Supporting Information

Pd(0)-catalysed asymmetric reductive Heck-type cyclization of (Z)-1-iodo-1,6-diene: enantioselective synthesis of quaternary tetrahydropyridines

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1. General Information

Unless otherwise noted, all reagents were obtained commercially and used without further purification.

NMR spectrum: ^{1}H and ^{13}C spectra are recorded on the Bruker AVANCEspectrometer, operating at 400 MHz (300 MHz or 500 MHz) for ^{1}H NMR and 100 MHz (75 MHz or 125 MHz) for ^{13}C NMR. Chemical shifts are reported in parts per million (ppm).Chemical shifts are reported downfield from $CDCl_3$ (δ: 7.26 ppm) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are reported in the scale relative to the solvent of $CDCl_3$ (δ: 77.0 ppm) used as an internal reference. Data are respresented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), intergration.

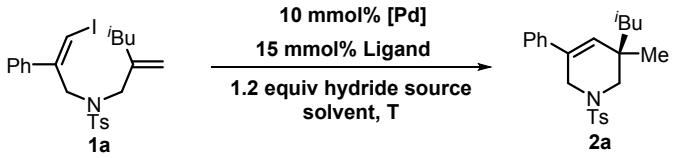
Mass spectroscopy: Mass spectra were in general recorded on an AMD 402/3 or a HP 5989A mass selective detector.

High Performance Liquid Chromatography: HPLC analysis was performed on Waters equipment using Daicel Chiralpak AD-H, OD-H, OJ-Hcolumn.

Spectropolarimeter: Optical rotations were measured on a AutopolIV-T polarimeter.

Chromatography: Column chromatography was performed with silica gel (200-300 mesh ASTM).

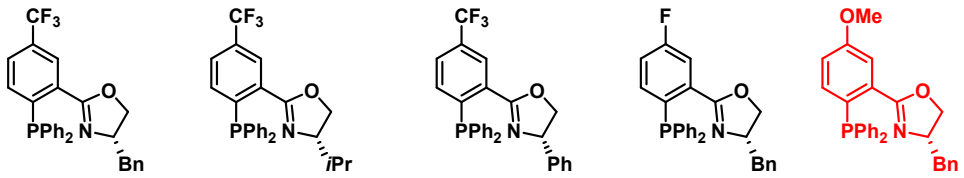
2. Optimization of Reaction Conditions



1a 2a

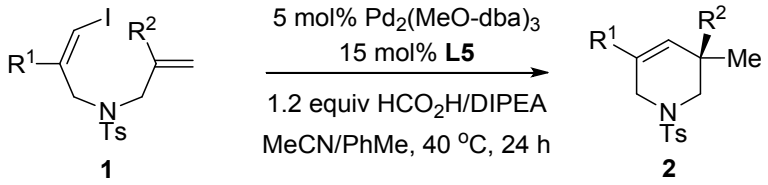
entry	catalyst	Ligand	"H"source	solvent	T/°C	yield/%	ee/%
1	Pd_2dba_3	*(R)*-BINAP	HCO_2H/Et_3N	toluene	40	46	52
2	$Pd_2(dba\text{-}OMe)_3$	*(R)*-BINAP	HCO_2H/Et_3N	toluene	40	53	55
3	$Pd_2(dba\text{-}OMe)_3$	L1	HCO_2H/Et_3N	toluene	40	55	65
4	$Pd_2(dba\text{-}OMe)_3$	L2	HCO_2H/Et_3N	toluene	40	55	60
5	$Pd_2(dba\text{-}OMe)_3$	L3	HCO_2H/Et_3N	toluene	40	67	43
6	$Pd_2(dba\text{-}OMe)_3$	L4	HCO_2H/Et_3N	toluene	40	61	64
7	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/Et_3N	toluene	40	62	70
8	$PdCl_2$	L5	HCO_2H/Et_3N	toluene	40	40	55
9	$Pd(OAc)_2$	L5	HCO_2H/Et_3N	toluene	40	42	63
10	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/Et_3N	toluene	40	75	79
11	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	toluene	40	80	82
12	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	THF	40	50	70
13	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN	40	91	69
14	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	DMF	40	68	72
15	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	dioxane	40	63	76
16	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(1:1)	40	87	85
17[a]	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(1:1)	40	80	67
18	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(2:1)	40	80	76
19	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(1:2)	40	77	64
20	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(1:1)	20	63	76
21	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2H/DIPEA	MeCN/toluene(1:1)	60	70	77
22	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2Na	MeCN/toluene(1:1)	40	80	68
23	$Pd_2(dba\text{-}OMe)_3$	L5	$(HCO_2)_2Ca$	MeCN/toluene(1:1)	40	76	57
24	$Pd_2(dba\text{-}OMe)_3$	L5	HCO_2NH_4	MeCN/toluene(1:1)	40	89	61

[a] **1a** (0.2 mmol), $Pd_2(dba\text{-}OMe)_3$ (0.01 mmol), ligand (0.03 mmol), hydride source (1.2 equiv), toluene:MeCN(1+1 mL), Ag_2CO_3 (2 equiv).

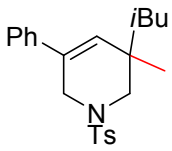


L1 L2 L3 L4 L5

3.Synthesis of Products 2 and Their Analytic Data



In a 25 mL Schlenk tube, the mixture of **1** (0.2 mmol), Pd_2(MeO-dba)$_3$ (0.01 mmol, 10.8 mg),**L5** (0.03 mmol, 14.7 mg) and HCO_2H (0.24 mmol, 11 mg), DIPEA (0.24 mmol, 31mg) were dissolved in MeCN:toluene (v/v = 1:1, v+ v = 2.0mL). The reaction mixture was thoroughly degassed by vacuum purge-and-refill with argon.The mixture was stirred at 40 °C. After completion of the reaction (monitored by TLC), the solvent was removed and the residue was directly subjected to silica gel column chromatography (petroleum ether/ethyl acetate as eluent) to give product **2**.



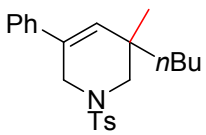
2a: 89% yield, 68.2mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 0.84 (d, *J* = 7.2 Hz, 3H), 0.87 (d, *J* = 7.2 Hz, 3H), 1.06 (s, 3H), 1.30 (dd, *J* = 6.0 Hz, *J* = 14.1 Hz, 1H), 1.43 (dd, *J* = 5.7 Hz, *J* = 14.1 Hz, 1H), 1.63-1.75 (m, 1H), 2.35 (s, 3H), 2.72 (d, *J* = 11.4 Hz, 1H), 2.92 (d, *J* = 11.4 Hz, 1H), 3.75-3.77 (m, 2H), 5.81 (dd, *J* = 1.8 Hz, *J* = 3.0 Hz, 1H), 7.17-7.28 (m, 7H), 7.64 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.58, 24.42, 24.92, 25.37, 25.41, 37.00, 46.46, 49.09, 53.63, 125.33, 127.72, 128.55, 129.76, 130.72, 132.73, 133.08, 138.62, 143.61.

ESI-MS: Calcd for$C_{23}H_{29}NO_2S$: [M+K$^+$] 422.1551, found 422.1550.

$[\alpha]^{25}_D$ = 36.3 (c = 0.34 in CH_2Cl_2); 85% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm,t_R = 13.9 min and 15.3 min].



2b: 90% yield, 68.9 mg, yellow oil.

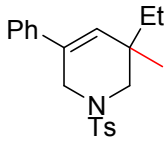
^{1}H NMR (300 MHz, $CDCl_3$): δ 0.80-0.85 (m, 3H), 1.02 (s, 3H), 1.18-1.22 (m, 4H), 1.30-1.44 (m, 2H), 2.35 (s, 3H), 2.73 (d, *J* = 11.1 Hz, 1H), 2.91 (d, *J* = 11.1 Hz, 1H), 3.73 (dd, *J* = 1.8 Hz, *J* = 15.6 Hz, 1H), 3.80 (dd,

J= 1.8 Hz, *J* = 15.6 Hz, 1H), 5.79 (s, 1H), 7.18-7.28 (m, 7H), 7.64 (d, *J* = 8.1 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 14.12, 21.57, 23.46, 24.44, 26.18, 36.49, 39.82, 46.50, 53.00, 125.38, 127.73, 128.53, 129.75, 131.14, 132.52, 133.30, 138.62, 143.57.

ESI-MS: Calcd for$C_{23}H_{29}NO_2S$: [M+K$^+$] 422.1551, found 422.1555.

$[\alpha]^{25}_D$ = 4.5 (c = 3.4 in CH_2Cl_2); 84% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 12.7 min and 15.7 min].



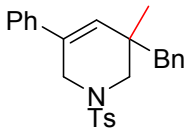
2c: 92% yield, 65.3 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.94 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 3H), 1.53 (q, *J* = 7.2 Hz, 2H), 2.45 (s, 3H), 2.82 (d, *J* = 11.2 Hz, 1H), 3.03 (d, *J* = 11.2 Hz, 1H), 3.84 (d, *J* = 15.6 Hz, 1H), 3.90 (d, *J* = 15.6 Hz, 1H), 5.88 (s, 1H), 7.26-7.37 (m, 7H), 7.74 (d, *J* = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 8.37, 21.57, 23.82, 32.39, 36.61, 46.51, 52.56, 125.38, 127.71, 128.52, 129.75, 131.33, 132.29, 133.16, 138.58, 143.58.

ESI-MS: Calcd for$C_{21}H_{25}NO_2S$: [M+H$^+$] 356.1679, found 356.1680.

$[\alpha]^{25}_D$ = 7.7 (c = 3.3 in CH_2Cl_2); 87% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 19.8 min and 21.8 min].



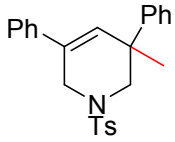
2d:83% yield, 75.1 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 0.94 (s, 3H), 2.36 (s, 3H), 2.47 (d, *J* = 11.4 Hz, 1H), 2.73 (d, *J* = 13.2 Hz, 1H), 2.78 (d, *J* = 13.2 Hz, 1H), 3.25 (d, *J* = 11.4 Hz, 1H), 3.58 (dd, *J* = 1.8 Hz, *J* = 15.3 Hz, 1H), 4.03 (dd, *J* = 1.5 Hz, *J* = 15.3 Hz, 1H), 5.71 (s, 1H), 7.14-7.29 (m, 12H), 7.64 (d, *J* = 8.1 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 21.57, 24.01, 37.51, 45.51, 46.71, 52.84, 125.36, 126.36, 127.83, 128.04, 128.57, 129.78, 130.84, 131.96, 132.92, 137.39, 138.44, 143.71.

ESI-MS: Calcd for$C_{26}H_{27}NO_2S$: [M+H$^+$] 418.1835, found 418.1837.

$[\alpha]^{25}_D$ = 23.6 (c = 3.7 in CH_2Cl_2); 90% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 22.8 min and 28.3 min].



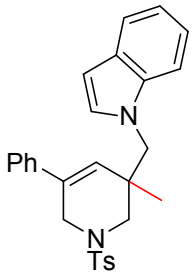
2e: 80% yield, 64.1 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 1.64 (s, 3H), 2.43 (s, 3H), 3.03 (d, *J* = 11.4 Hz, 1H), 3.39 (d, *J* = 11.4 Hz, 1H), 3.76 (dd, *J* = 2.1 Hz, *J* = 15.6 Hz, 1H), 4.22 (d, *J* = 15.6 Hz, 1H), 6.19 (t, *J* = 1.8 Hz, 1H), 7.27-7.43 (m, 12H), 7.64 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.55, 25.23, 41.22, 46.36, 55.47, 125.43, 126.45, 126.79, 127.30, 127.69, 128.02, 128.43, 128.52, 128.65, 129.75, 131.51, 132.19, 133.22, 138.32, 143.62, 145.46.

ESI-MS: Calcd for$C_{25}H_{25}NO_2S$: [M+H$^+$] 404.1679, found 404.1679.

$[\alpha]^{25}_D$ = 29.3 (c = 3.2 in CH_2Cl_2); 85% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 30.3 min and 38.4 min].



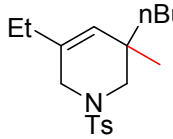
2f:81% yield, 72.9 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 1.07 (s, 3H), 2.46-2.49 (m, 4H), 3.59 (d, J = 15.6 Hz, 1H), 3.67 (d, J = 11.2 Hz, 1H), 4.26-4.36 (m, 3H), 5.79 (s, 1H), 6.57 (d, J = 2.4 Hz, 1H), 7.10-7.14 (m, 1H), 7.19-7.40 (m, 10H), 7.65 (d, J = 7.6 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.60, 23.44, 40.03, 46.84, 51.52, 52.92, 101.76, 110.12, 119.31, 120.85, 121.50, 125.39, 127.83, 128.18, 128.31, 128.63, 129.23, 129.74, 129.92, 132.40, 133.56, 137.22, 137.88, 144.04.

ESI-MS: Calcd for$C_{28}H_{28}N_2O_2S$ [M+H$^+$] 457.1944, found 457.1943.

$[\alpha]^{25}_D$ = -7.2 (c = 3.6 in CH_2Cl_2); 85% ee [Chiralcel OJ-H column, n-hexane/i-PrOH = 95:5, 0.8 mL/min, λ_{max} 254 nm,t_R = 9.1 min and 10.9 min].



2g:87% yield, 58.2 mg, yellow oil.

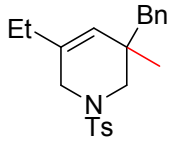
^{1}H NMR (300 MHz, $CDCl_3$): δ 0.89 (t, *J* = 7.2 Hz, 3H), 0.98 (t, *J* = 7.5 Hz, 6H), 1.18-1.36 (m, 6H), 1.92 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 2.68 (d, *J* = 11.1 Hz, 1H), 2.86 (d, *J* = 11.1 Hz, 1H), 3.32 (dd, *J* = 1.5 Hz, *J* = 18.0 Hz,

1H), 3.38 (dd, *J* = 1.2 Hz, *J* = 18.0 Hz, 1H), 5.21 (s, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.67 (d, *J*= 8.1 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 12.15, 14.12, 21.55, 23.45, 24.50, 26.08, 27.15, 35.65, 39.84, 47.33, 53.34, 127.69, 128.12, 129.63, 132.95, 143.36.

ESI-MS: Calcd for$C_{19}H_{29}NO_2S$: [M+H$^+$] 336.1992, found 336.1995.

$[\alpha]^{25}_D$ = -4.0 (c = 2.9 in CH_2Cl_2); 71% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 16.4 min and 27.1 min].



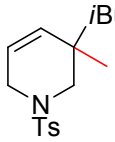
2h: 82% yield, 79.4 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (s, 3H), 1.00 (t, *J* = 7.6 Hz, 3H), 1.95 (q, *J* = 7.6 Hz, 2H), 2.42-2.46 (m, 4H), 2.70 (d, *J* = 13.2 Hz, 1H), 2.74 (d, *J* = 13.2 Hz, 1H), 3.18-3.25 (m, 2H), 3.61 (d, *J* = 15.6 Hz, 1H), 5.17 (s, 1H), 7.20-7.36 (m, 7H), 7.69 (d, *J* = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 12.11, 21.57, 24.08, 27.12, 36.73, 45.46, 47.55, 53.04, 126.16, 127.80, 127.87, 129.67, 130.84, 132.83, 133.32, 137.72, 143.53.

ESI-MS: Calcd for$C_{22}H_{27}NO_2S$: [M+ Na$^+$] 392.1655, found 392.1653.

$[\alpha]^{25}_D$ = -53.0 (c = 3.9 in CH_2Cl_2); 71% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 14.3 min and 16.6 min].



2i: 75% yield, 46.0 mg, yellow oil.

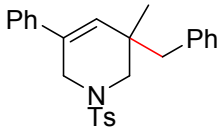
^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (d, *J* = 6.8 Hz, 3H), 0.93 (d, *J* = 6.8 Hz, 3H), 1.05 (s, 3H), 1.29 (dd, *J* = 5.6 Hz, *J* = 14.0 Hz, 1H), 1.42 (dd, *J* = 5.6 Hz, *J* = 14.0 Hz, 1H), 1.66-1.77 (m, 4H), 2.45 (s, 3H), 2.74 (d, *J* = 10.8 Hz, 1H), 2.95 (d, *J* = 10.8 Hz, 1H), 3.43-3.54 (m, 2H), 5.47-5.52 (m, 1H), 5.59 (d, *J* = 10.4 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.55, 24.29, 24.93, 25.05, 25.28, 36.64, 44.84, 48.74, 53.94, 119.84, 127.68, 129.63, 133.18, 135.51, 143.44.

ESI-MS: Calcd for$C_{17}H_{25}NO_2S$: [M+ Na$^+$] 330.1498, found 330.1500.

$[\alpha]^{25}_D$ = -13.1 (c = 2.3 in CH_2Cl_2); 77% ee [Chiralcel OD-H column, n-hexane/i-

PrOH= 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 24.2 min and 27.8 min].



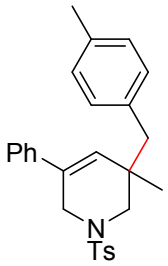
2j: 88% yield, 71.7 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 0.94 (s, 3H), 2.36 (s, 3H), 2.47 (d, *J* = 11.4 Hz, 1H), 2.73 (d, *J* = 13.2 Hz, 1H), 2.78 (d, *J* = 13.2 Hz, 1H), 3.25 (d, *J* = 11.4 Hz, 1H), 3.58 (dd, *J* = 1.8 Hz, *J* = 15.3 Hz, 1H), 4.03 (dd, *J* = 1.5 Hz, *J* = 15.3 Hz, 1H), 5.71 (s, 1H), 7.14-7.29 (m, 12H), 7.64 (d, *J* = 8.1 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 21.57, 24.01, 37.51, 45.51, 46.71, 52.84, 125.36, 126.36, 127.83, 128.04, 128.57, 129.78, 130.84, 131.96, 132.92, 137.39, 138.44, 143.71.

ESI-MS: Calcd for$C_{26}H_{27}NO_2S$: [M+H$^+$] 418.1835, found 418.1837.

$[\alpha]^{25}_D$ = -29.3 (c = 3.5 in CH_2Cl_2); 98% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 22.6 min and 28.7 min].



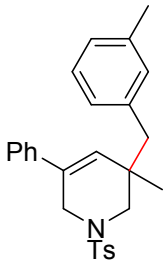
2k:80% yield, 68.6 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 0.94 (s, 3H), 2.27 (s, 3H), 2.36 (s, 3H), 2.47 (d, *J* = 11.4 Hz, 1H), 2.71 (s, 2H), 3.22 (d, *J* = 11.4 Hz, 1H), 3.59 (dd, *J* = 1.8 Hz, *J* = 15.6 Hz, 1H), 4.01 (dd, *J* = 0.9 Hz, *J* = 15.6 Hz, 1H), 5.72 (s, 1H), 7.05 (s, 4H), 7.18-7.29 (m, 7H), 7.65 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.10, 21.58, 23.97, 37.48, 45.03, 46.69, 52.80, 125.34, 127.82, 128.55, 128.73, 129.77, 130.72, 131.17, 132.07, 132.81, 134.18, 135.84, 138.45, 143.70.

ESI-MS: Calcd for$C_{27}H_{29}NO_2S$: [M+ Na$^+$] 454.1811, found 454.1812.

$[\alpha]^{25}_D$ = 42.7 (c = 3.4 in CH_2Cl_2); 98% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 21.6 min and 26.2 min].



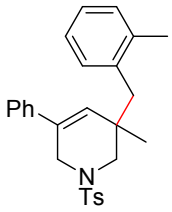
2l: 75% yield, 64.6 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.05 (s, 3H), 2.38 (s, 3H), 2.46 (s, 3H), 2.59 (d, *J* = 11.2 Hz, 1H), 2.81 (s, 2H), 3.32 (d, *J* = 11.2 Hz, 1H), 3.70 (d, *J* = 15.6 Hz, 1H), 4.09 (d, *J* = 15.6 Hz, 1H), 5.81 (s, 1H), 7.05-7.10 (m, 3H), 7.20-7.24 (m, 1H), 7.27-7.38 (m, 7H), 7.75 (d, *J* = 9.2 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.46, 21.58, 24.05, 37.44, 45.43, 46.70, 52.82, 125.33, 127.07, 127.83, 127.88, 128.55, 129.76, 131.17, 131.74, 132.09, 132.80, 137.24, 137.52, 138.47, 143.71.

ESI-MS: Calcd for$C_{27}H_{29}NO_2S$: [M+ Na^+] 454.1811, found 454.1808.

$[\alpha]^{25}_D$ = 22.6 (c = 3.2 in CH_2Cl_2); 89% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm,t_R = 14.0 min and 15.4 min].



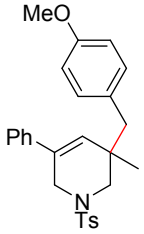
2m: 60% yield, 51.2 mg, yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 1.02 (s, 3H), 2.22 (s, 3H), 2.37 (s, 3H), 2.62 (d, *J* = 11.2 Hz, 1H), 2.64 (d, *J* = 13.2 Hz, 1H), 3.04 (d, *J* = 13.2 Hz, 1H), 3.26 (d, *J* = 11.3 Hz, 1H), 3.64 (dd, *J* = 1.5 Hz, *J* = 15.6 Hz, 1H), 4.01 (dd, *J* = 1.8 Hz, *J* = 15.6 Hz, 1H), 5.62-5.64 (m, 1H), 7.06-7.08 (m, 2H), 7.12-7.21 (m, 3H), 7.21-7.30 (m, 6H), 7.67 (d, *J* = 8.1 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 20.39, 21.58, 24.31, 38.35, 41.91, 46.65, 54.01, 77.24, 125.24, 125.47, 126.43, 127.79, 128.56, 129.79, 130.52, 131.21, 131.56, 131.62, 132.98, 135.94, 137.21, 138.39, 143.73.

ESI-MS: Calcd for$C_{27}H_{29}NO_2S$: [M+ Na^+] 454.1811, found 454.1811.

$[\alpha]^{25}_D$ = 0.27 (c = 2.5 in CH_2Cl_2); 98% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 17.4 min and 20.0 min]



2n: 87% yield, 77.6 mg, yellow oil.

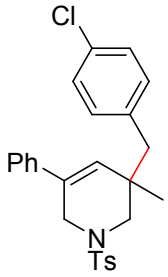
^{1}H NMR (400 MHz, $CDCl_3$): δ 1.02 (s, 3H), 2.45 (s, 3H), 2.53 (d, *J* = 11.2 Hz, 1H), 2.77 (d, *J* = 14.8 Hz, 1H), 2.80 (d, *J* = 14.8 Hz, 1H), 3.33

(d, J = 11.2 Hz, 1H), 3.66 (d, J = 15.6 Hz, 1H), 3.83 (s, 3H), 4.12 (d, J = 15.6 Hz, 1H), 5.80 (s, 1H), 6.87 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 7.27-7.38 (m, 7H), 7.74 (d, J = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.58, 23.94, 37.55, 44.45, 46.69, 52.62, 55.25, 113.42, 125.33, 127.82, 128.56, 129.36, 129.77, 131.21, 131.76, 132.09, 132.78, 138.43, 143.71, 158.18.

ESI-MS: Calcd for$C_{27}H_{29}NO_3S$: [M+ Na^+] 470.1760, found 470.1760.

