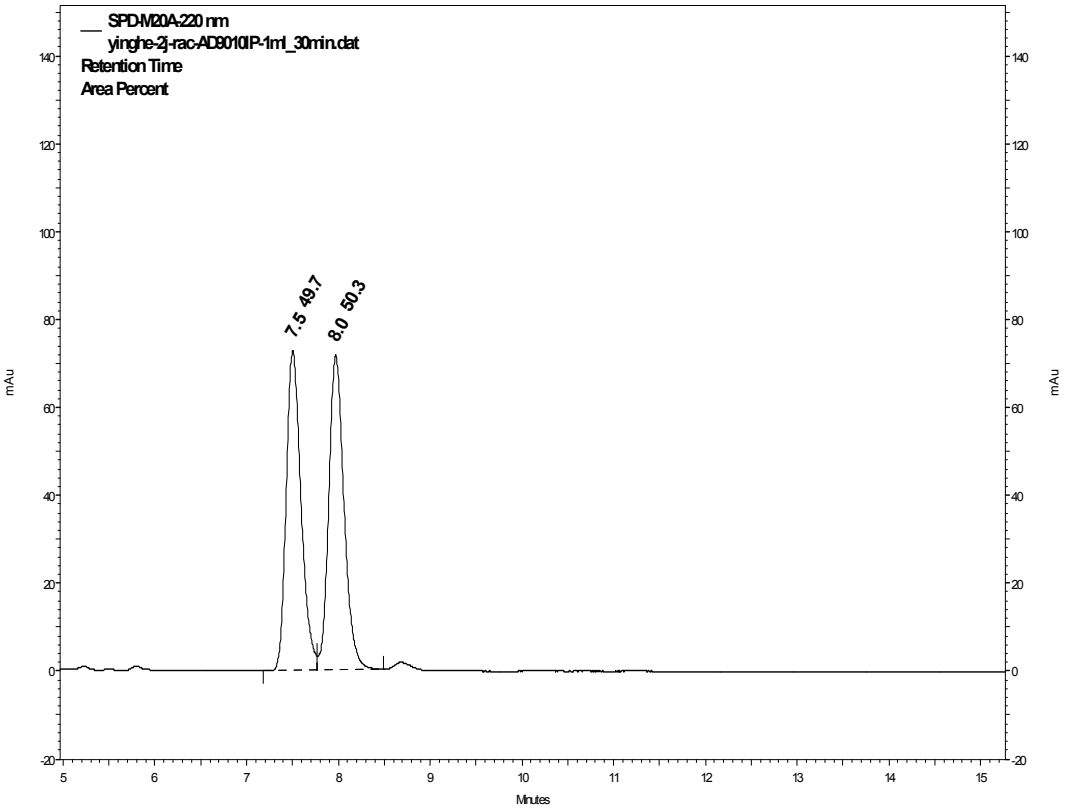
2i

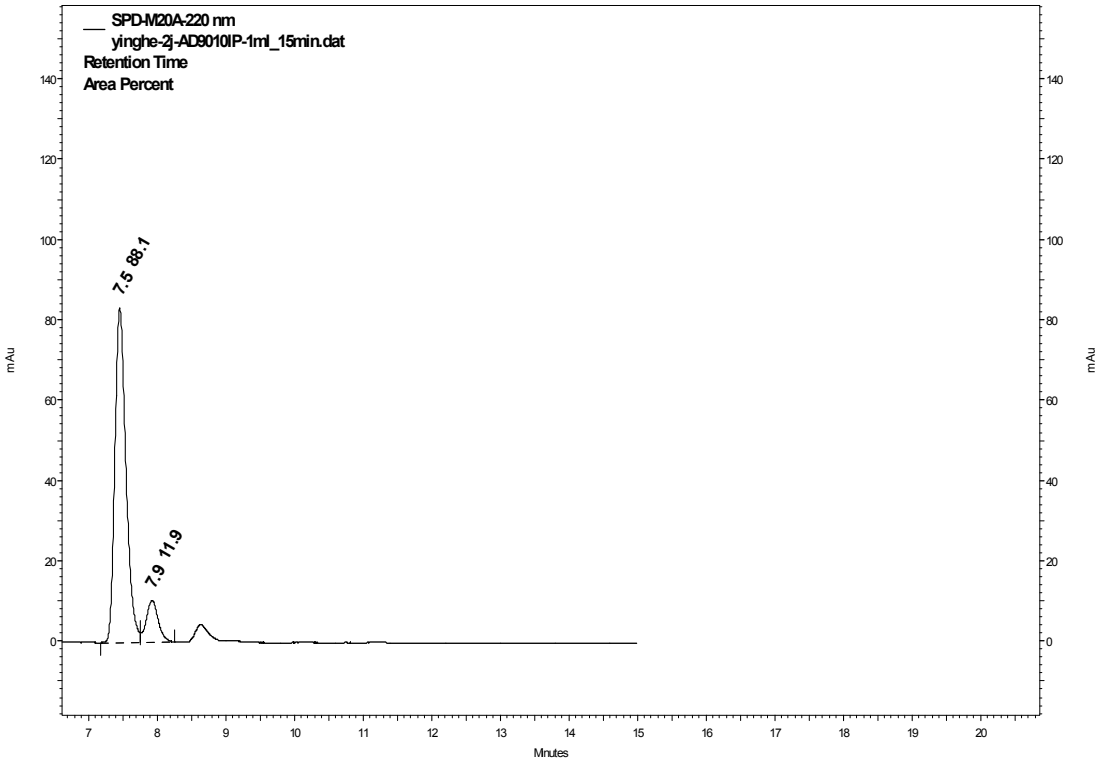

SPD-M20A-222 nm
yinghe-2i-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
5.5 49.6
16.9 50.4
mAu
Minutes

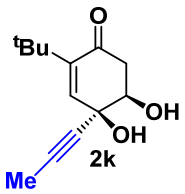

SPD-M20A-222 nm
yinghe-2i-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
5.5 94.4
17.1 5.6
mAu
Minutes