$[\alpha]^{25}_D$ = 19.2 (c = 3.9 in CH_2Cl_2); 89% ee [Chiralcel OD-Hcolumn, n-hexane/i-PrOH = 95:5, 1.0 mL/min, λ_{max} 254 nm,t_R = 11.9 min and 13.0 min]



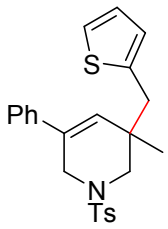
2o: 82% yield, 72.1mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (s, 3H), 2.45-2.48 (m, 4H), 2.84 (s, 2H), 3.39 (d, J = 11.2 Hz, 1H), 3.59 (d, J = 15.6 Hz, 1H), 4.20 (d, J = 15.6 Hz, 1H), 5.76 (s, 1H), 7.20 (d, J = 8.4 Hz, 2H), 7.27-7.38 (m, 9H), 7.73 (d, J = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.58, 23.87, 37.44, 44.62, 46.70, 52.51, 125.32, 127.80, 127.95, 128.17, 128.61, 129.62, 131.56, 131.68, 132.13, 132.89, 132.67, 135.85, 138.23, 143.81.

ESI-MS: Calcd for$C_{26}H_{26}ClNO_2S$: [M+ Na^+] 474.1265, found 474.1264.

$[\alpha]^{25}_D$ = 29.9 (c = 3.6 in CH_2Cl_2); 92 % ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 28.1min and 30.5 min].



2p:60% yield, 71.0 mg, yellow oil.

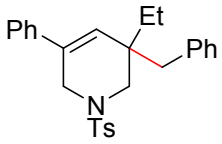
^{1}H NMR (400 MHz, $CDCl_3$): δ 1.12 (s, 3H), 2.45 (s, 3H), 2.66 (d, J = 11.2 Hz, 1H), 3.07 (s, 2H), 3.32 (d, J = 11.2 Hz, 1H), 3.73 (d, J = 15.6 Hz, 1H), 4.05 (d, J = 15.6 Hz, 1H), 5.88 (s, 1H), 6.94-6.96 (m, 1H), 6.98-7.01 (m, 1H), 7.18 (d, J = 4.8 Hz, 1H), 7.29-7.38 (m, 7H), 7.74 (d, J = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.58, 24.19, 37.36, 39.52, 46.64, 52.54, 124.14,

125.40, 126.90, 127.67, 127.77, 127.91, 128.57, 129.80, 131.40, 131.99, 132.87, 138.30, 139.09, 143.75.

ESI-MS: Calcd for$C_{24}H_{25}NO_2S_2$: [M+ Na^+] 446.1219, found 446.1218.

$[\alpha]^{25}_D$ = 0.53 (c = 3.6 in CH_2Cl_2); 89% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 21.4 min and 23.2 min].



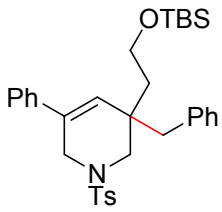
2q: 80% yield, 68.7 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.92 (t, *J* = 7.2 Hz, 3H), 1.50 (q, *J* = 7.2 Hz, 2H), 2.46 (s, 3H), 2.75 (d, *J* = 11.2 Hz, 1H), 2.86 (d, *J* = 13.6 Hz, 1H), 2.93 (d, *J* = 13.6 Hz, 1H), 3.24 (d, *J* = 11.2 Hz, 1H), 3.70 (d, *J* = 15.6 Hz, 1H), 4.07 (d, *J* = 15.6 Hz, 1H), 5.77 (s, 1H), 7.22-7.38 (m, 12H), 7.74 (d, *J* = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 8.42, 21.59, 29.14, 40.39, 43.27, 46.70, 50.59, 125.33, 126.30, 127.78, 128.00, 128.56, 129.79, 130.75, 131.05, 132.06, 132.88, 137.48, 138.56, 143.70.

ESI-MS: Calcd for$C_{27}H_{29}NO_2S$: [M+ Na^+] 454.1811, found 454.1810.

$[\alpha]^{25}_D$ = 41.3 (c = 3.4 in CH_2Cl_2); 99% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm,t_R = 79.7 min and 86.6 min].



2r: 86% yield, 96.5 mg, yellow oil.

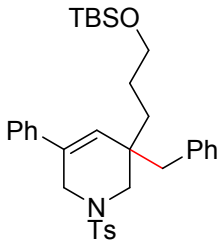
^{1}H NMR (400 MHz, $CDCl_3$): δ 0.01 (s, 3H), 0.01 (s, 3H), 0.84 (s, 9H), 1.72 (t, *J* = 6.4 Hz, 2H), 2.46 (s, 3H), 2.91 (d, *J* = 13.2 Hz, 1H), 2.93 (d, *J* = 11.6 Hz, 1H), 3.04 (d, *J* = 13.2 Hz, 1H), 3.30 (d, *J* = 11.6 Hz, 1H), 3.67-3.72 (m, 3H), 4.10 (d, *J* = 15.2 Hz, 1H), 5.79 (s, 1H), 7.23-7.37 (m, 12H), 7.74 (d, *J* = 8.0 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 24.42, 24.91, 25.51, 28.44, 32.98, 35.77, 38.38, 52.39, 52.72, 52.88, 53.05, 125.85, 126.97, 128.30, 132.27, 133.26, 142.02, 172.22, 172.62.

ESI-MS: Calcd for$C_{33}H_{43}NO_3SSi$: [M+ Na^+] 584.2625, found 584.2621.

$[\alpha]^{25}_D$ = 0.8 (c = 4.8 in CH_2Cl_2); 93% ee [Chiralcel AD-H column, n-hexane/i-PrOH=

98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 38.3 min and 47.3 min].



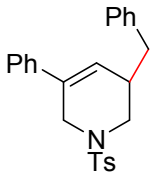
2s: 82% yield, 92.0 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.05 (s, 6H), 0.90 (s, 9H), 1.48-1.60 (m, 4H), 2.46 (s, 3H), 2.70 (d, J = 11.6 Hz, 1H), 2.86 (d, J = 13.2 Hz, 1H), 2.95 (d, J = 13.2 Hz, 1H), 3.29 (d, J = 11.6 Hz, 1H), 3.54-3.57 (m, 2H), 3.66 (d, J = 15.2 Hz, 1H), 4.10 (d, J = 15.2 Hz, 1H), 5.75 (s, 1H), 7.22-7.38 (m, 12H), 7.73 (d, J = 8.0 Hz, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 5.29, 18.41, 21.58, 26.01, 27.35, 32.70, 40.02, 43.88, 46.70, 50.91, 63.45, 125.32, 126.32, 127.79, 127.82, 128.03, 128.55, 129.80, 130.79, 131.04, 132.02, 132.77, 137.34, 138.48, 143.73.

ESI-MS: Calcd for$C_{34}H_{45}NO_3SSi$ [M+ Na^+] 598.2782, found 598.2780.

$[\alpha]^{25}_D$ = 90 (c = 4.6 in CH_2Cl_2);85% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 31.7 min and 37.6 min].



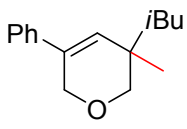
2t: 66% yield, 53.1 mg, yellow

^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H), 2.74-2.85 (m, 3H), 3.06 (dd, *J* = 5.2 Hz, *J* = 11.6 Hz, 1H), 3.13 (dd, *J* = 4.4 Hz, *J* = 11.6 Hz, 1H), 3.85 (d, *J* = 15.6 Hz, 1H), 4.03 (d, *J* = 15.6 Hz, 1H), 6.02-6.04 (m, 1H), 7.24-7.38 (m, 12H), 7.71 (d, *J* = 8.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 21.56, 37.90, 39.42, 46.68, 46.81, 125.38, 126.39, 127.78, 127.89, 128.58, 129.31, 129.75, 133.43, 138.48, 139.34, 143.69.

ESI-MS: Calcd for$C_{25}H_{25}NO_2S$: [M+ Na^+] 426.1498, found 426.1496.

$[\alpha]^{25}_D$ = 0.6 (c = 2.7 in CH_2Cl_2); 49% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm,t_R = 17.0 min and 19.4 min].



2v: 73% yield, 33.6 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.96 (d, *J* = 5.6 Hz, 6H), 1.09 (s, 3H),

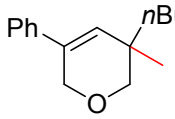
1.33 (dd, J = 6.4 Hz, J = 14.0 Hz, 1H), 1.47 (dd, J = 5.2 Hz, J = 14.0 Hz, 1H), 1.78-1.89 (m, 1H), 3.46 (d, J = 10.8 Hz, 1H), 3.63 (d, J = 10.8 Hz, 1H), 4.45 (d, J = 16.8 Hz, 1H), 4.49 (d, J = 16.8 Hz, 1H), 6.02 (s, 1H), 7.27-7.37 (m, 5H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 24.45, 24.74,

24.96, 25.41, 35.32, 48.86, 66.91, 74.77, 124.83, 127.37, 128.51, 131.62, 133.45, 138.28.

ESI-MS: Calcd for$C_{16}H_{22}O$: [M+H$^+$] 231.1743, found 231.1743.

$[\alpha]^{25}_D$ = 6.2 (c = 1.7 in CH_2Cl_2); 58% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm, t_R = 4.0 min and 4.7 min].



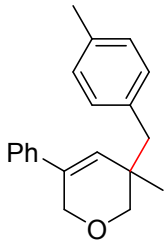
2w: 75% yield, 34.5 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.80-0.86 (m, 3H), 0.97 (s, 3H), 1.18-1.32 (m, 6H), 3.36 (d, J = 11.1 Hz, 1H), 3.52 (d, J = 11.1 Hz, 1H), 4.38 (s, 1H), 4.38 (s, 1H), 5.91 (t, J = 1.5 Hz, 1H), 7.18-7.26 (m, 5H).

^{13}C NMR (75 MHz, $CDCl_3$): δ14.16, 23.61, 23.75, 26.28, 34.73, 39.43, 66.96, 74.36, 124.86, 127.40, 128.50, 131.26, 133.81, 138.23.

ESI-MS: Calcd for$C_{16}H_{22}O$ [M+H$^+$] 231.1743, found 231.1743.

$[\alpha]^{25}_D$ = 5.2 (c = 1.7 in CH_2Cl_2); 63% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm,t_R = 3.8 min and 4.8 min].



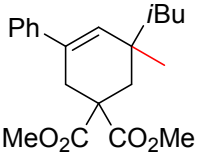
2x: 75% yield, 41.7 mg, yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (s, 3H), 2.36 (s, 3H), 2.71 (d, J = 13.2 Hz, 1H), 2.80 (d, J = 13.2 Hz, 1H), 3.41 (d, J = 11.2 Hz, 1H), 3.70 (d, J = 11.2 Hz, 1H), 4.50 (d, J = 16.0 Hz, 1H), 4.54 (d, J = 16.0 Hz, 1H), 5.93 (s, 1H), 7.08-7.14 (m, 4H), 7.27-7.37 (m, 5H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.07, 22.76, 29.73, 35.69, 44.96, 67.12, 73.88, 124.84, 127.48, 128.52, 128.63, 130.53, 130.93, 133.87, 134.70, 135.63, 138.10.

ESI-MS: Calcd for$C_{27}H_{29}NO_2S$: [M+ Na$^+$] 301.1563, found 301.1563.

$[\alpha]^{25}_D$ = -0.4 (c = 2.1 in CH_2Cl_2); 53% ee [Chiralcel OD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm, t_R = 6.3 min and 10.6 min].



2y: 70% yield, 48.1mg, yellow oil.

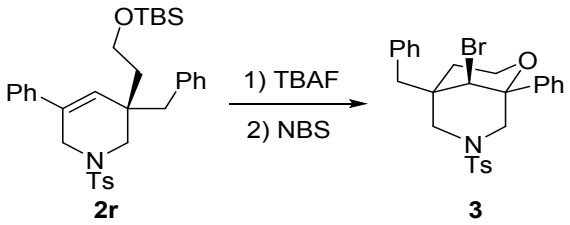
^{1}H NMR (300 MHz, $CDCl_3$): δ0.94 (d, *J* = 3.9 Hz, 3H), 0.96 (d, *J* = 4.2 Hz, 3H), 0.98 (s, 3H), 1.28 (dd, *J* = 6.3 Hz, *J* = 14.1 Hz, 1H), 1.37 (dd, *J* = 4.8 Hz, *J* = 14.1 Hz, 1H), 1.69-1.87 (m, 1H), 2.21 (d, *J* = 15.2 Hz, 1H), 2.27 (d, *J* = 15.2 Hz, 1H), 2.55 (dd, *J* = 3.6 Hz, *J* = 16.8 Hz, 1H), 3.12 (d, *J* = 16.8 Hz, 1H), 3.73 (s, 3H), 3.76 (s, 3H), 5.71 (d, *J* = 2.1 Hz, 1H), 7.23-7.27 (m, 1H), 7.32-7.38 (m, 2H), 7.42-7.46 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 24.42, 24.91, 25.31, 28.44, 32.98, 35.77, 38.38, 52.39, 52.72, 52.88, 53.05, 125.85, 126.97, 128.30, 132.27, 133.26, 142.02, 172.22, 172.62.

ESI-MS: Calcd for$C_{21}H_{28}O_4$ [M+ Na^+] 367.1880, found 367.1881.

$[\alpha]^{25}_D$ = 20 (c = 2.4 in CH_2Cl_2); 8% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 99:1, 0.8 mL/min, λ_{max} 254 nm, t_R = 6.3 min and 14.6 min].

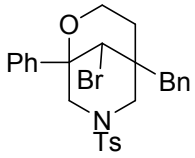
4. Synthetic Application



2r **3**

To a solution of **2r** (0.19mmol) in Et_2O (2mL) at 0°C was added of TBAF (0.3mL, 1 mol/L). After 2 h,the reaction was concentrated in vacuum. The residue was used for the next stepwithoutpurification.

To a solution of NBS (35.5 mg,0.2 mmol) in CH_2Cl_2 (5.0 mL) was added the solutionof alcoholin CH_2Cl_2 (2.0 mL). The reaction was stirred atroom temperature for 5 min, and then was quenched by aq.$Na_2S_2O_3$solution (5 mL). The resulted mixture was diluted with H_2O, and was extracted with CH_2Cl_2. Thecombinedorganic extracts were dried over $MgSO_4$ and then was concentrated in vacuum. The residue waspurified by column chromatography (silica gel, PE/EA) to give a white solid (79.4 mg 71%).



3: 71% yield, 79.4 mg, yellow solid.mp. 196-197°C

^{1}H NMR (300 MHz, $CDCl_3$): δ 1.89 (dd, *J* = 4.2 Hz, *J* = 13.8 Hz, 1H), 1.98-2.11 (m, 1H), 2.41 (s, 3H), 2.55 (d, *J* = 13.5 Hz, 1H), 2.75 (d, *J* = 13.5 Hz, 1H), 3.00 (dd, *J* = 2.1 Hz, *J* = 11.4 Hz, 1H), 3.67-3.78 (m, 3H), 4.16 (s, 1H), 4.20 (d, *J* = 12.0 Hz, 1H), 4.88-4.98 (m, 1H), 7.13-7.17 (m, 2H), 7.22-7.39 (m, 8H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.1 Hz, 2H).

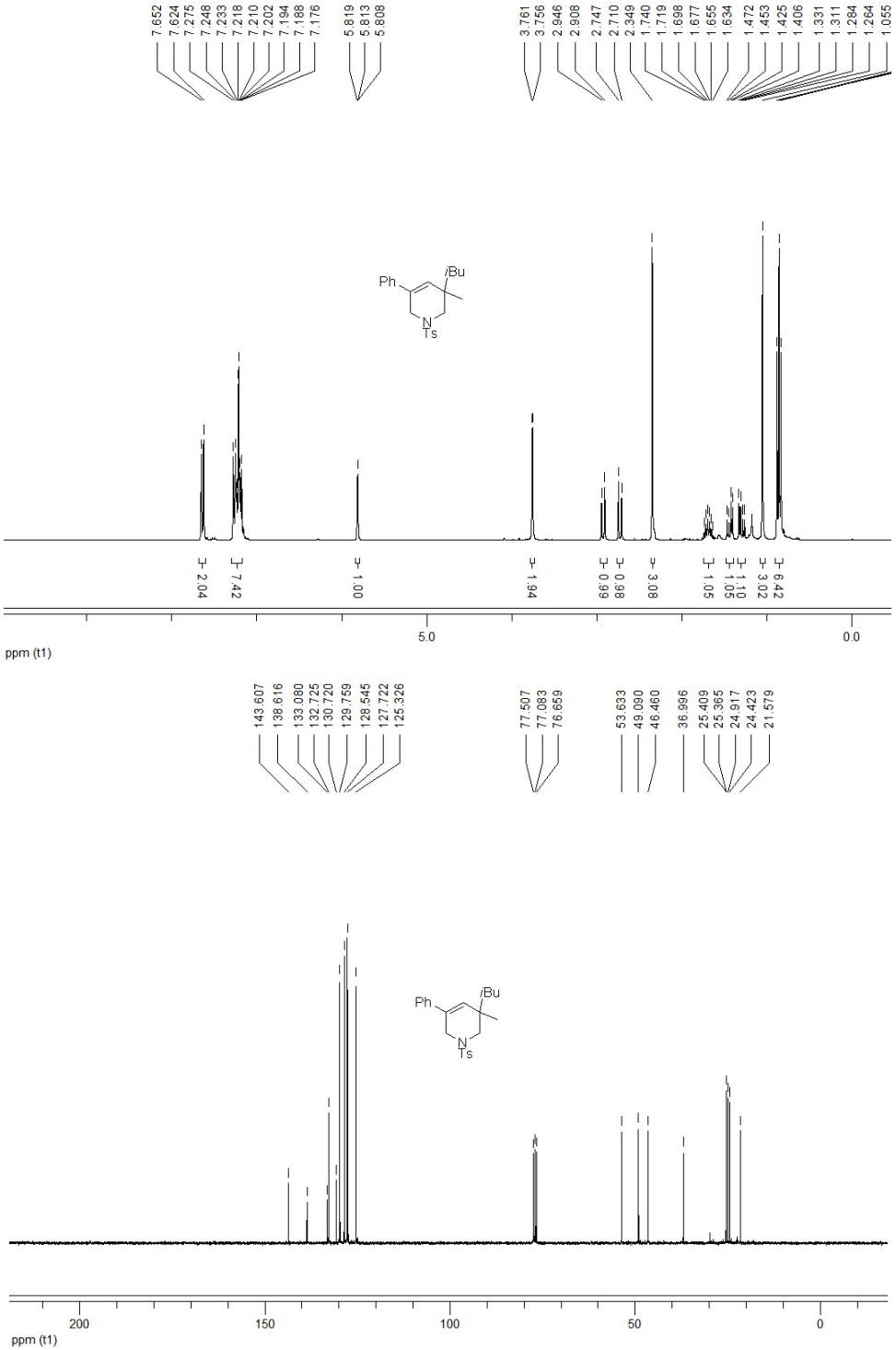
^{13}C NMR (75 MHz, $CDCl_3$): δ 21.67, 35.82, 38.69, 45.05, 47.19, 49.31, 63.31, 63.92, 73.98, 125.41, 127.15, 127.58, 128.24, 128.35, 128.52, 129.99, 130.61, 132.41, 135.03, 141.54, 143.97.

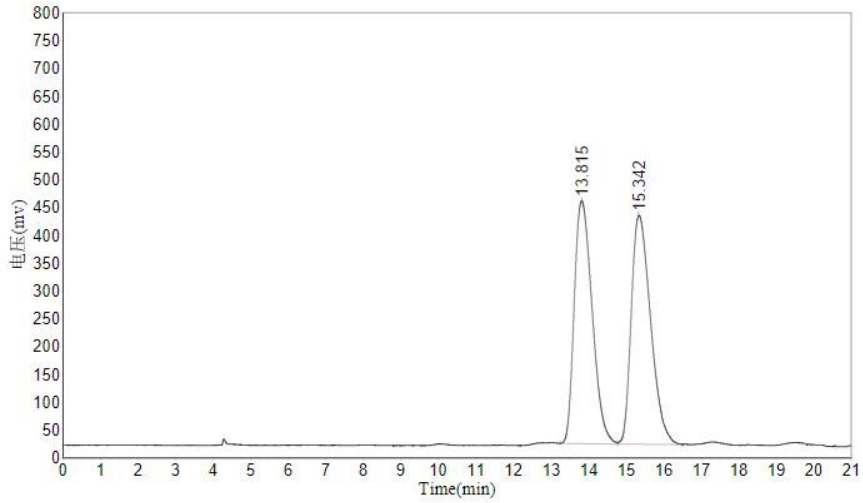
ESI-MS: Calcd for$C_{27}H_{28}BrNO_3S$ [M+Na^+] 548.0865, found 548.0863.

$[\alpha]^{25}_D$ = 0.7 (c = 3.3 in CH_2Cl_2); 93.6% ee [Chiralcel AD-H column, n-hexane/i-PrOH = 98:2, 0.8 mL/min, λ_{max} 254 nm, t_R = 9.3 min and 10.0 min].

5. NMR and HPLC Spectra ofNew Compounds

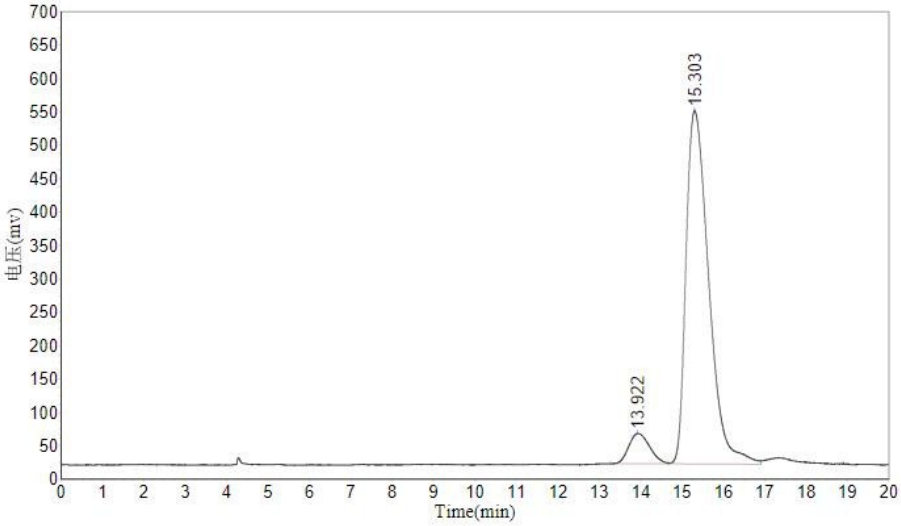
2a





Results

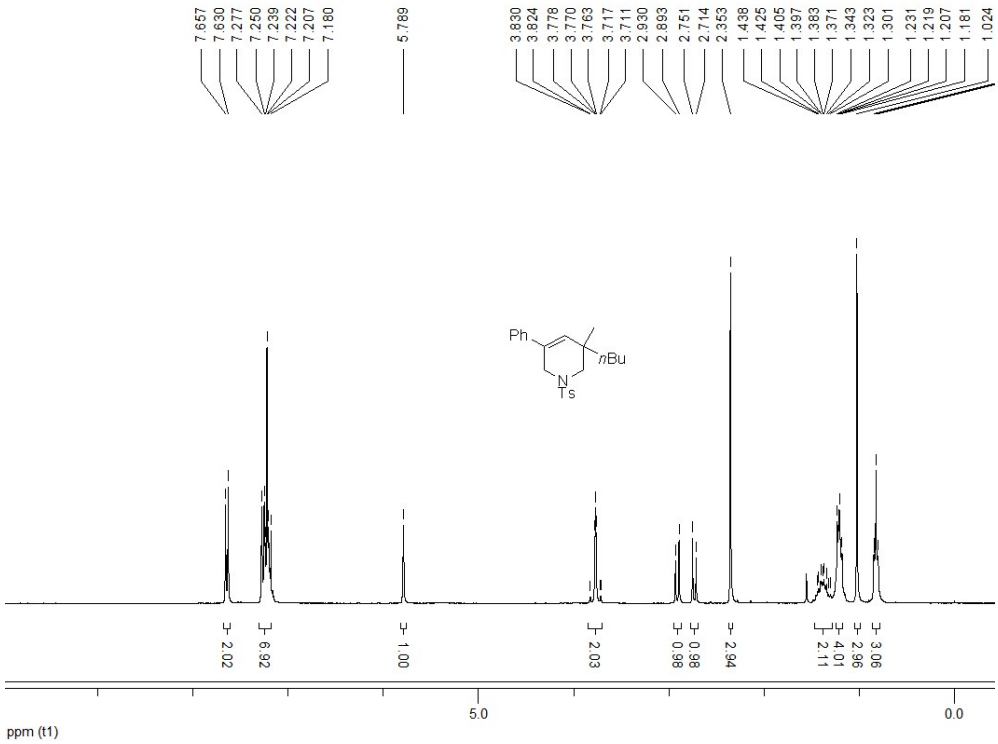
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		13.815	436262.156	14477421.000	49.5977
2		15.342	410956.125	14712297.000	50.4023
Total			847218.281	29189718.000	100.0000



Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		13.922	45563.320	1609037.625	7.4097
2		15.303	528522.313	20106362.000	92.5903
Total			574085.633	21715399.625	100.0000

2b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7.277
7.250
7.239
7.222
7.207
7.180
5.789
3.830
3.824
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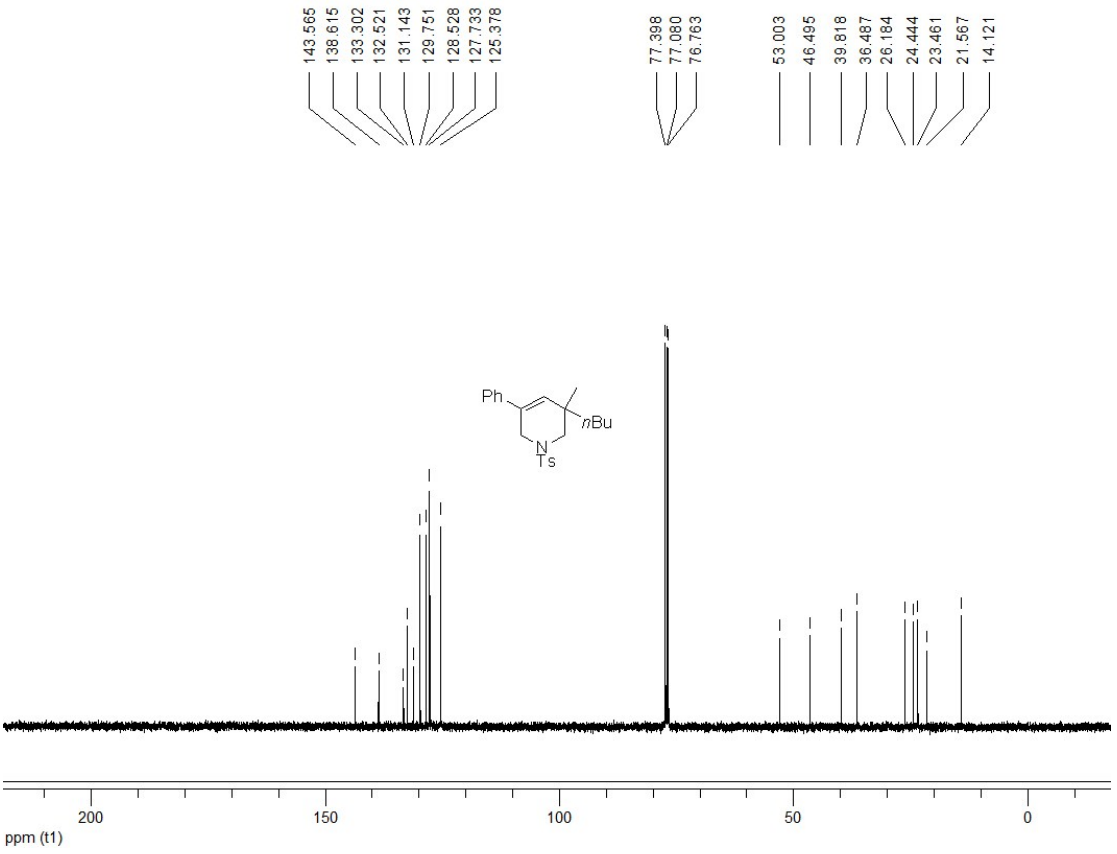
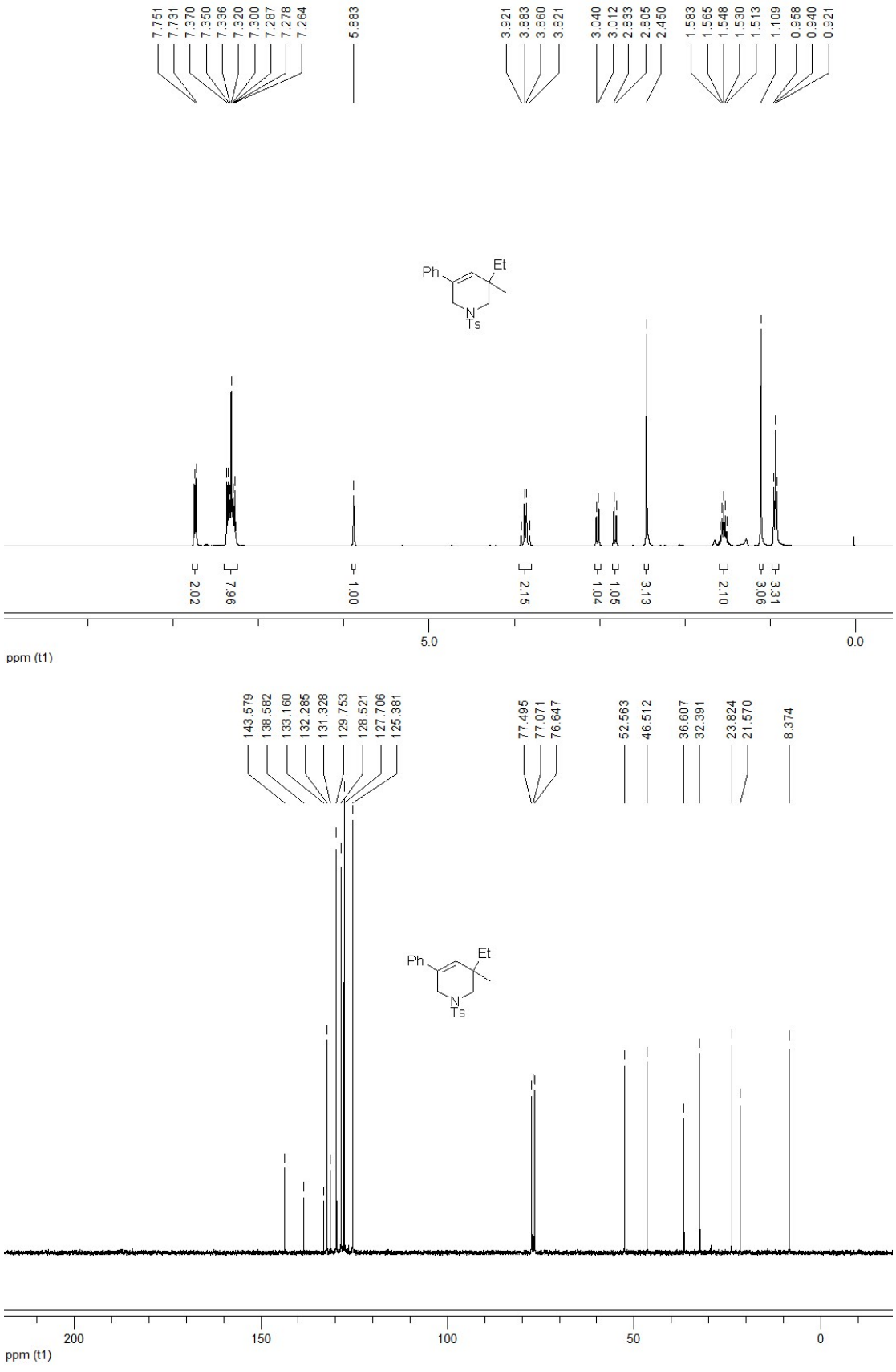
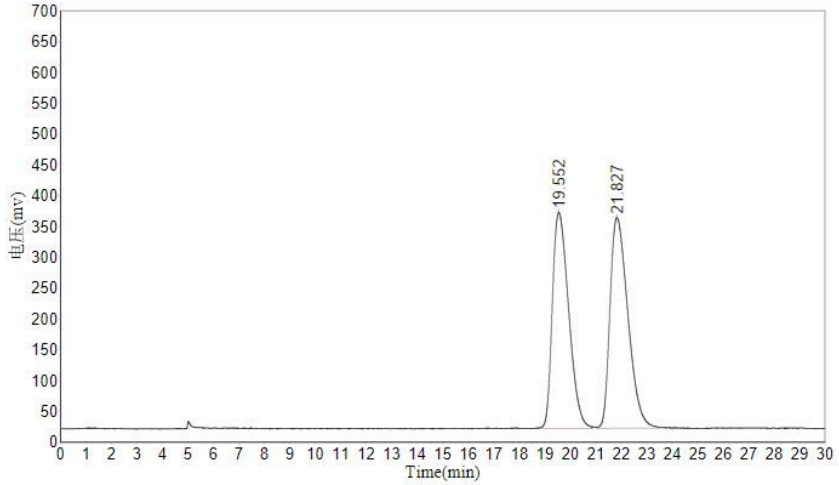
3.770
3.763
3.717
3.711
2.930
2.893
2.751
2.714
2.353
1.438
1.425
1.405
1.397
1.383
1.371
1.343
1.323
1.301
1.231
1.219
1.207
1.181
1.024
Ph
nBu
N
Ts
2.02
6.92
1.00
2.03
0.98
0.98
2.94
2.11
4.01
2.96
3.06
5.0
0.0
ppm (t1)


143.565
138.615
133.302
132.521
131.143
129.751
128.528
127.733
125.378
77.398
77.080
76.763
53.003
46.495
39.818
36.487
26.184
24.444
23.461
21.567
14.121
Ph
nBu
N
Ts
200
150
100
50
0
ppm (t1)

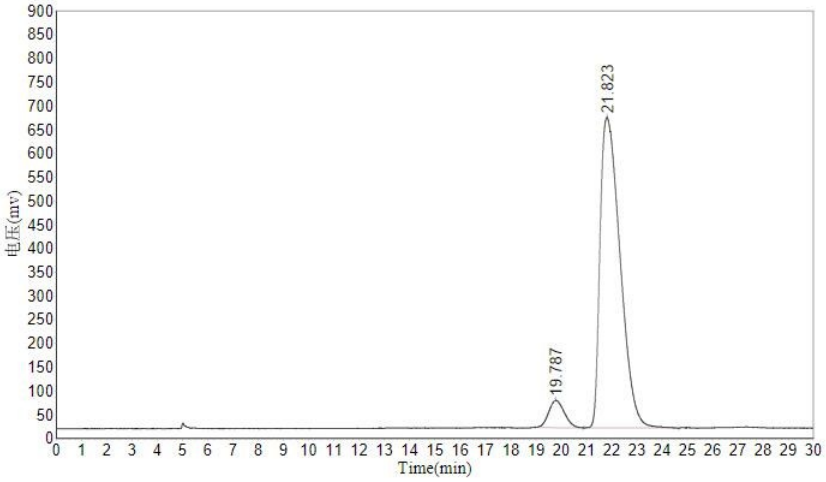
2c


7.751
7.731
7.370
7.350
7.336
7.320
7.300
7.287
7.278
7.264
5.883
3.921
3.883
3.860
3.821
3.040
3.012
2.833
2.805
2.450
1.583
1.565
1.548
1.530
1.513
1.109
0.958
0.940
0.921
Ph
Et
N
Ts
2.02
7.96
1.00
2.15
1.04
1.05
3.13
2.10
3.08
3.31
5.0
0.0
ppm (t1)
143.579
138.582
133.160
132.285
131.328
129.753
128.521
127.706
125.381
77.495
77.071
76.647
52.563
46.512
36.607
32.391
23.824
21.570
8.374
Ph
Et
N
Ts
200
150
100
50
0
ppm (t1)



Results

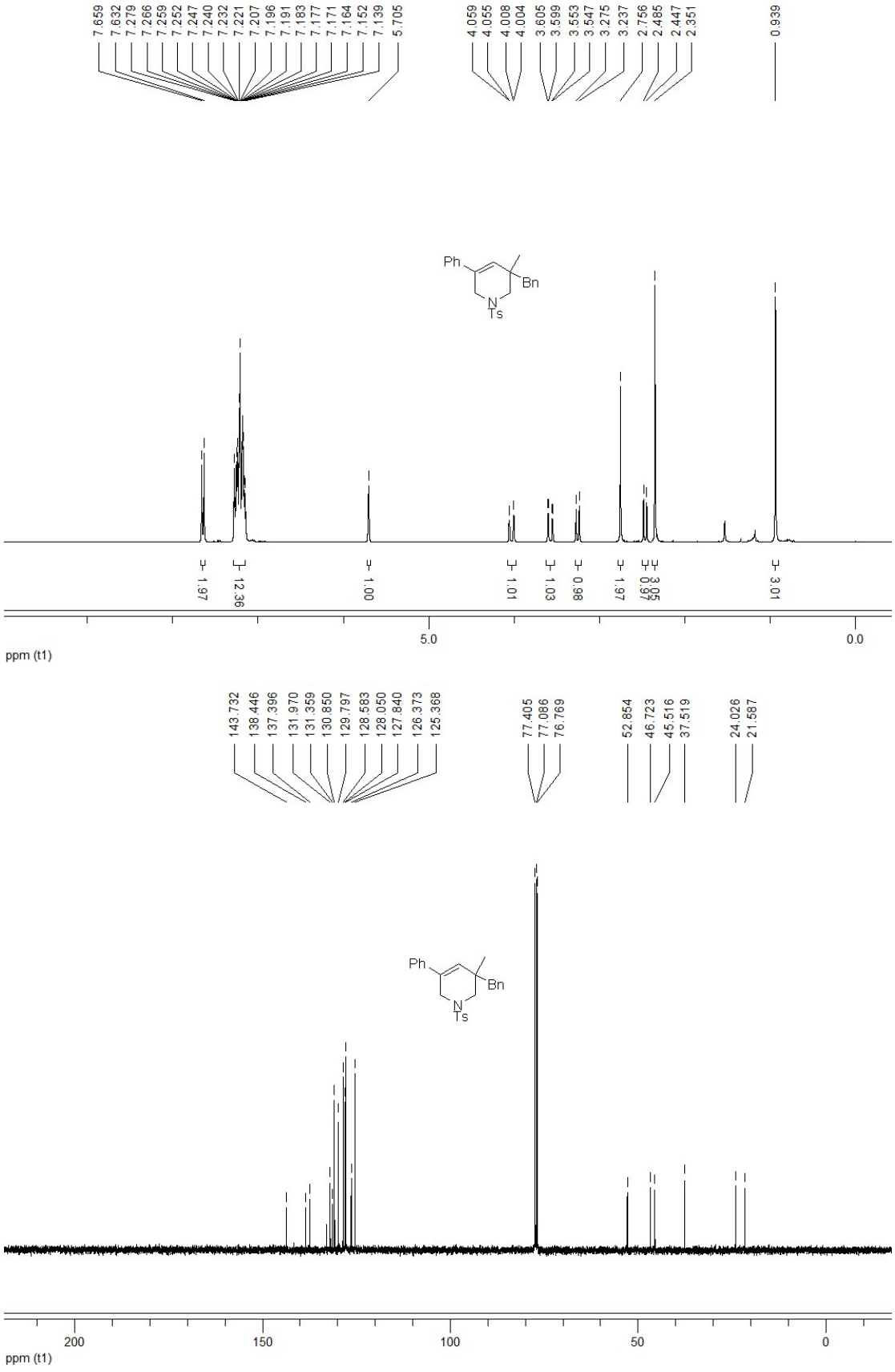
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		19.552	350231.688	15567532.000	48.2326
2		21.827	341480.938	16708432.000	51.7674
Total			691712.625	32275964.000	100.0000



Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		19.787	57194.172	2465226.500	6.4011
2		21.823	653859.000	36047516.000	93.5989
Total			711053.172	38512742.500	100.0000

2d


7.659
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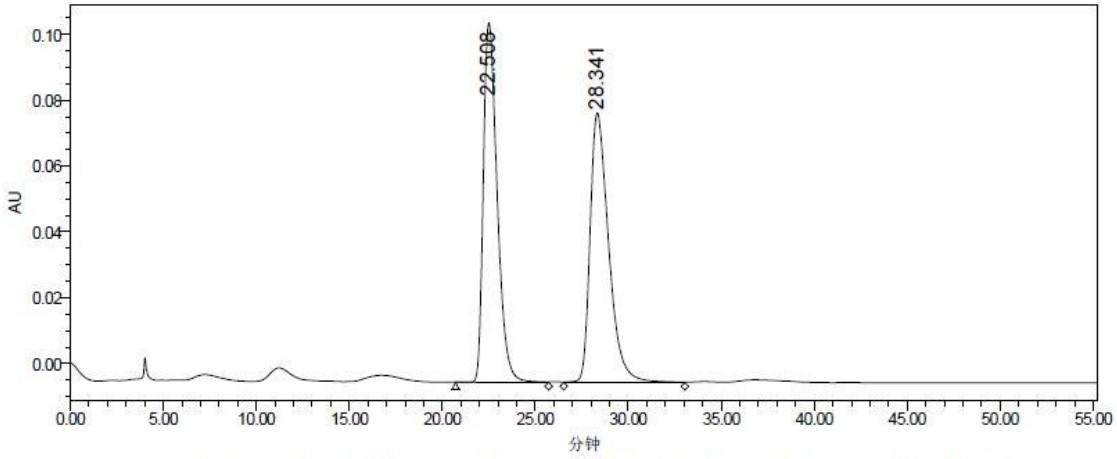
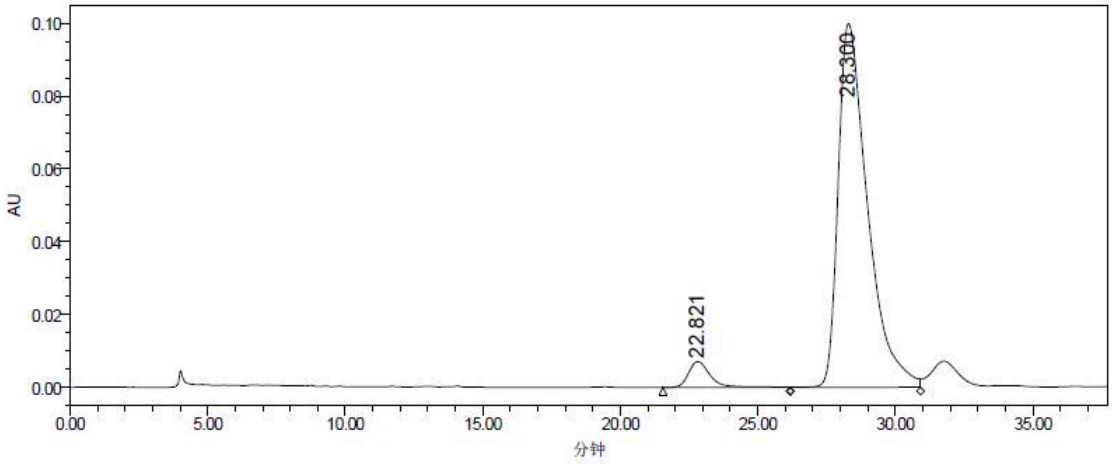
7.279
7.266
7.259
7.252
7.247
7.240
7.232
7.221
7.207
7.196
7.191
7.183
7.177
7.171
7.164
7.152
7.139
5.705
4.059
4.055
4.008
4.004
3.605
3.599
3.553
3.547
3.275
3.237
2.756
2.485
2.447
2.351
0.939
Ph
Bn
N
Ts
1.97
12.36
1.00
1.01
1.03
0.98
1.97
3.06
0.97
3.01
5.0
0.0
ppm (t1)
143.732
138.446
137.396
131.970
131.359
130.850
129.797
128.583
128.050
127.840
126.373
125.368
77.405
77.086
76.769
52.854
46.723
45.516
37.519
24.026
21.587
Ph
Bn
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

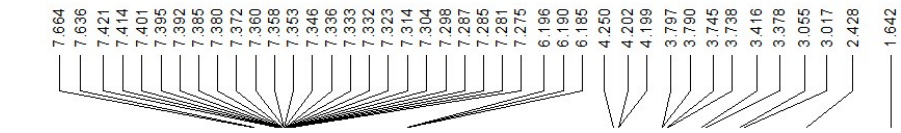
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	22.508	5648897	49.84	109248
2	W2489 ChA 254nm	28.341	5686081	50.16	81871



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	22.821	390500	5.00	7109
2	W2489 ChA 254nm	28.300	7414428	95.00	99928

2e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7.414
7.401
7.395
7.392
7.385
7.380
7.372
7.360
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7.353
7.346
7.336
7.333
7.332
7.323
7.314
7.304
7.298
7.287
7.285
7.281
7.275
6.196
6.190
6.185
4.250
4.202
4.199
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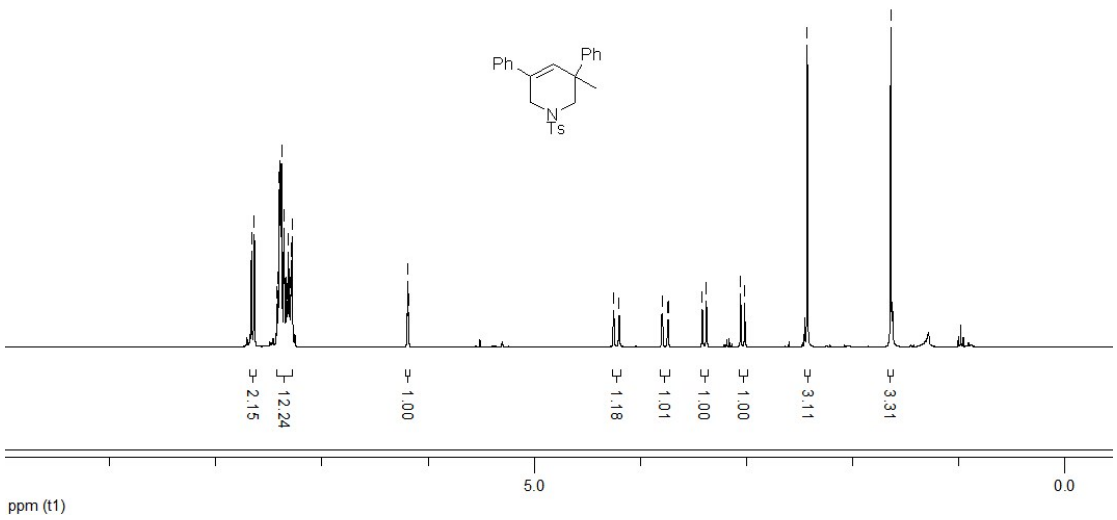
3.790
3.745
3.738
3.416
3.378
3.055
3.017
2.428
1.642