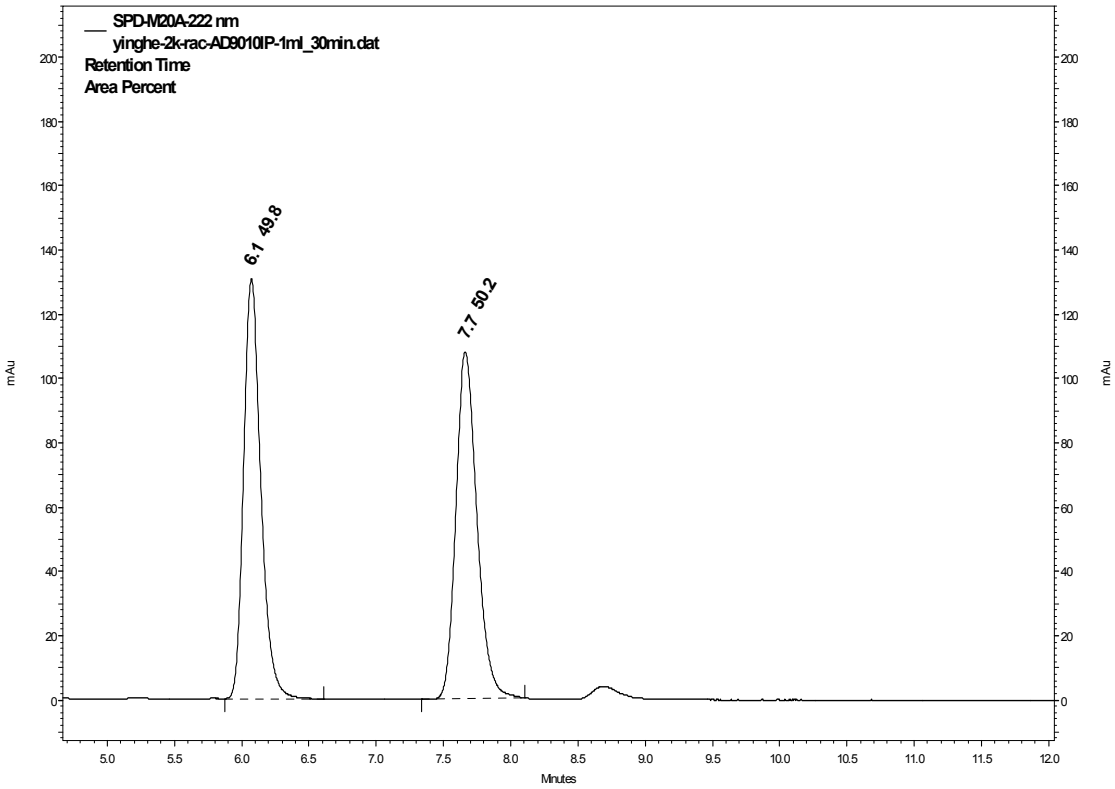

O
iPr
OH
iPrOOC
OH

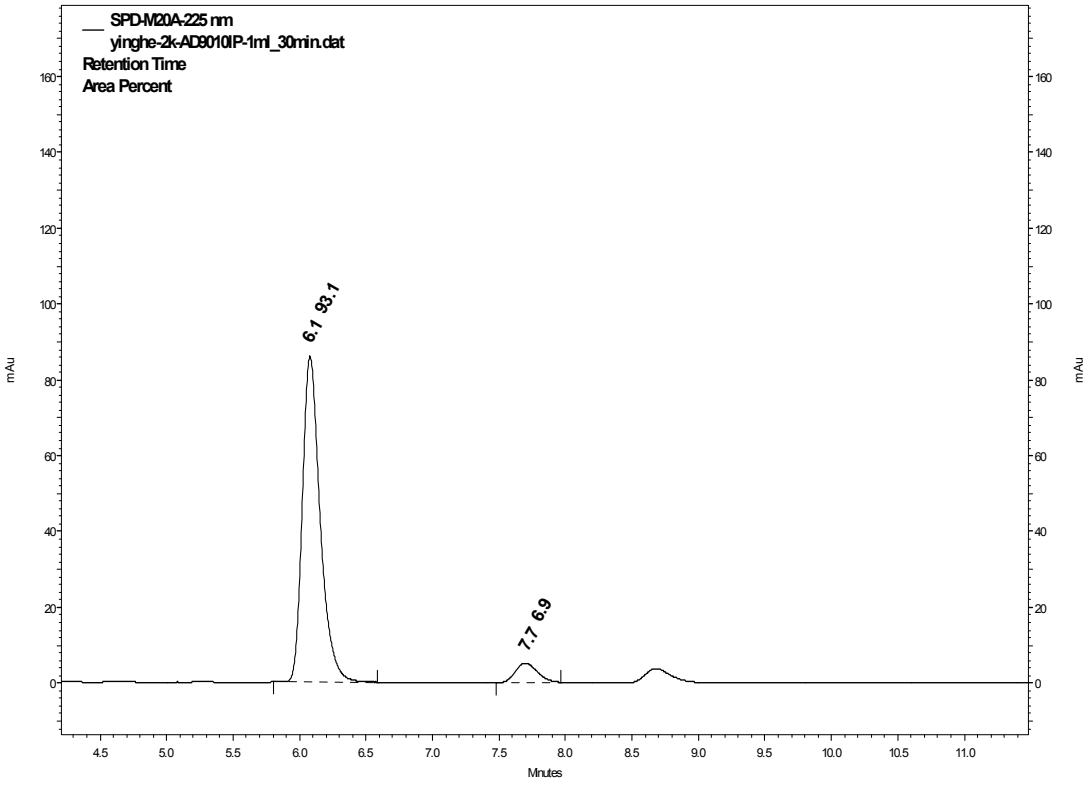
2j

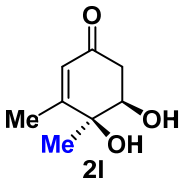

SPD-M20A-220 nm
yinghe-2j-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
7.5 49.7
8.0 50.3
mAu
Minutes


SPD-M20A-220 nm
yinghe-2j-AD9010IP-1ml_15min.dat
Retention Time
Area Percent
7.5 88.1
7.9 11.9
mAu
Minutes