Ph
Ph
N
Ts
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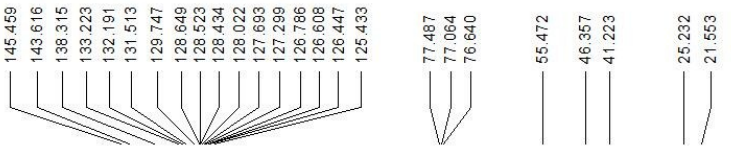
12.24
1.00
1.18
1.01
1.00
1.00
3.11
3.31
5.0
0.0
ppm (t1)


145.459
143.616
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133.223
132.191
131.513
129.747
128.649
128.523
128.434
128.022
127.693
127.299
126.786
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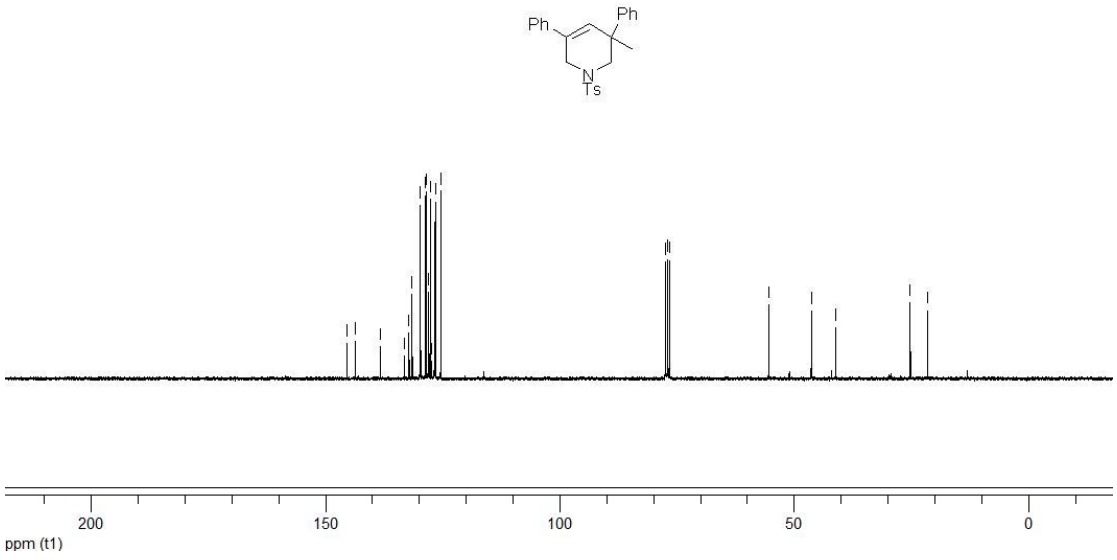
126.447
125.433
77.487
77.064
76.640
55.472
46.357
41.223
25.232
21.553


Ph
Ph
N
Ts
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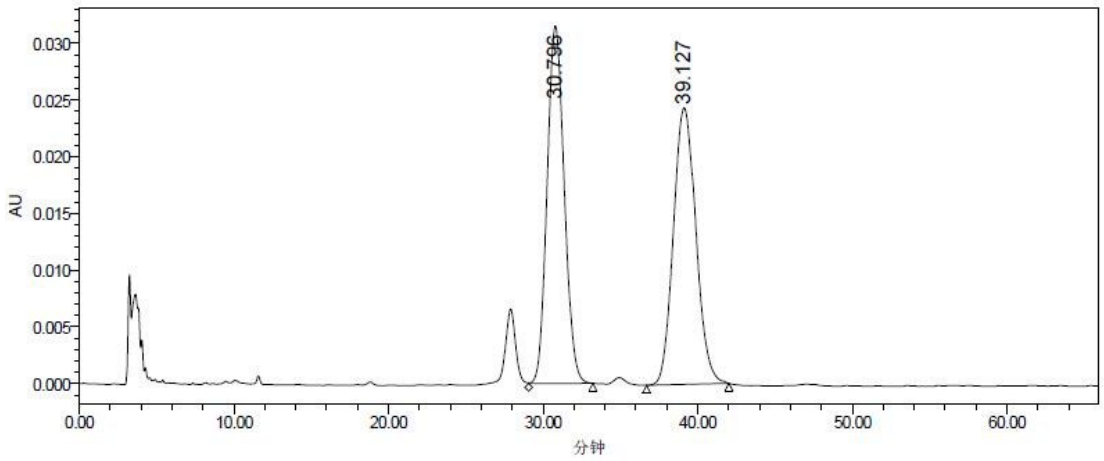
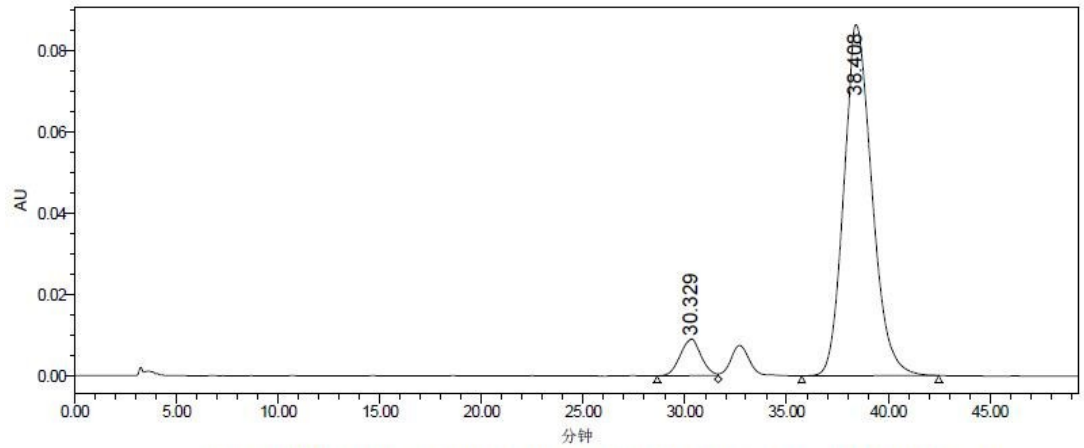
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

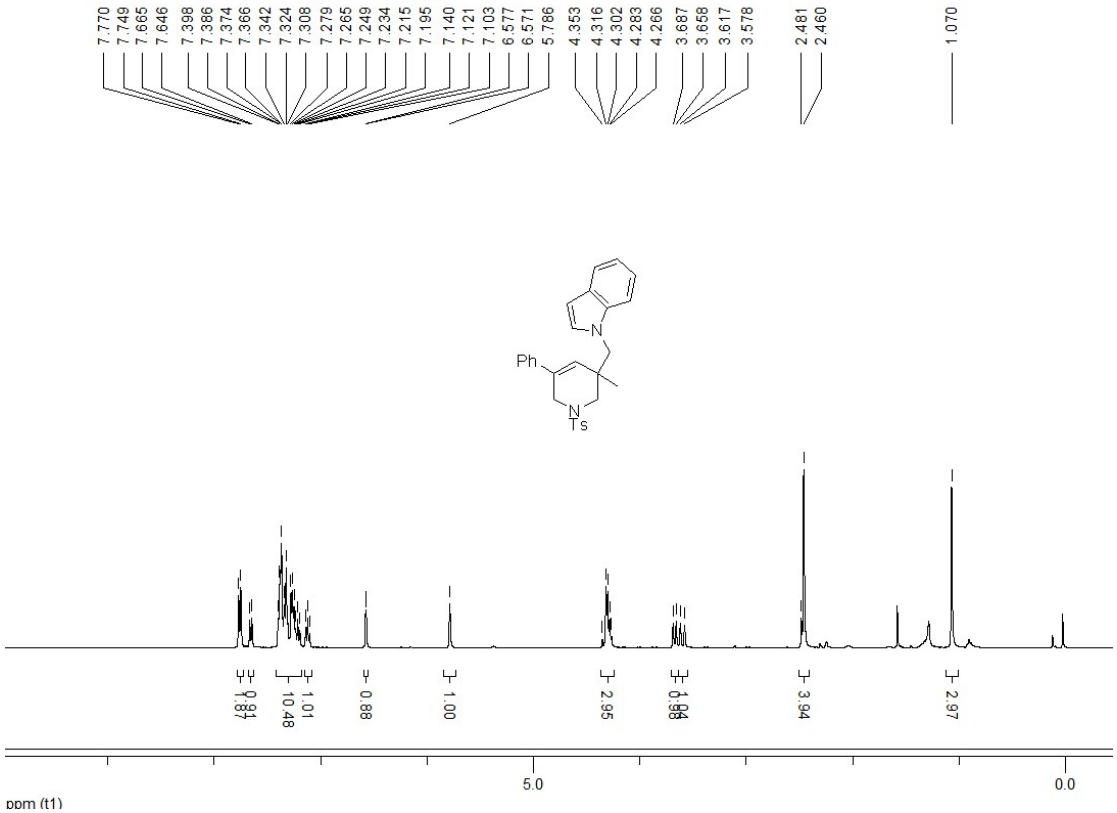
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	30.796	2428188	49.60	31512
2	W2489 ChA 254nm	39.127	2467366	50.40	24392



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	30.329	638778	7.16	9019
2	W2489 ChA 254nm	38.408	8283304	92.84	86247

2f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7.646
7.398
7.386
7.374
7.366
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7.324
7.308
7.279
7.265
7.249
7.234
7.215
7.195
7.140
7.121
7.103
6.577
6.571
5.786
4.353
4.316
4.302
4.283
4.266
3.687
3.658
3.617
3.578
2.481
2.460
1.070
Ph
N
Ts
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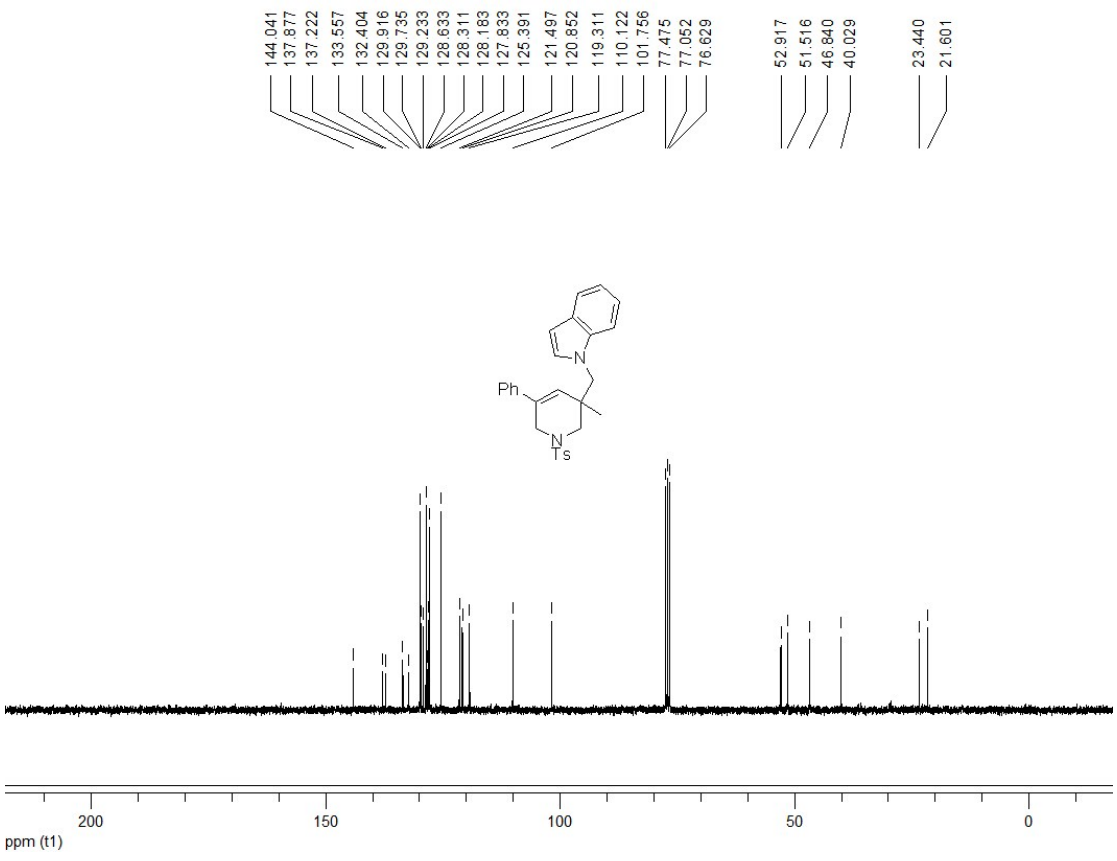
0.88
1.00
2.95
0.98
3.94
2.97
5.0
0.0
ppm (t1)


144.041
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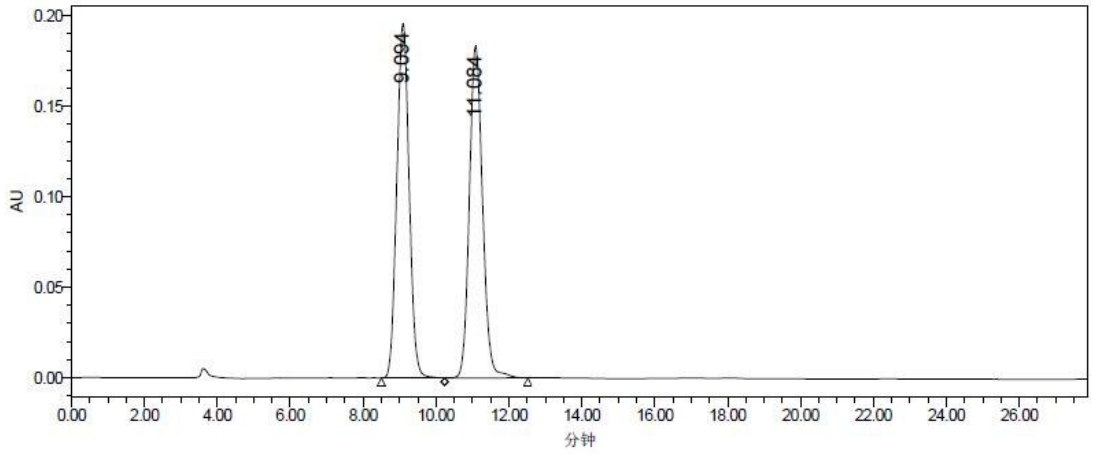
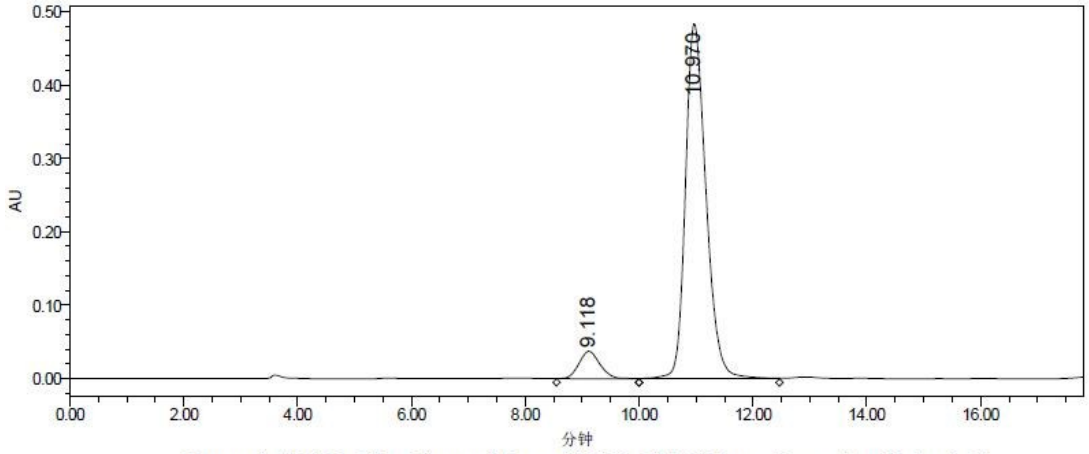
137.222
133.557
132.404
129.916
129.735
129.233
128.633
128.311
128.183
127.833
125.391
121.497
120.852
119.311
110.122
101.756
77.475
77.052
76.629
52.917
51.516
46.840
40.029
23.440
21.601
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

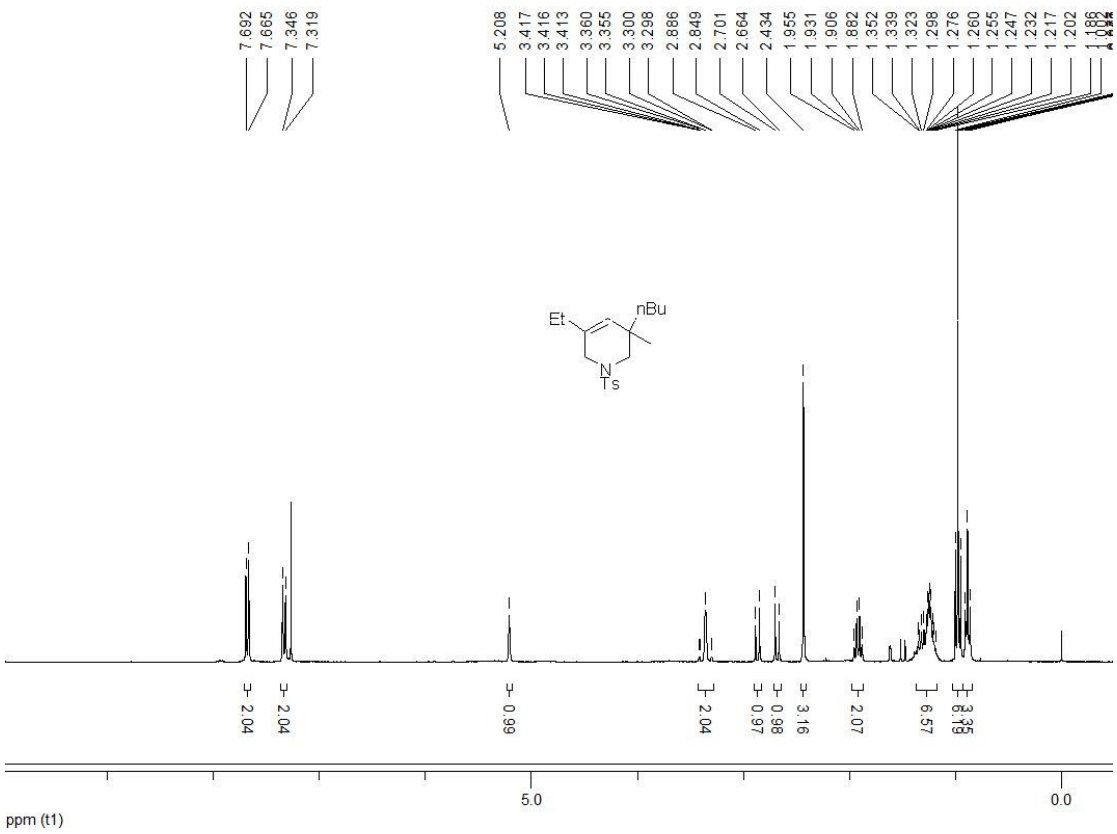
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	9.094	4605814	50.00	195820
2	W2489 ChA 254nm	11.084	4604991	50.00	183142



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	9.118	955922	7.30	37326
2	W2489 ChA 254nm	10.970	12146196	92.70	483620

2g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7.346
7.319
5.208
3.417
3.416
3.413
3.360
3.355
3.300
3.298
2.886
2.849
2.701
2.664
2.434
1.955
1.931
1.906
1.882
1.352
1.339
1.323
1.298
1.276
1.260
1.255
1.247
1.232
1.217
1.202
Et
nBu
N
Ts
2.04
2.04
0.99
2.04
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0.98
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2.07
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6.18
3.35
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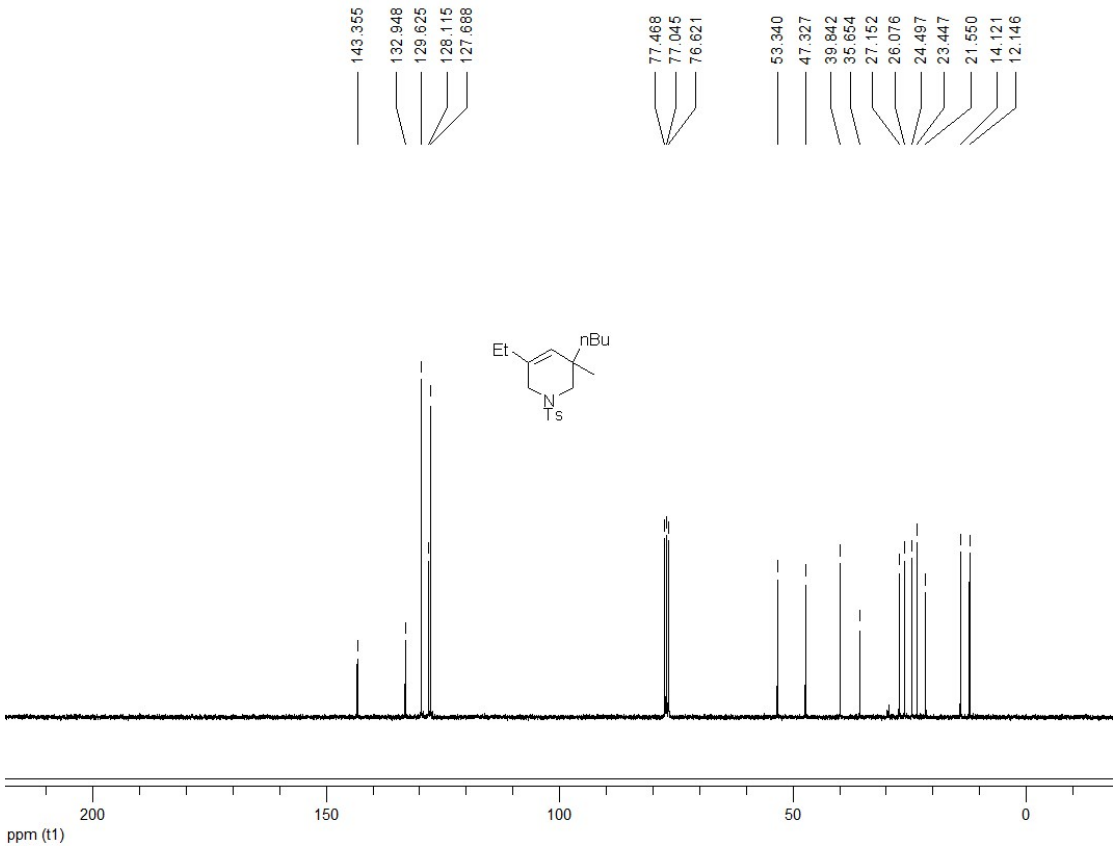
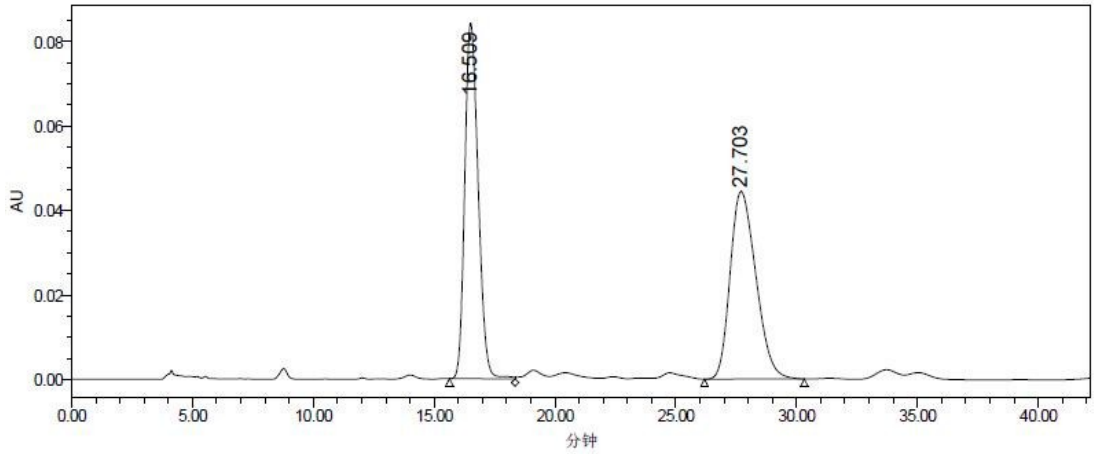
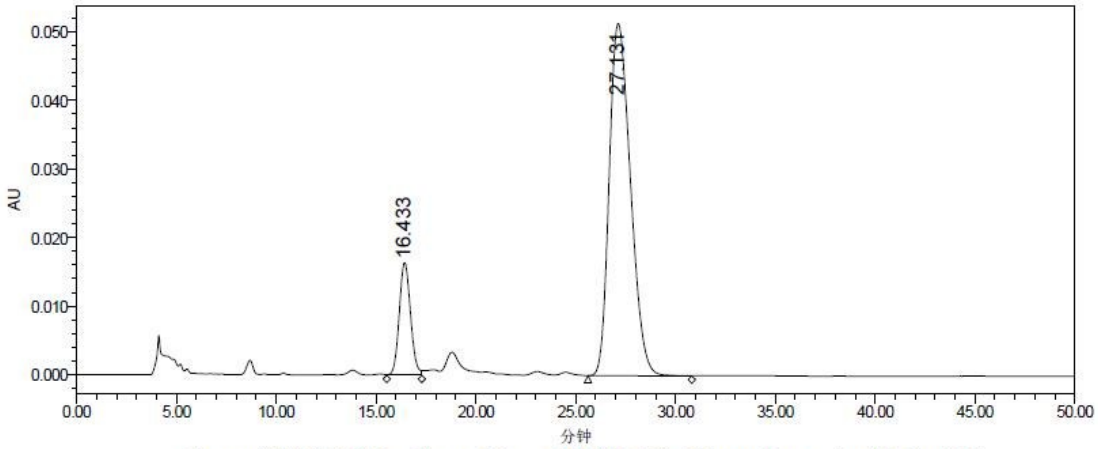
0.0
ppm (t1)


143.355
132.948
129.625
128.115
127.688
77.468
77.045
76.621
53.340
47.327
39.842
35.654
27.152
26.076
24.497
23.447
21.550
14.121
12.146
Et
nBu
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

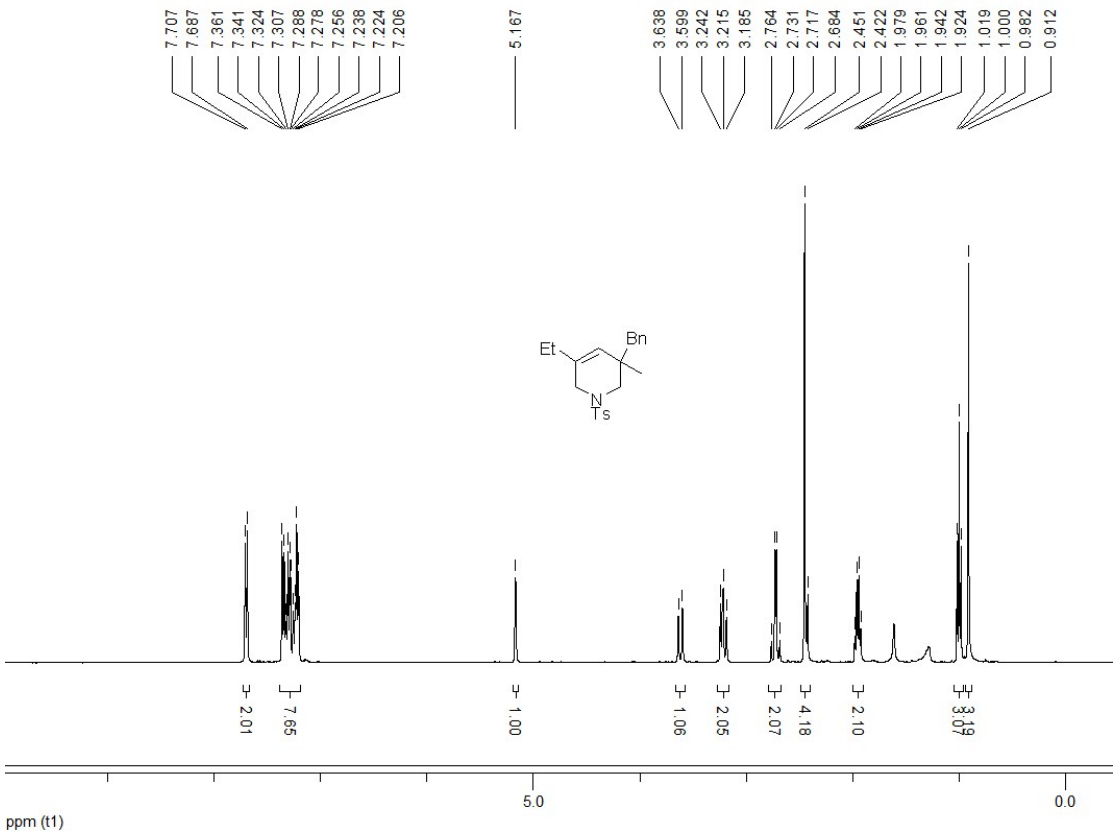
	Channel Description	RT (min)	Area (碘*sec)	% Area	Height (碘)
1	W2489 ChA 254nm	16.509	3243009	49.64	84202
2	W2489 ChA 254nm	27.703	3289605	50.36	44374



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (碘*sec)	% Area	Height (碘)
1	W2489 ChA 254nm	16.433	644029	14.49	16431
2	W2489 ChA 254nm	27.131	3801367	85.51	51372

2h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7.341
7.324
7.307
7.288
7.278
7.256
7.238
7.224
7.206
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3.638
3.599
3.242
3.215
3.185
2.764
2.731
2.717
2.684
2.451
2.422
1.979
1.961
1.942
1.924
1.019
1.000
0.982
0.912
Et
Bn
N
Ts
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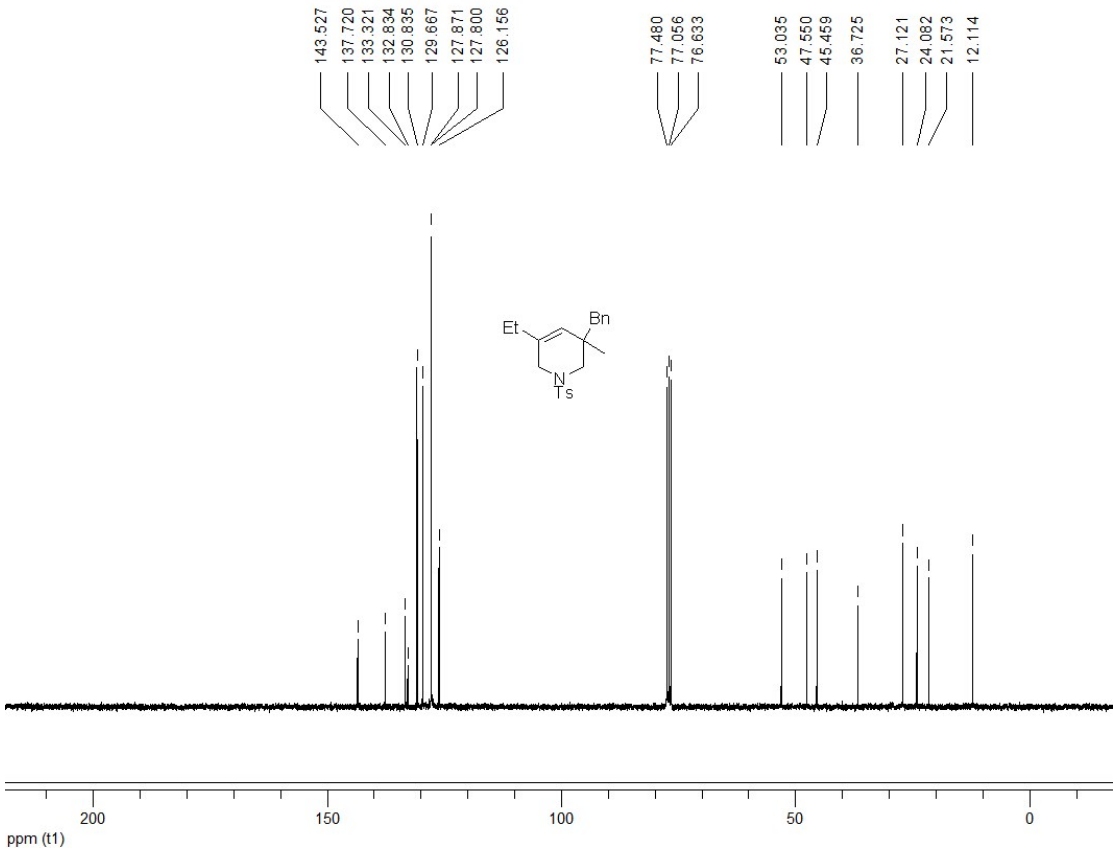
7.66
1.00
1.06
2.06
2.07
4.18
2.10
3.07
5.0
0.0
ppm (t1)


143.527
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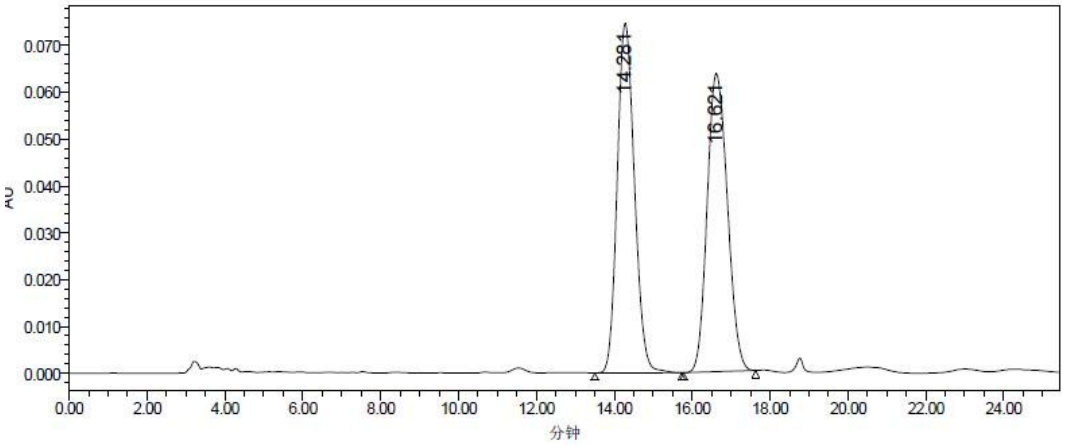
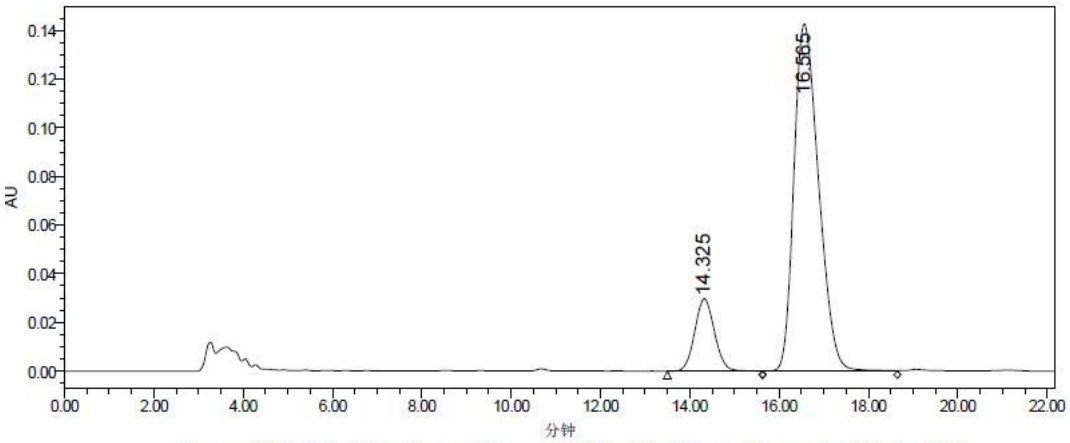
132.834
130.835
129.667
127.871
127.800
126.156
77.480
77.056
76.633
53.035
47.550
45.459
36.725
27.121
24.082
21.573
12.114
Et
Bn
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

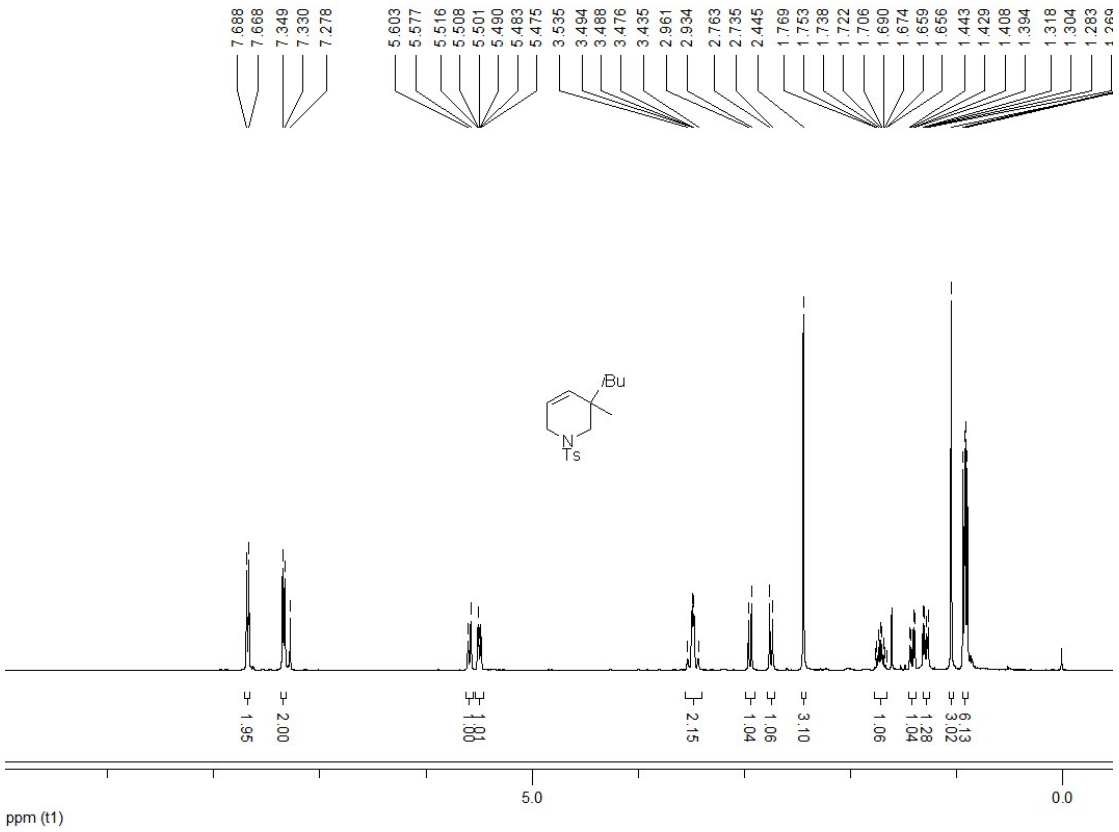
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	14.281	2298063	49.99	74704
2	W2489 ChA 254nm	16.621	2299369	50.01	63671

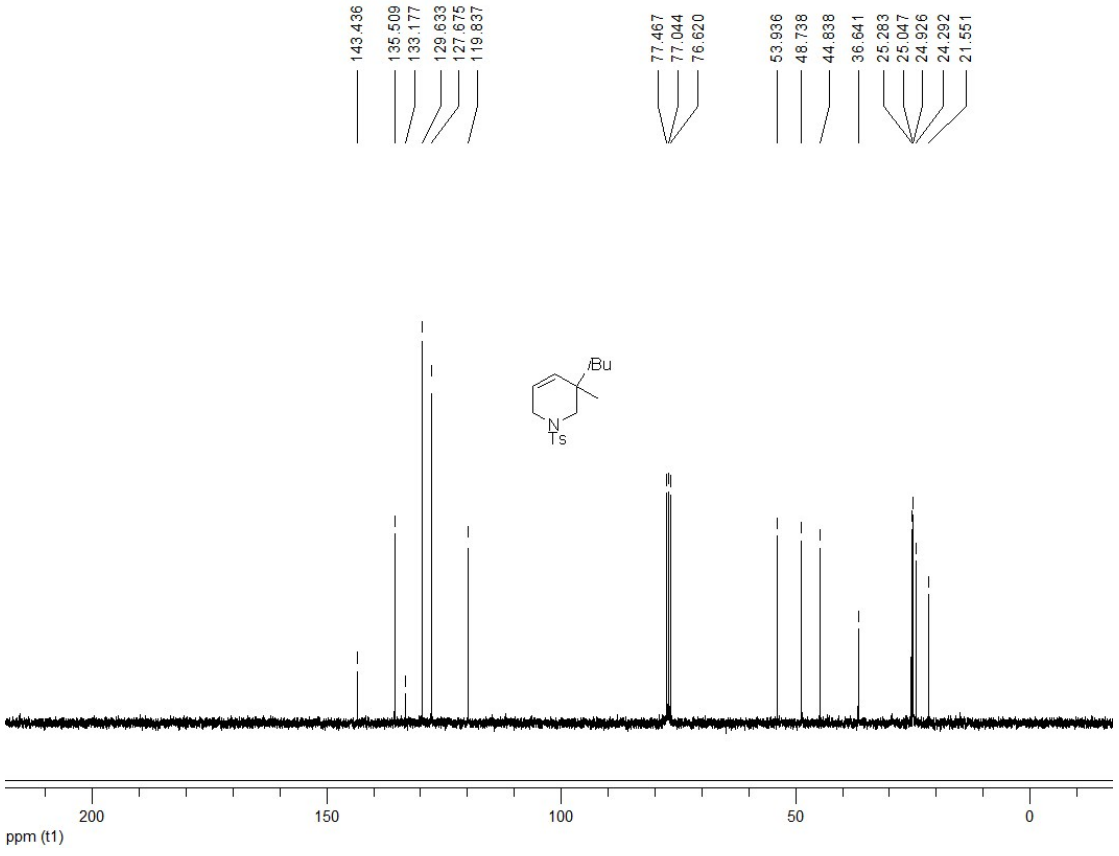


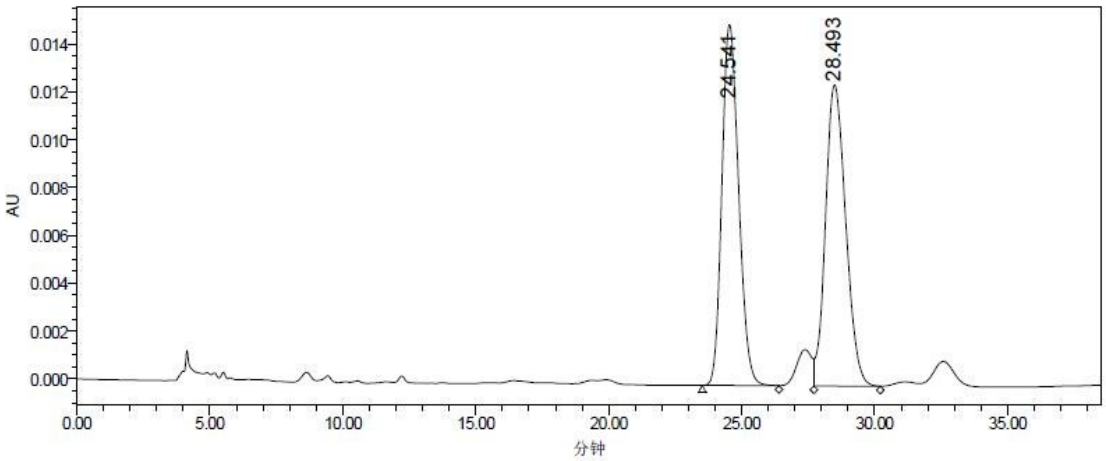
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	14.325	911491	14.26	29718
2	W2489 ChA 254nm	16.565	5481595	85.74	142622

2i

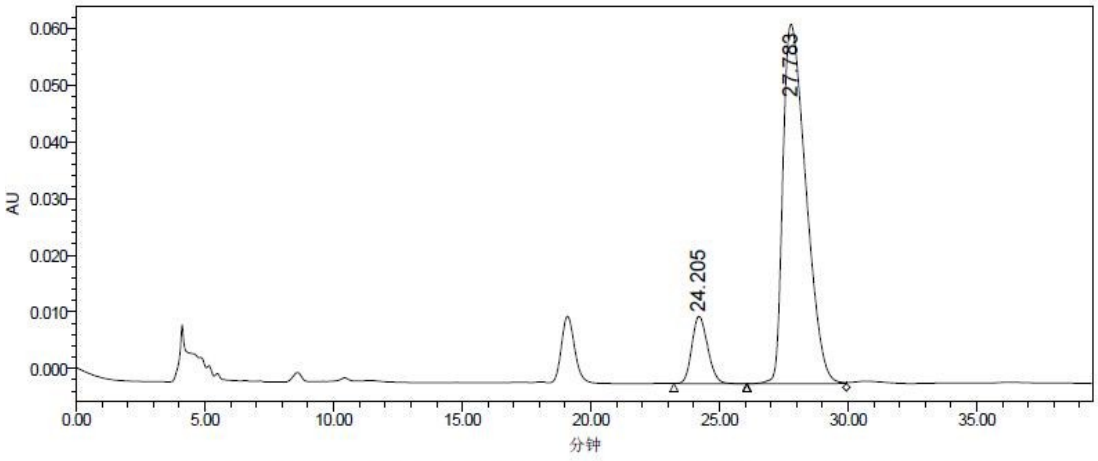

7.688
7.668
7.349
7.330
7.278
5.603
5.577
5.516
5.508
5.501
5.490
5.483
5.475
3.535
3.494
3.488
3.476
3.435
2.961
2.934
2.763
2.735
2.445
1.769
1.753
1.738
1.722
1.706
1.690
1.674
1.659
1.656
1.443
1.429
1.408
1.394
1.318
1.304
1.283
tBu
N
Ts
1.95
2.00
1.80
2.15
1.04
1.06
3.10
1.06
1.04
3.02
6.13
5.0
0.0
ppm (t1)