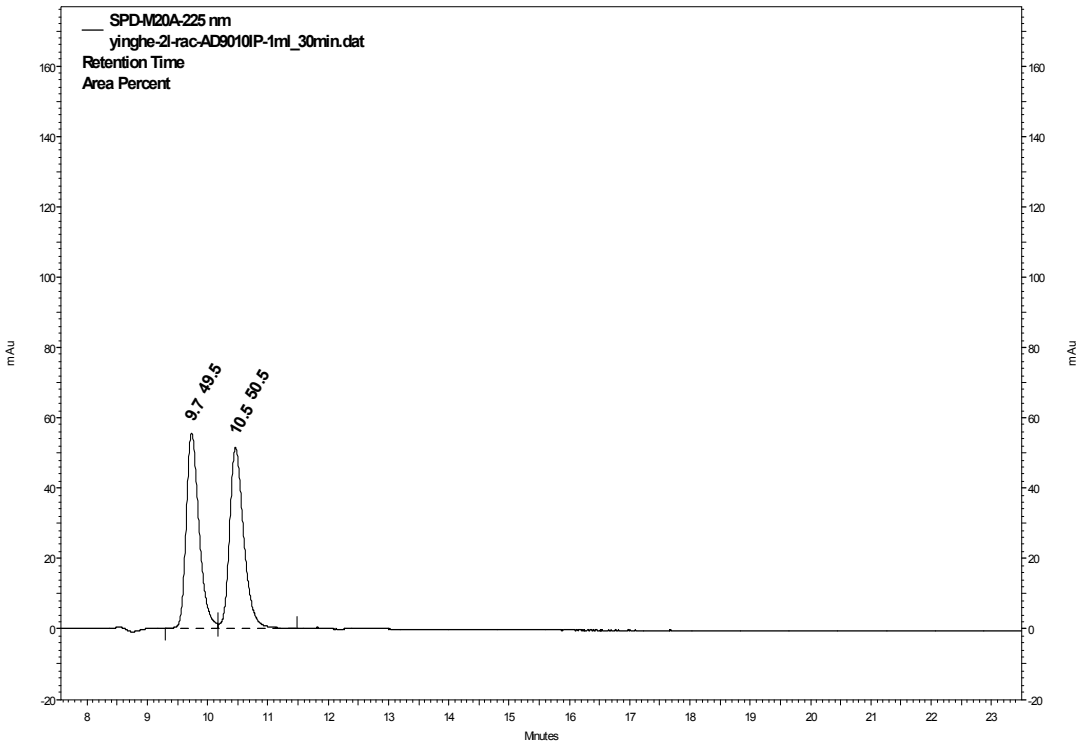

O
tBu
OH
OH
2k
Me

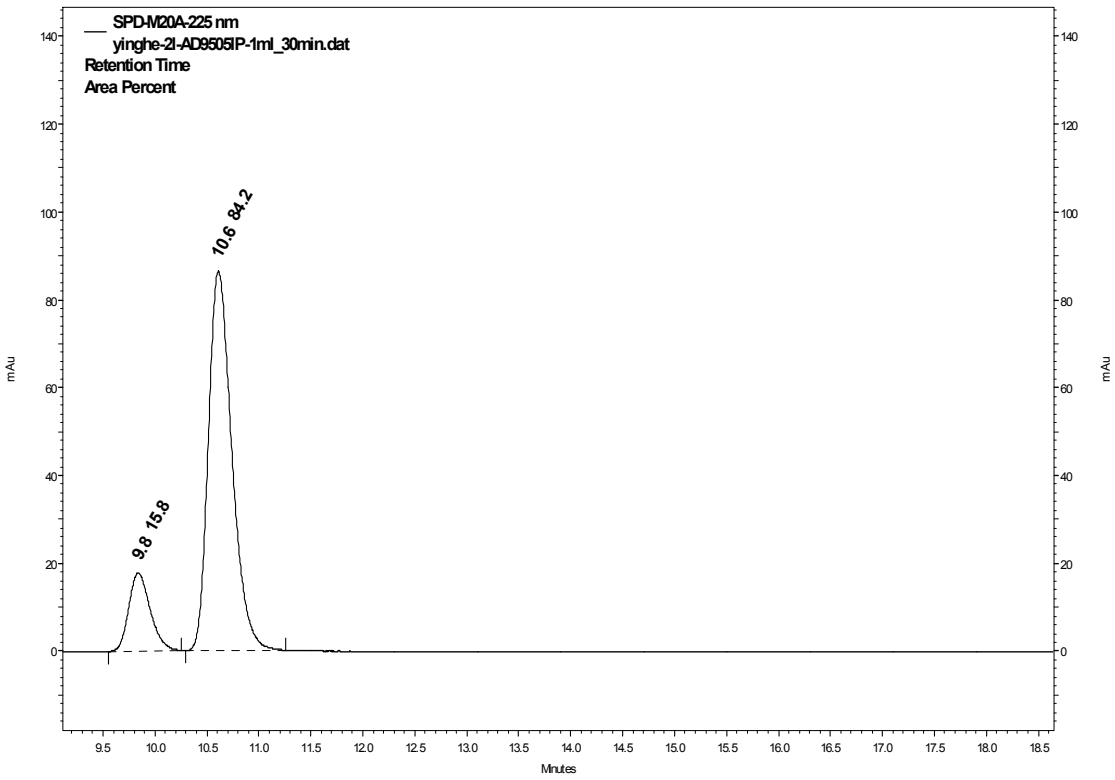

SPD-M20A-222 nm
yinghe-2k-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.1 49.8
7.7 50.2
mAu
Mnutes

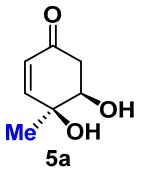

SPD-M20A-225 nm
yinghe-2k-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
6.1 93.1
7.7 6.9
mAu
Mnutes