143.436
135.509
133.177
129.633
127.675
119.837
77.467
77.044
76.620
53.936
48.738
44.838
36.641
25.283
25.047
24.926
24.292
21.551
tBu
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

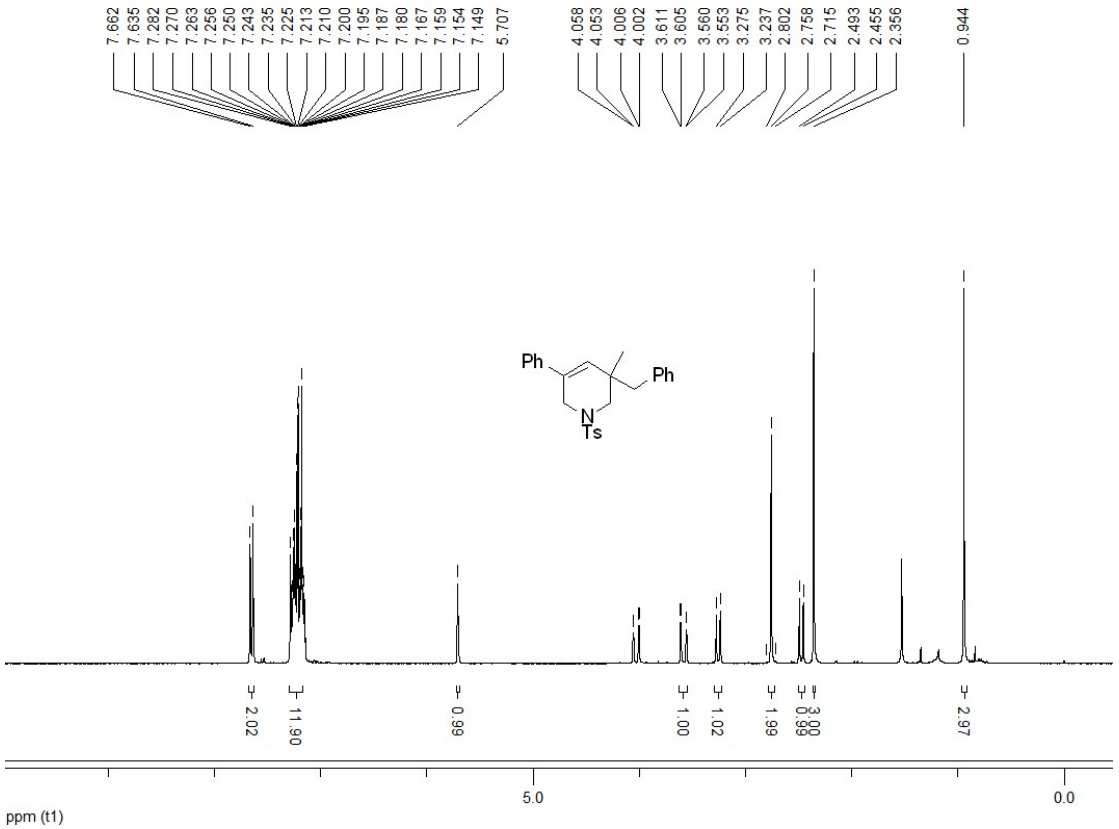
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	24.541	658662	49.70	15076
2	W2489 ChA 254nm	28.493	666548	50.30	12589

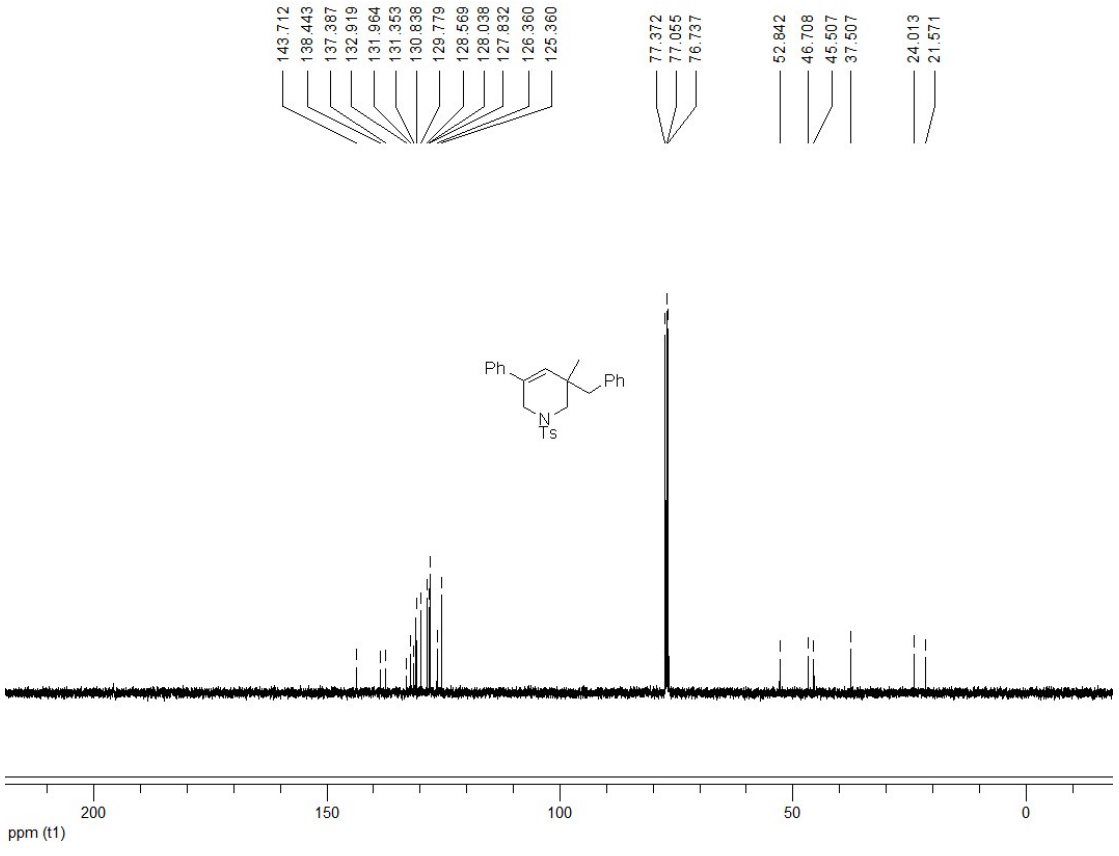


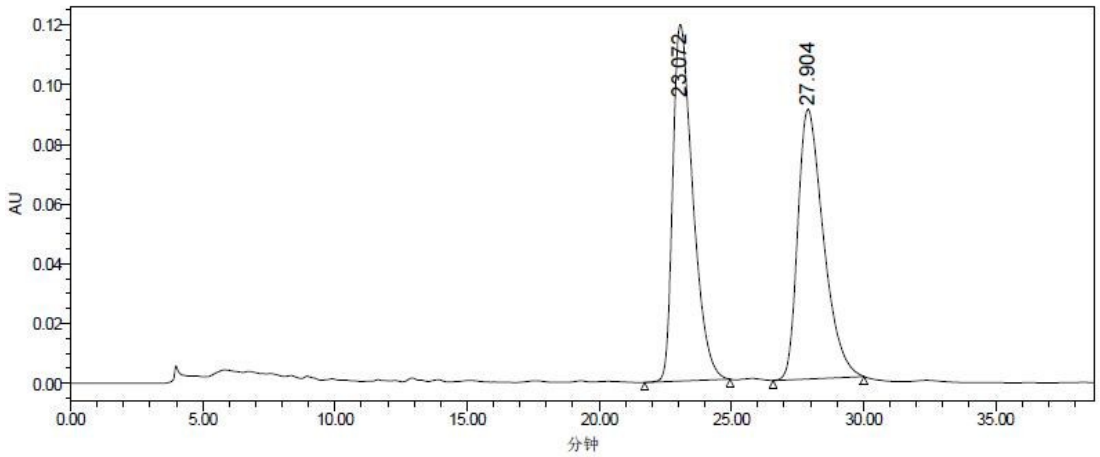
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	24.205	506998	11.40	11884
2	W2489 ChA 254nm	27.783	3940250	88.60	63427

2j

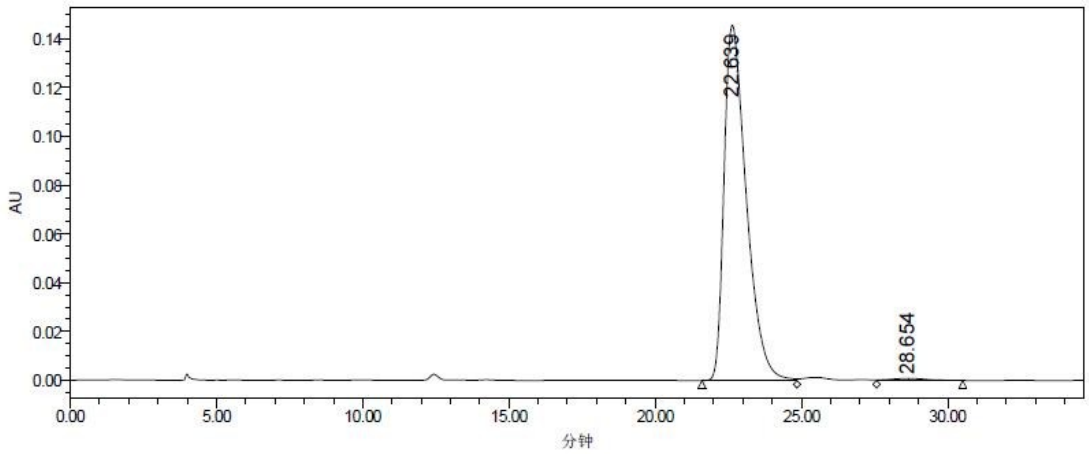

7.662
7.635
7.282
7.270
7.263
7.256
7.250
7.243
7.235
7.225
7.213
7.210
7.200
7.195
7.187
7.180
7.167
7.159
7.154
7.149
5.707
4.058
4.053
4.006
4.002
3.611
3.605
3.560
3.553
3.275
3.237
2.802
2.758
2.715
2.493
2.455
2.356
0.944
Ph
Ph
N
Ts
2.02
11.90
0.99
1.00
1.02
1.99
3.00
0.99
2.97
5.0
0.0
ppm (t1)


143.712
138.443
137.387
132.919
131.964
131.353
130.838
129.779
128.569
128.038
127.832
126.360
125.360
77.372
77.055
76.737
52.842
46.708
45.507
37.507
24.013
21.571
Ph
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

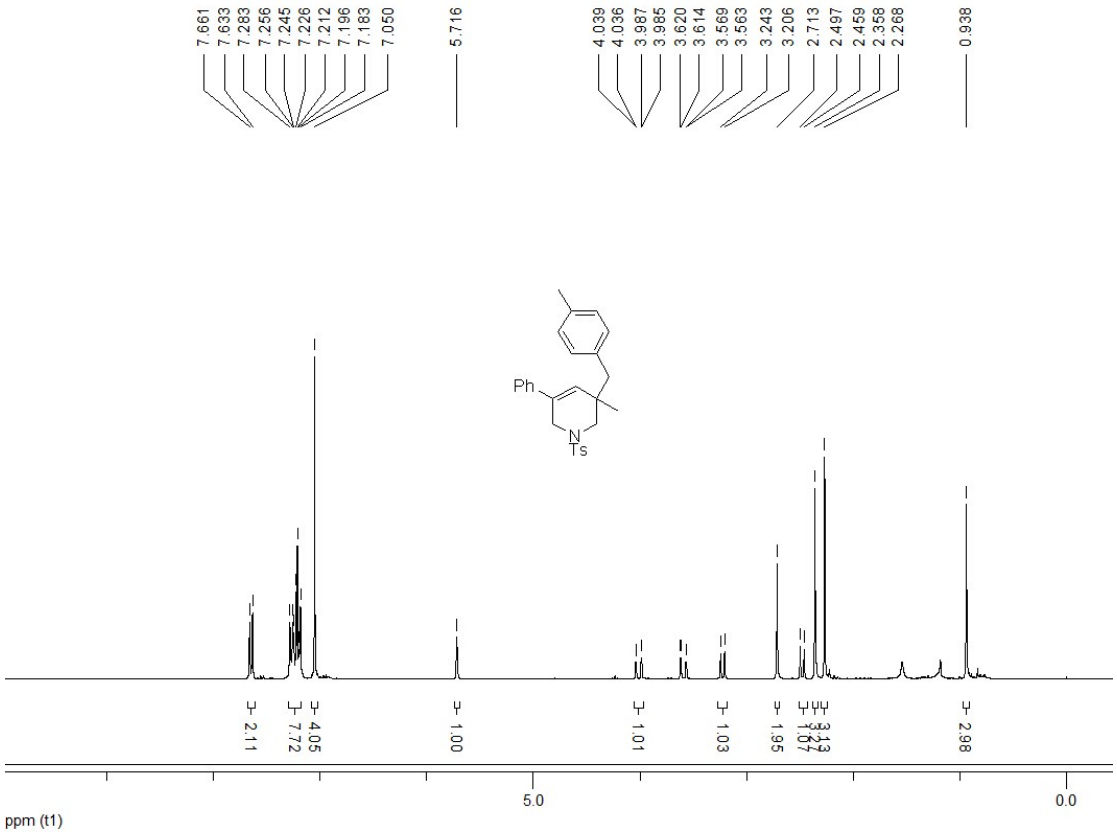
	Channel Description	RT (min)	Area (磺*sec)	% Area	Height (磺)
1	W2489 ChA 254nm	23.072	6295859	50.78	119375
2	W2489 ChA 254nm	27.904	6102773	49.22	90229

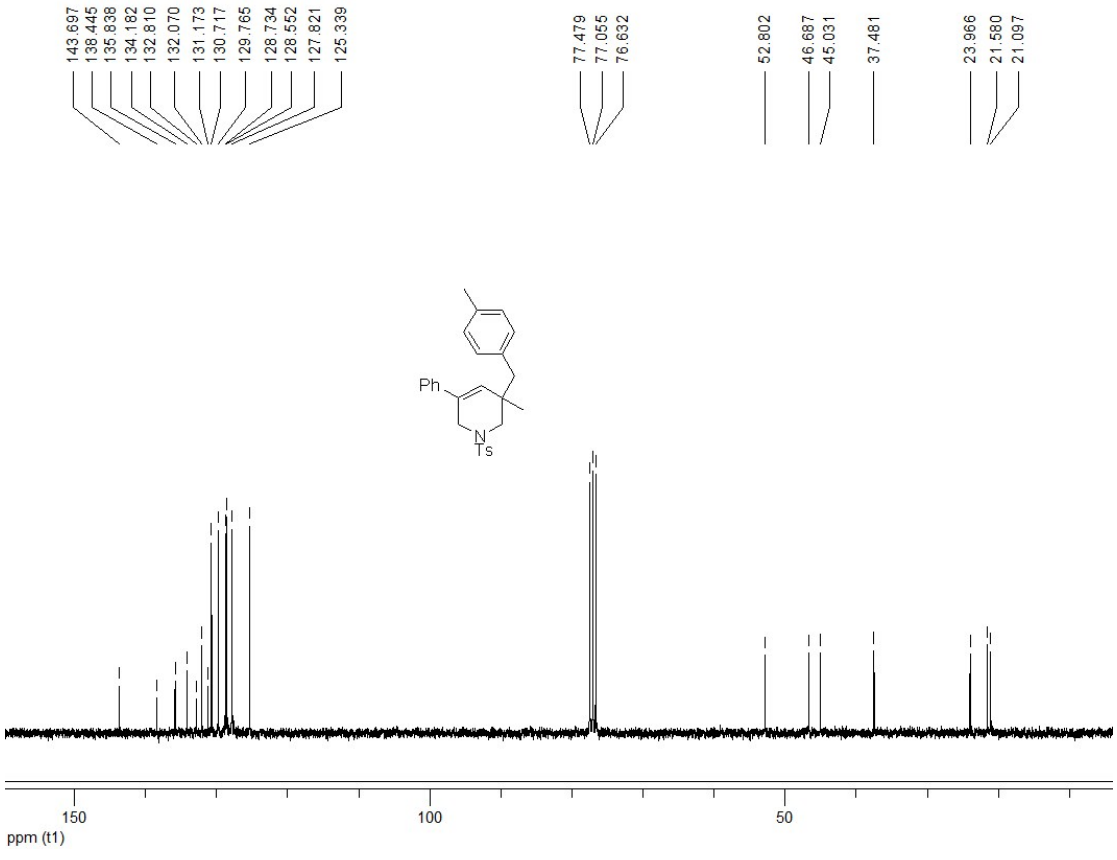


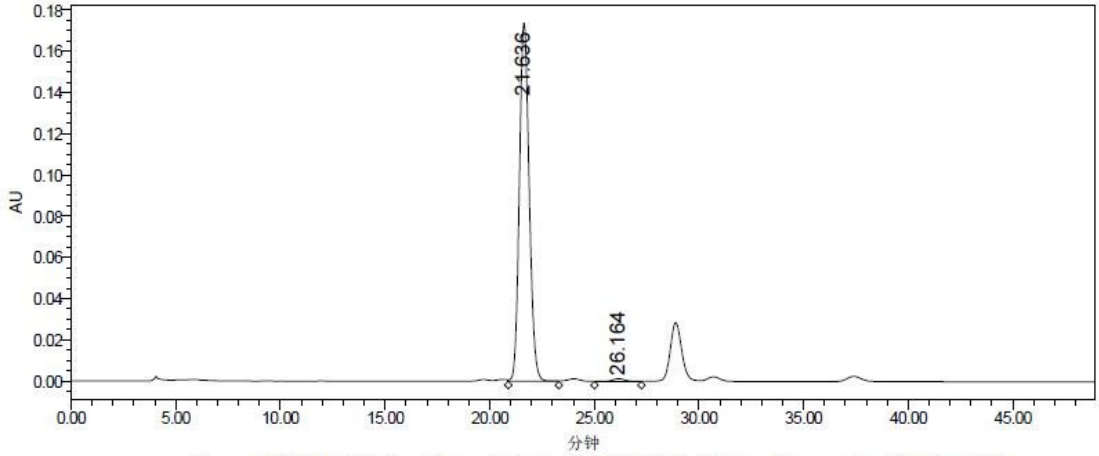
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (磺*sec)	% Area	Height (磺)
1	W2489 ChA 254nm	22.639	7702457	99.07	145763
2	W2489 ChA 254nm	28.654	72248	0.93	855

2k

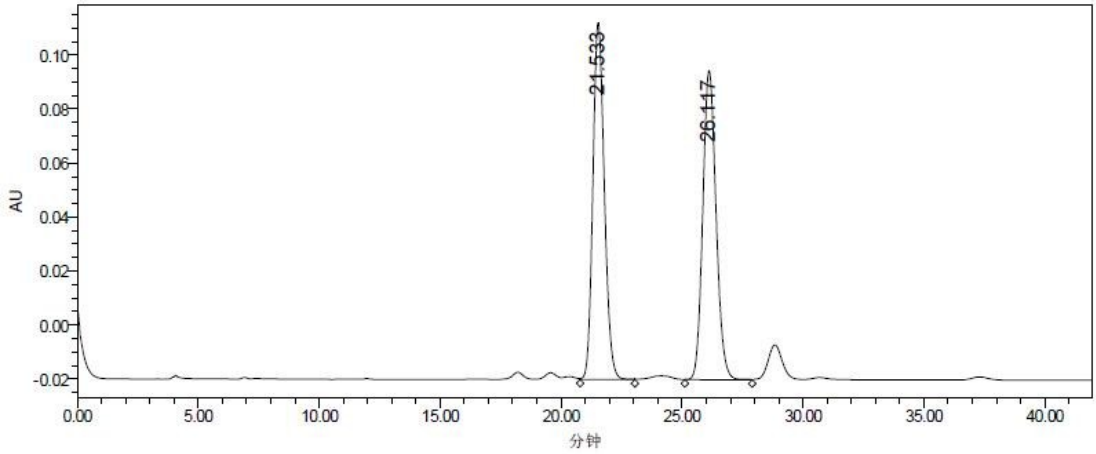

7.661
7.633
7.283
7.256
7.245
7.226
7.212
7.196
7.183
7.050
5.716
4.039
4.036
3.987
3.985
3.620
3.614
3.569
3.563
3.243
3.206
2.713
2.497
2.459
2.358
2.268
0.938
Ph
N
Ts
2.11
7.72
4.05
1.00
1.01
1.03
1.96
3.13
2.98
5.0
0.0
ppm (t1)


143.697
138.445
135.838
134.182
132.810
132.070
131.173
130.717
129.765
128.734
128.552
127.821
125.339
77.479
77.055
76.632
52.802
46.687
45.031
37.481
23.966
21.580
21.097
Ph
N
Ts
150
100
50
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

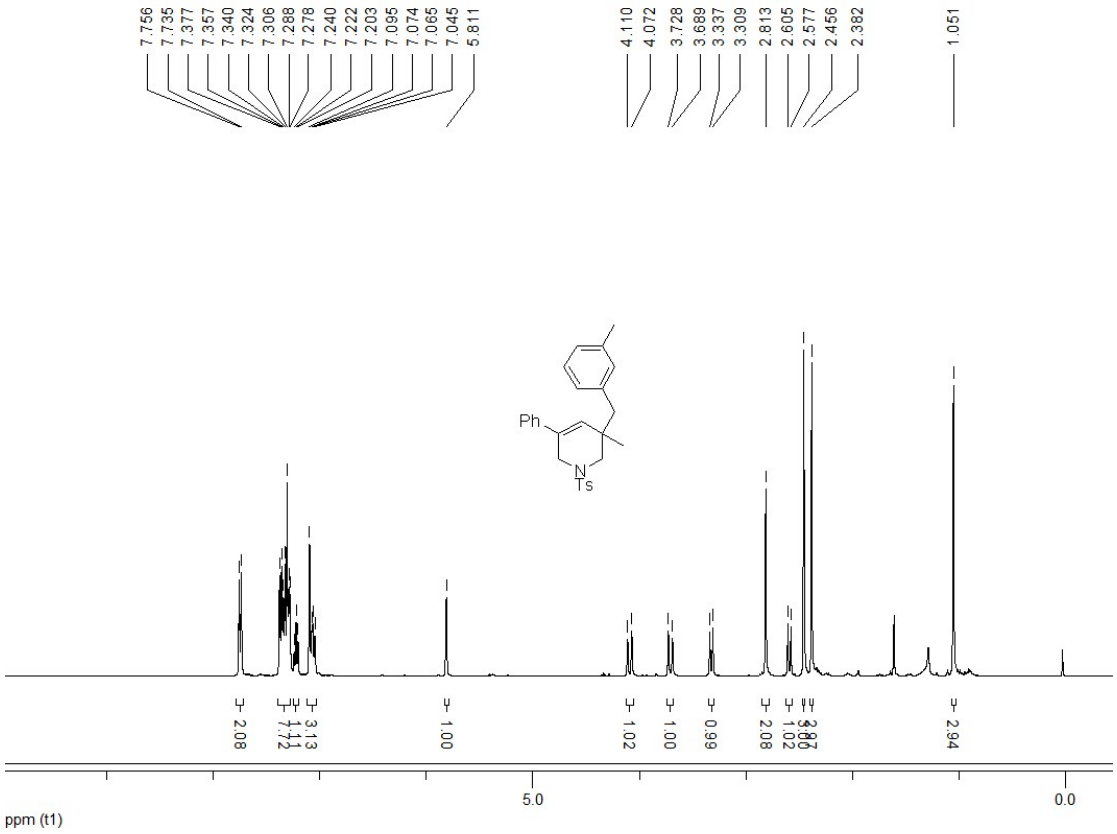
	Channel Description	RT (min)	Area (磺*sec)	% Area	Height (磺)
1	W2489 ChA 254nm	21.636	5659263	99.01	173819
2	W2489 ChA 254nm	26.164	56429	0.99	1371

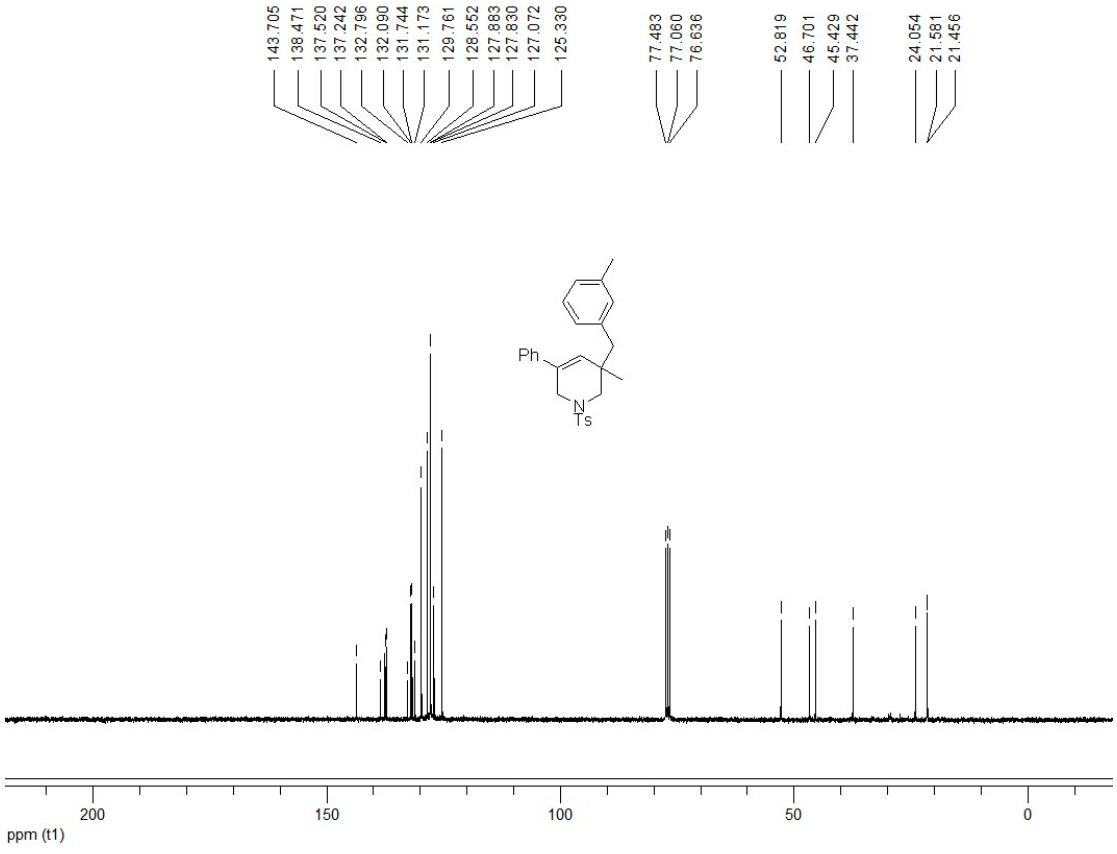


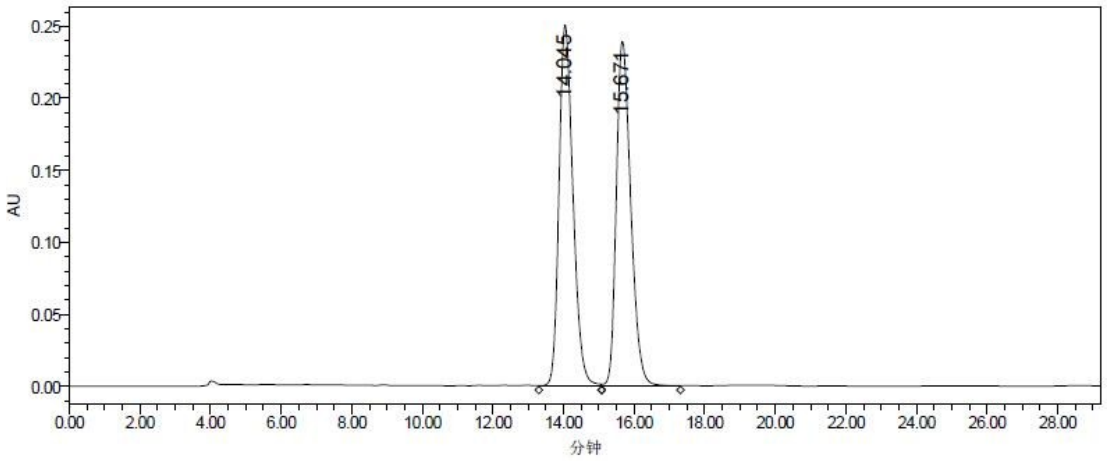
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (磺*sec)	% Area	Height (磺)
1	W2489 ChA 254nm	21.533	4358325	49.94	132170
2	W2489 ChA 254nm	26.117	4368024	50.06	114511

2l

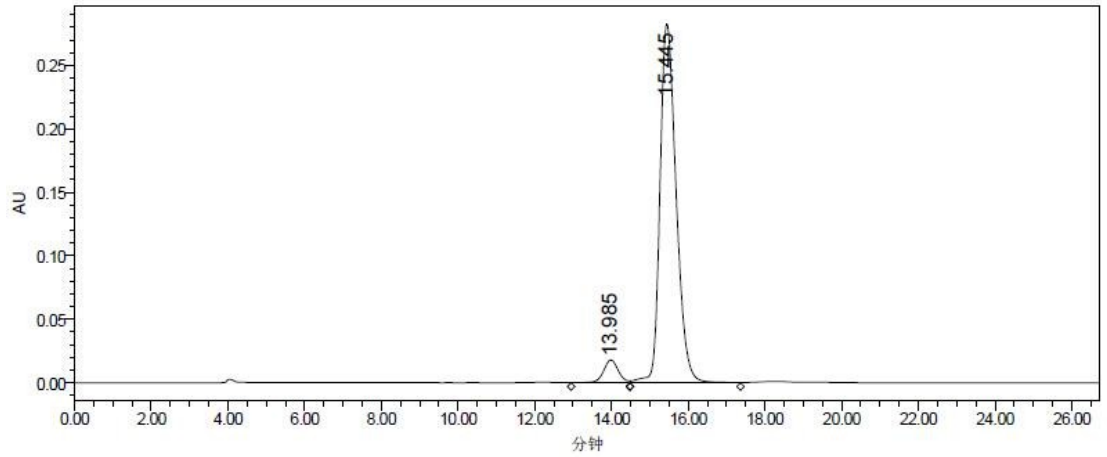

7.756
7.735
7.377
7.357
7.340
7.324
7.306
7.288
7.278
7.240
7.222
7.203
7.095
7.074
7.065
7.045
5.811
4.110
4.072
3.728
3.689
3.337
3.309
2.813
2.605
2.577
2.456
2.382
1.051
Ph
N
Ts
2.08
3.13
1.00
1.02
1.00
0.99
2.08
2.94
5.0
0.0
ppm (t1)


143.705
138.471
137.520
137.242
132.796
132.090
131.744
131.173
129.761
128.552
127.883
127.830
127.072
125.330
77.483
77.060
76.636
52.819
46.701
45.429
37.442
24.054
21.581
21.456
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

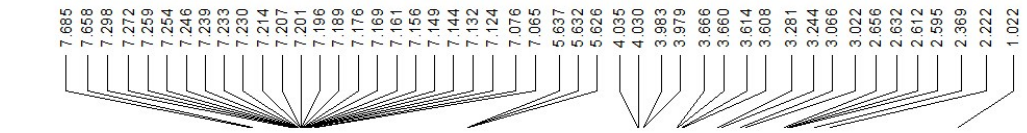
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	14.045	6916771	50.27	250925
2	W2489 ChA 254nm	15.671	6842900	49.73	239501

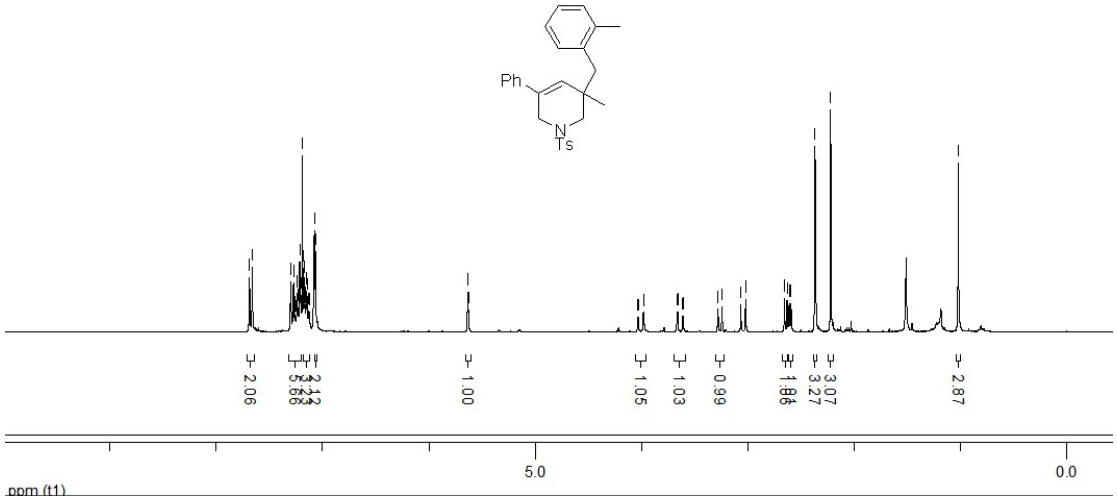


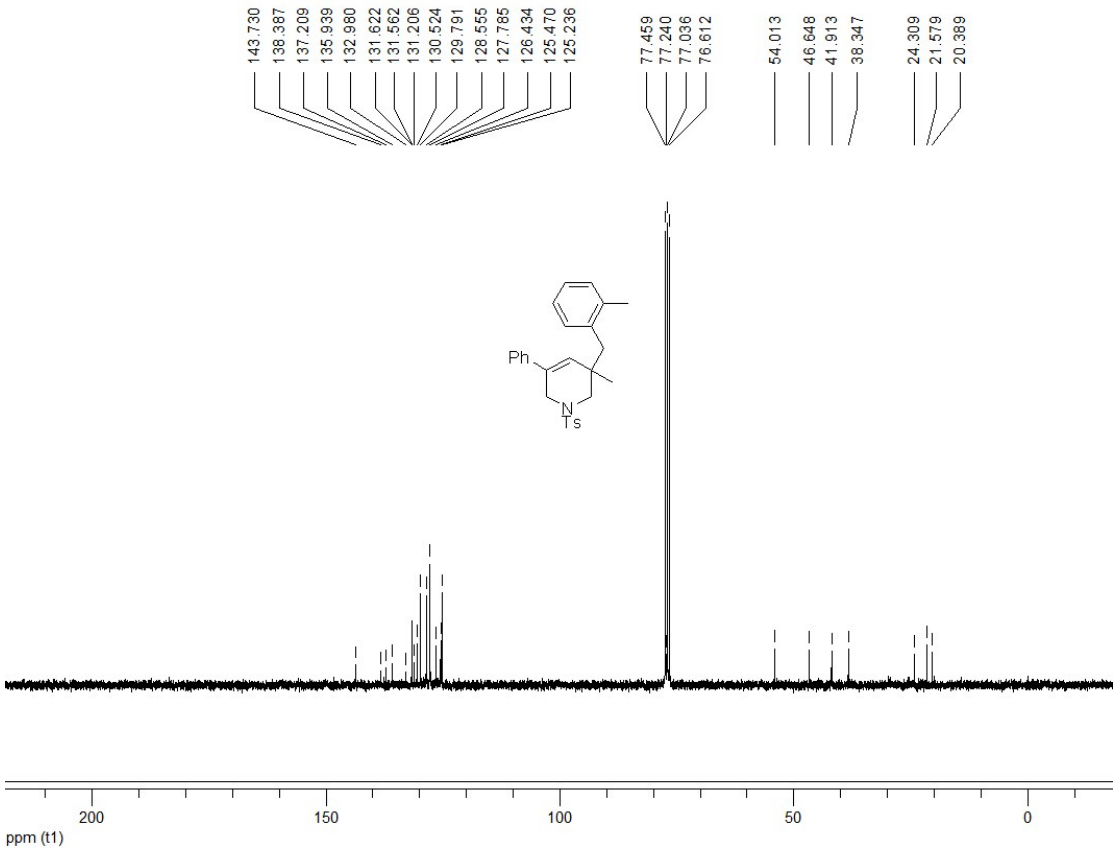
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

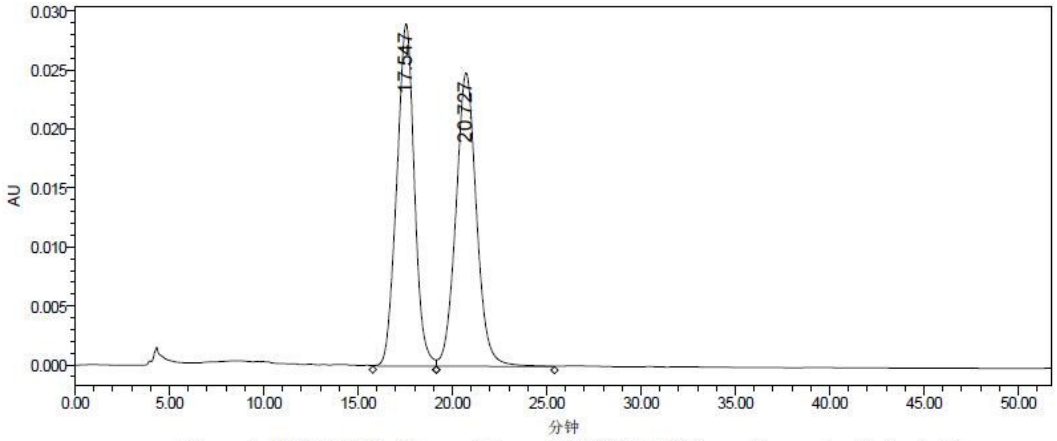
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	13.985	483016	5.51	18063
2	W2489 ChA 254nm	15.445	8280059	94.49	282780

2m


7.685
7.658
7.298
7.272
7.259
7.254
7.246
7.239
7.233
7.230
7.214
7.207
7.201
7.196
7.189
7.176
7.169
7.161
7.156
7.149
7.144
7.132
7.124
7.076
7.065
5.637
5.632
5.626
4.035
4.030
3.983
3.979
3.666
3.660
3.614
3.608
3.281
3.244
3.066
3.022
2.656
2.632
2.612
2.595
2.369
2.222
1.022

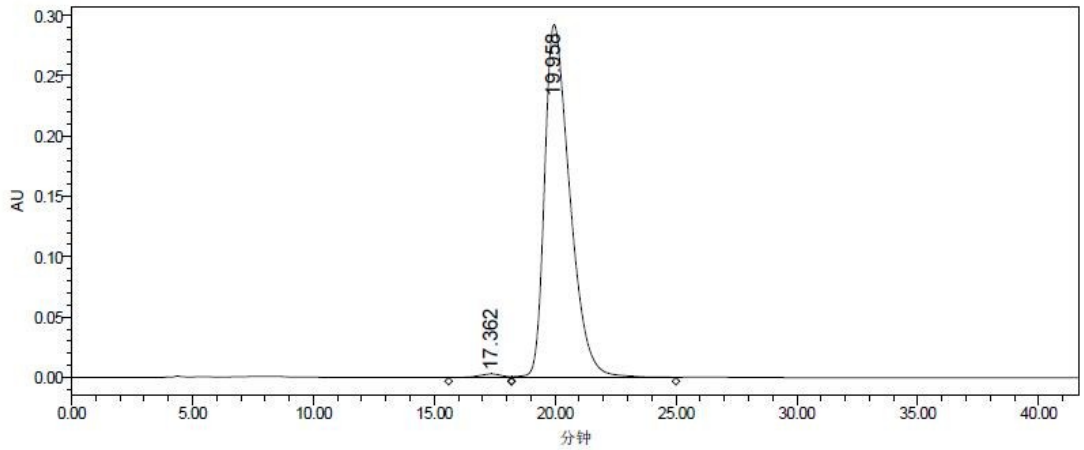

Ph
N
Ts
2.06
3.13
1.00
1.05
1.03
0.99
1.88
3.27
3.07
2.87
5.0
0.0
ppm (t1)


143.730
138.387
137.209
135.939
132.980
131.622
131.562
131.206
130.524
129.791
128.555
127.785
126.434
125.470
125.236
77.459
77.240
77.036
76.612
54.013
46.648
41.913
38.347
24.309
21.579
20.389
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

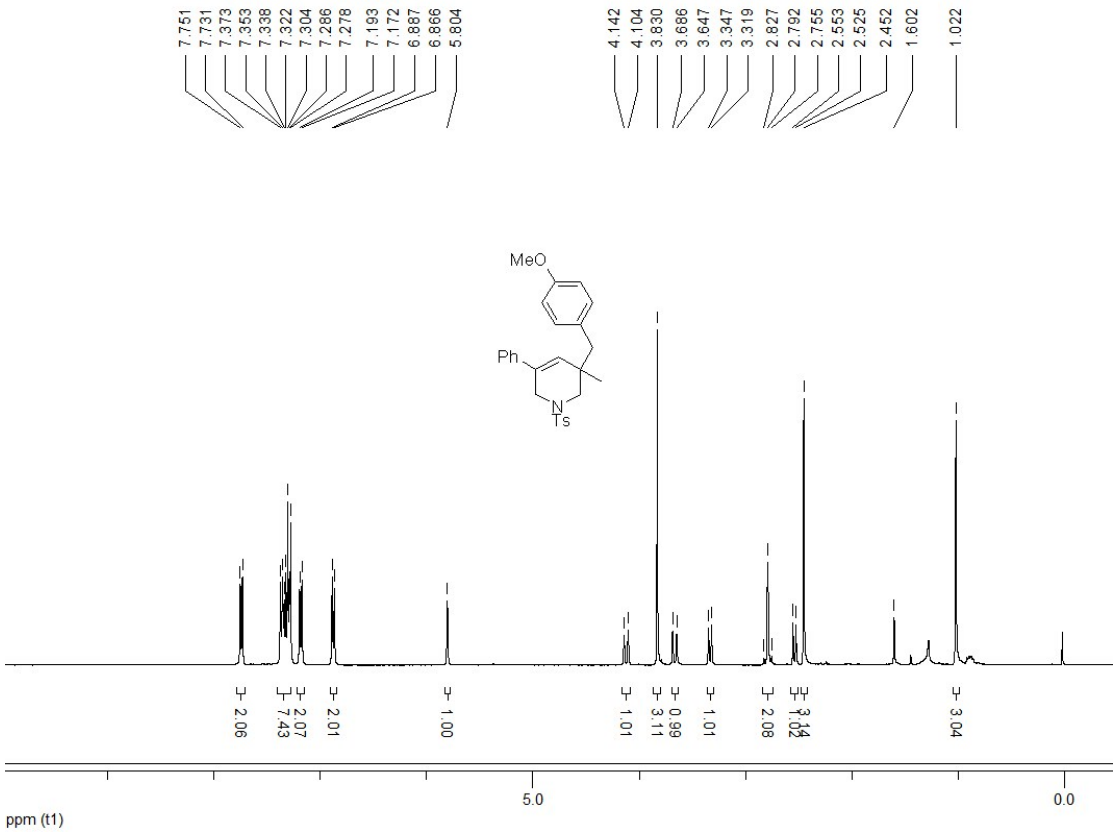
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	17.547	1886013	49.89	28988
2	W2489 ChA 254nm	20.727	1894217	50.11	24848

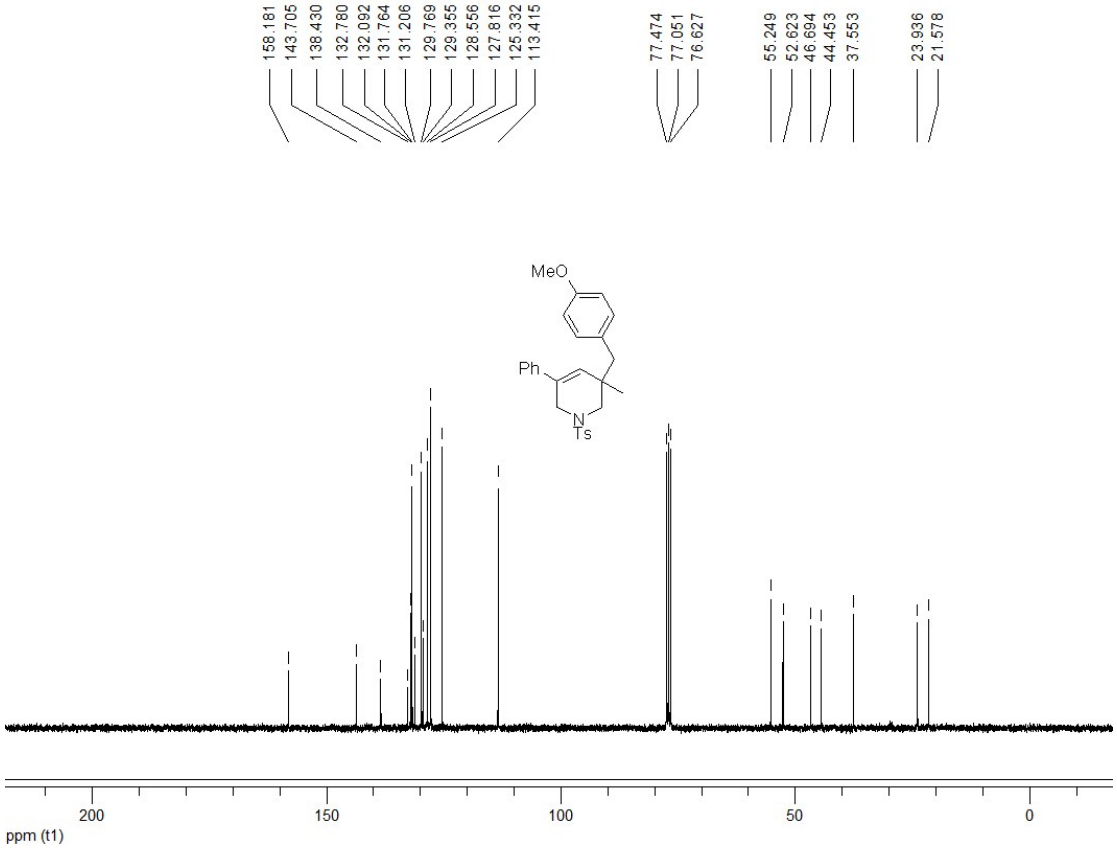


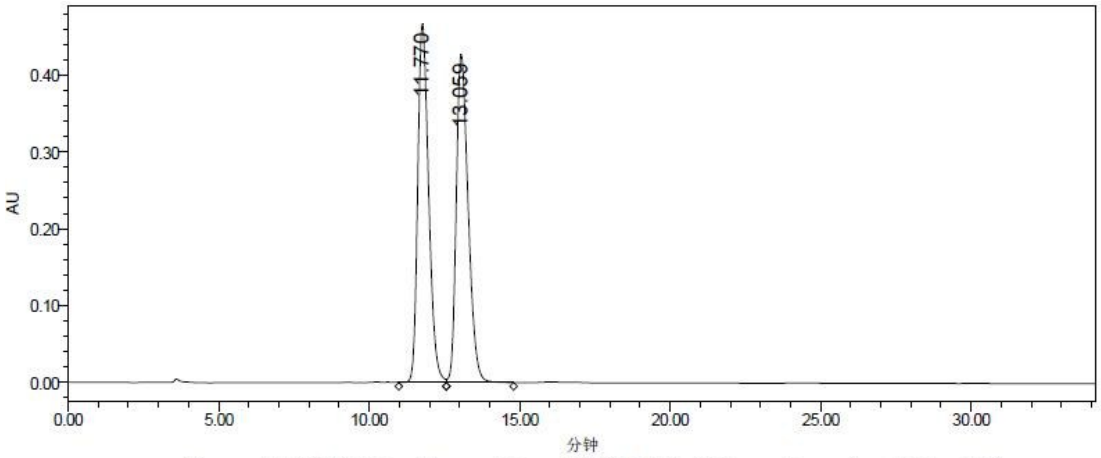
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	17.362	196202	0.91	3049
2	W2489 ChA 254nm	19.958	21295104	99.09	292500