O
Me
OH
Me
OH

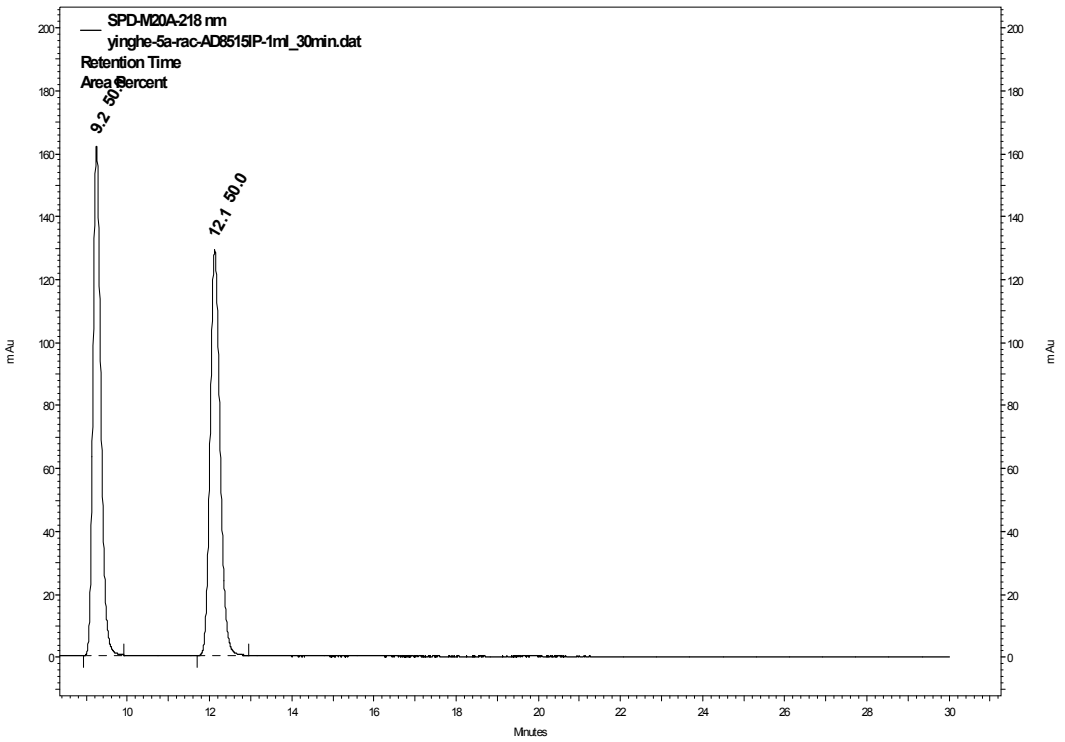
2l

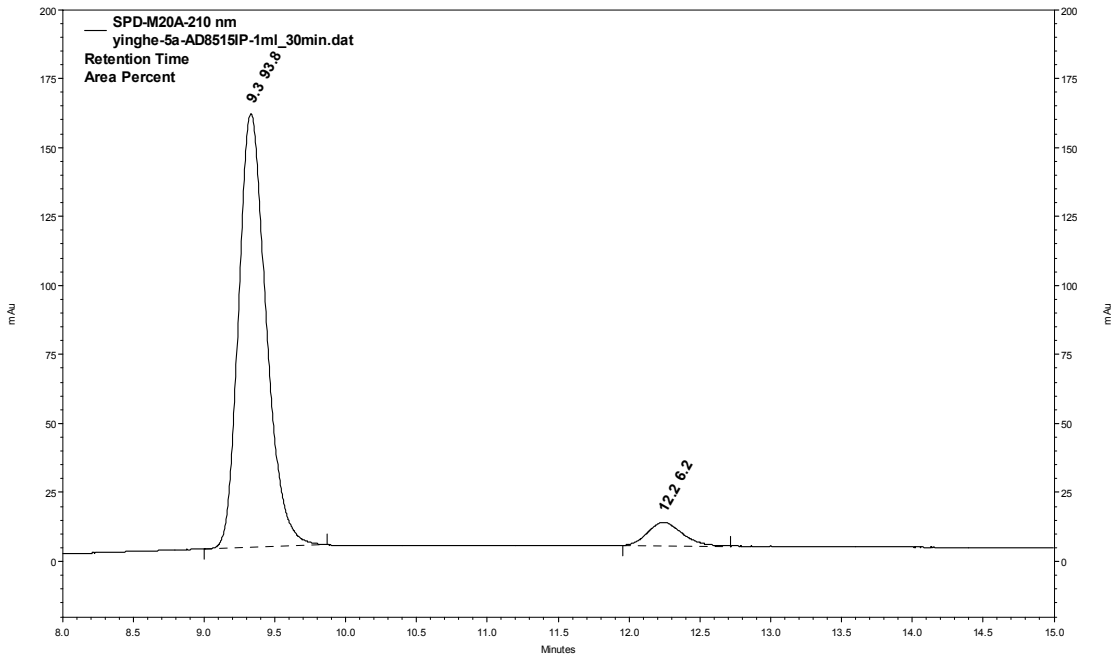

SPD-M20A-225 nm
yinghe-2l-rac-AD9010IP-1ml_30min.dat
Retention Time
Area Percent
9.7 49.5
10.5 50.5
mAu
Minutes

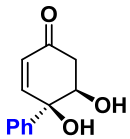

SPD-M20A-225 nm
yinghe-2l-AD9505IP-1ml_30min.dat
Retention Time
Area Percent
9.8 15.8
10.6 84.2
mAu
Minutes


O
OH
Me
OH

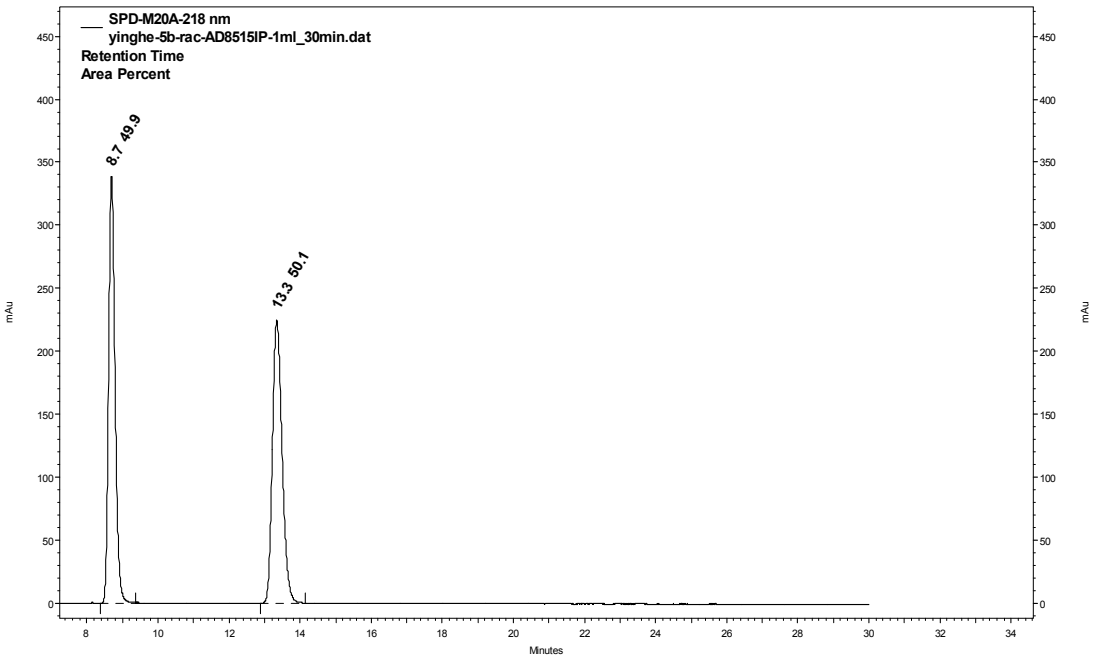
5a

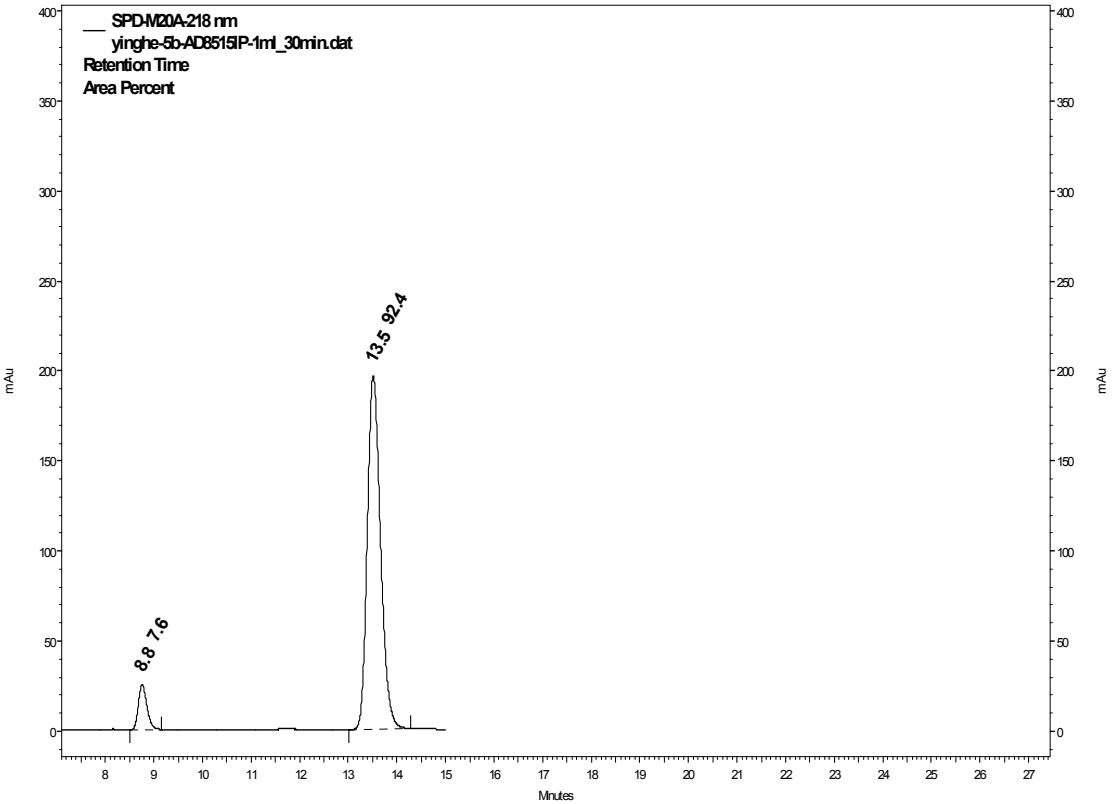

SPD-M20A-218 nm
yinghe-5a-rac-AD8515IP-1ml_30min.dat
Retention Time
Area Percent
9.2 50.0
12.1 50.0
mAu
Minutes


SPD-M20A-210 nm
yinghe-5a-AD8515IP-1ml_30min.dat
Retention Time
Area Percent
9.3 93.8
12.2 6.2
mAu
Minutes


O
OH
Ph
OH

5b


SPD-M20A-218 nm
yinghe-5b-rac-AD8515IP-1ml_30min.dat
Retention Time
Area Percent
8.7 49.9
13.3 50.1
mAu
Minutes


SPD-M20A-218 nm
yinghe-5b-AD8515IP-1ml_30min.dat
Retention Time
Area Percent
8.8 7.6
13.5 92.4
mAu
Mnutes