2n

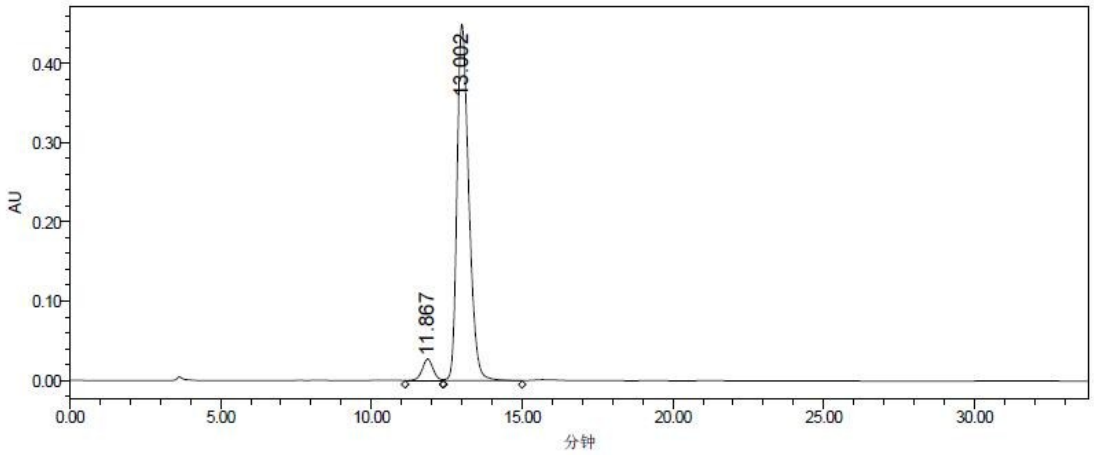

7.751
7.731
7.373
7.353
7.338
7.322
7.304
7.286
7.278
7.193
7.172
6.887
6.866
5.804
4.142
4.104
3.830
3.686
3.647
3.347
3.319
2.827
2.792
2.755
2.553
2.525
2.452
1.602
1.022
MeO
Ph
N
Ts
2.06
7.43
2.07
2.01
1.00
1.01
3.11
0.99
1.01
2.08
3.02
3.14
3.04
5.0
0.0
ppm (t1)


158.181
143.705
138.430
132.780
132.092
131.764
131.206
129.769
129.355
128.556
127.816
125.332
113.415
77.474
77.051
76.627
55.249
52.623
46.694
44.453
37.553
23.936
21.578
MeO
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	11.770	11804615	50.12	467459
2	W2489 ChA 254nm	13.059	11749875	49.88	427201

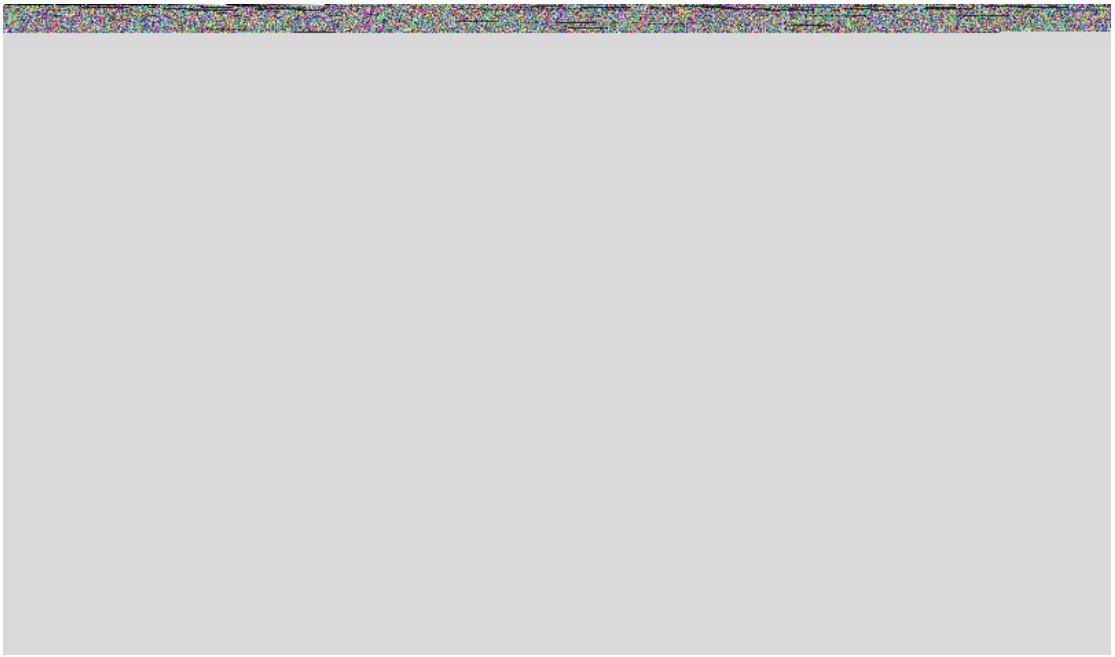


Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

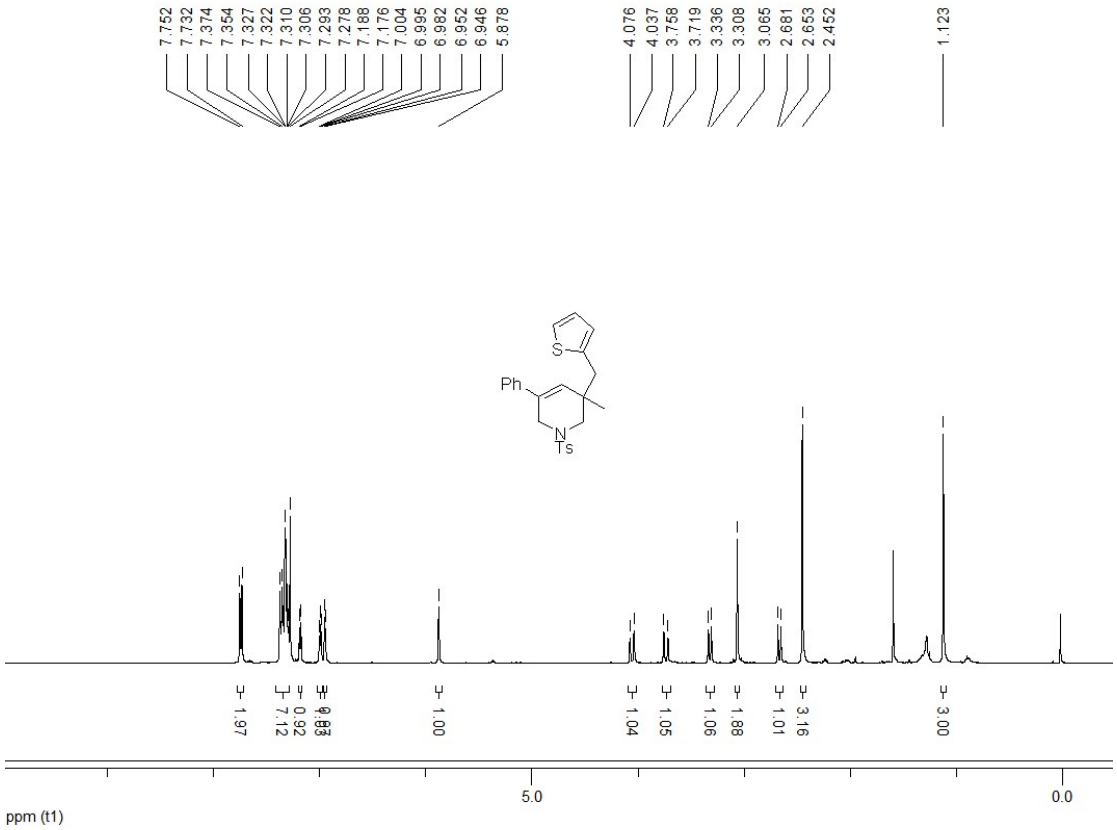
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	11.867	687053	5.33	27184
2	W2489 ChA 254nm	13.002	12191262	94.67	449470

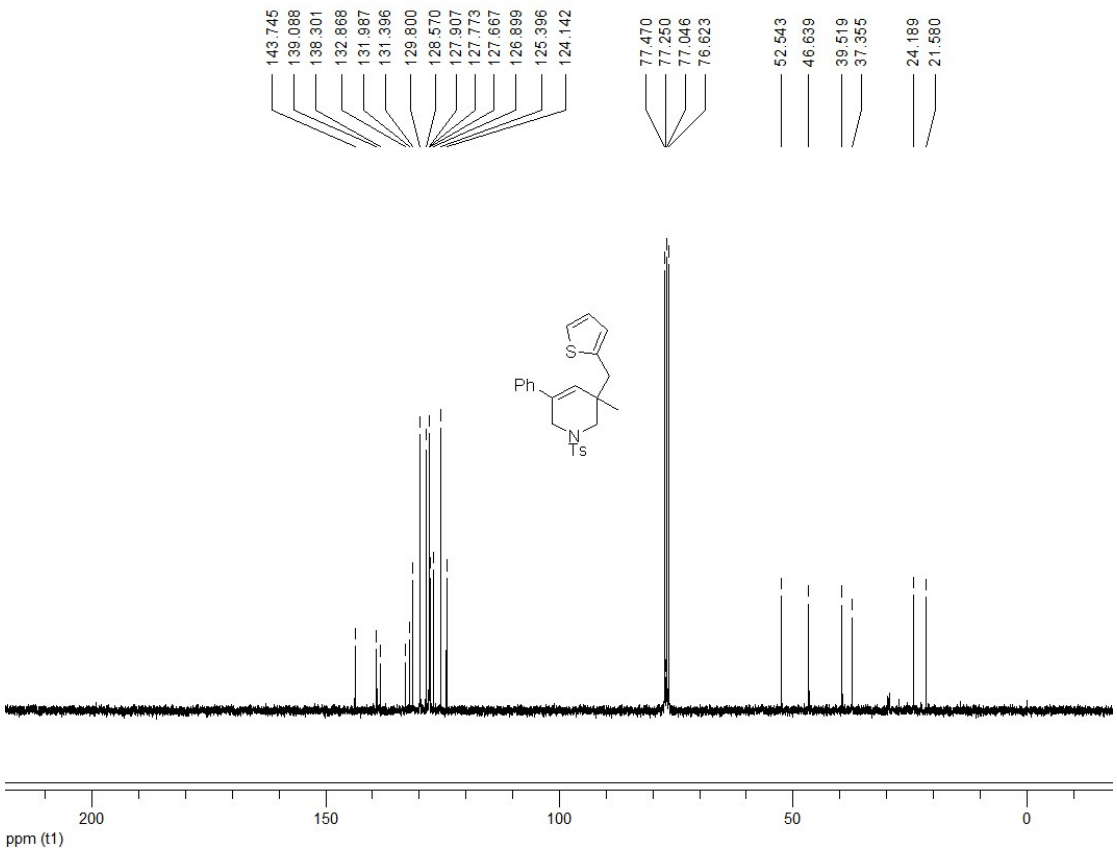
2o

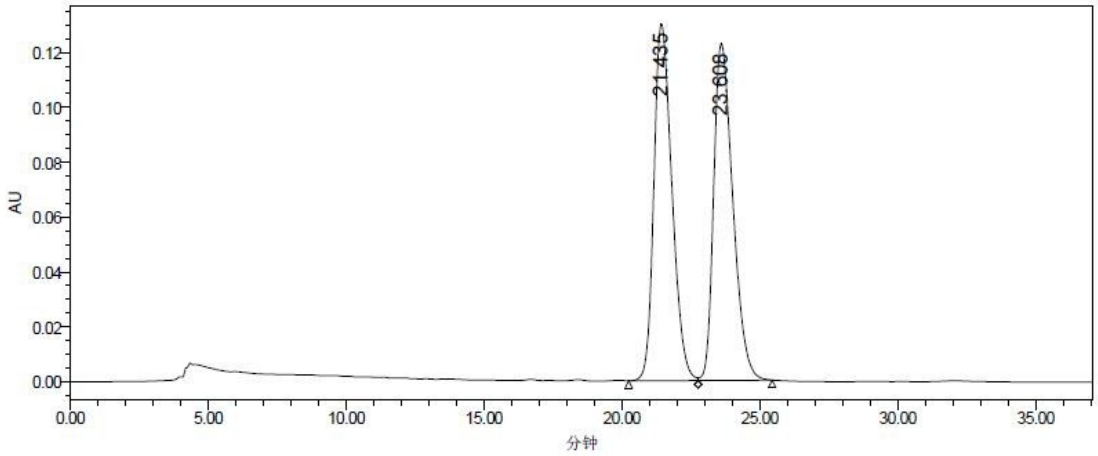
\



2p

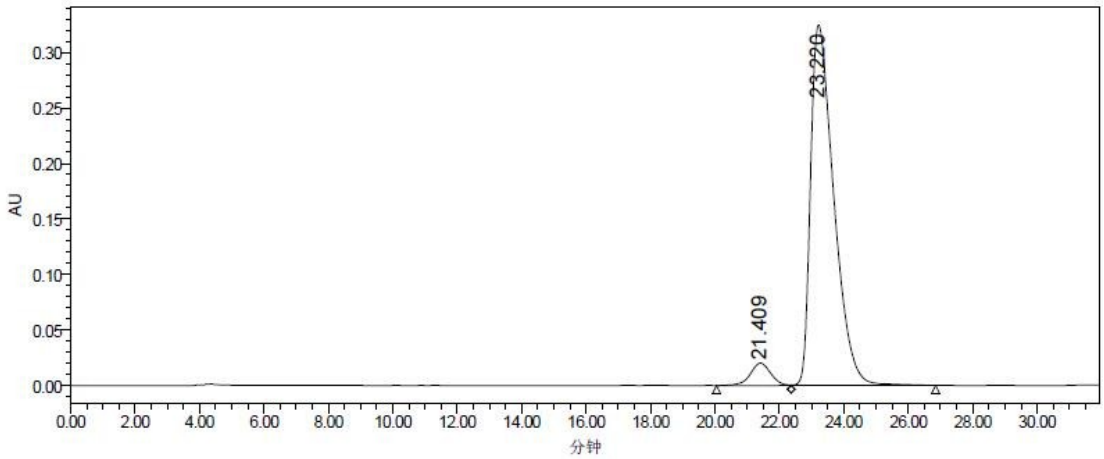

7.752
7.732
7.374
7.354
7.327
7.322
7.310
7.306
7.293
7.278
7.188
7.176
7.004
6.995
6.982
6.952
6.946
5.878
4.076
4.037
3.758
3.719
3.336
3.308
3.065
2.681
2.653
2.452
1.123
Ph
S
N
Ts
1.97
7.12
0.92
1.03
1.00
1.04
1.05
1.06
1.88
1.01
3.16
3.00
5.0
0.0
ppm (t1)


143.745
139.088
138.301
132.868
131.987
131.396
129.800
128.570
127.907
127.773
127.667
126.899
125.396
124.142
77.470
77.250
77.046
76.623
52.543
46.639
39.519
37.355
24.189
21.580
Ph
S
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

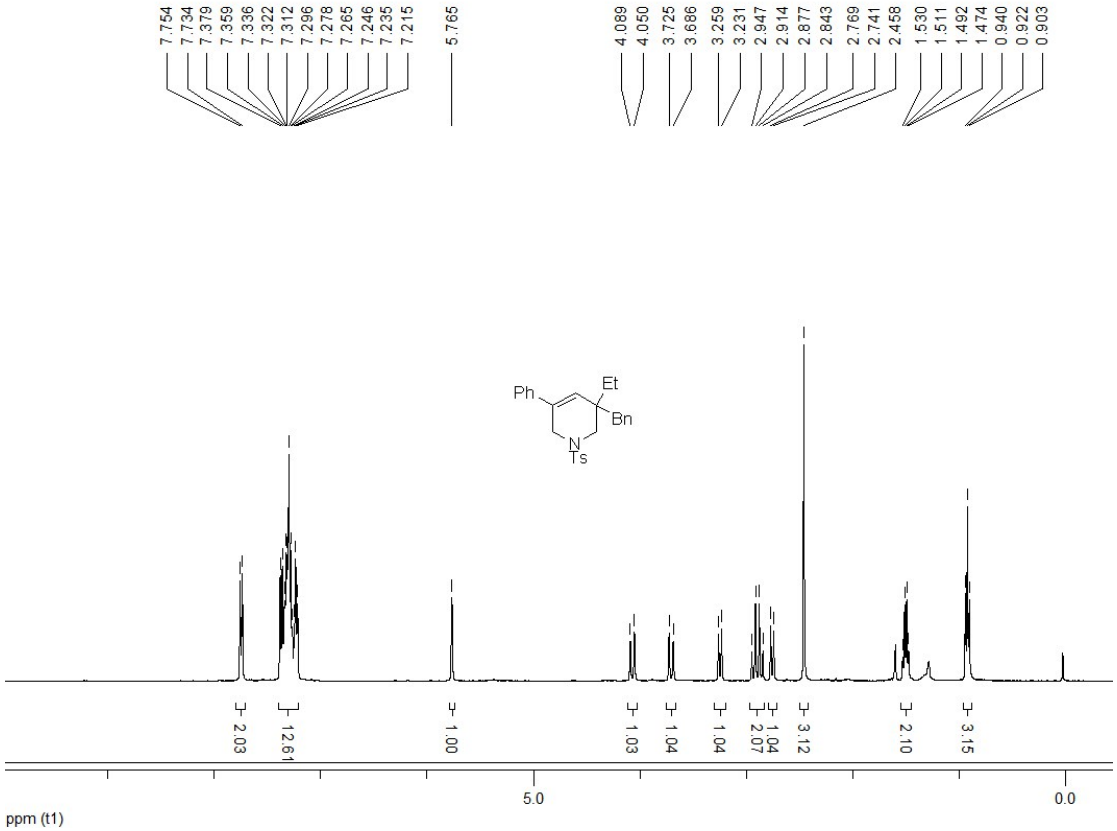
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	21.435	5913758	49.94	130083
2	W2489 ChA 254nm	23.608	5927979	50.06	122697

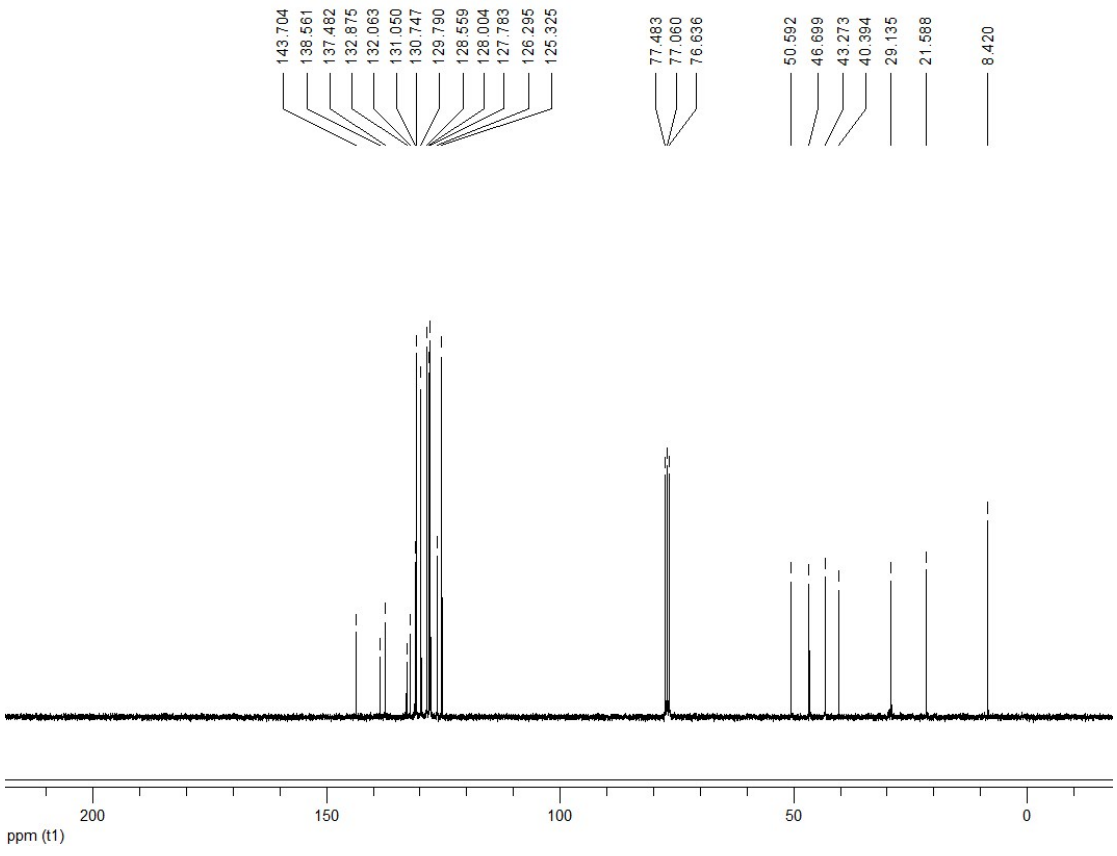


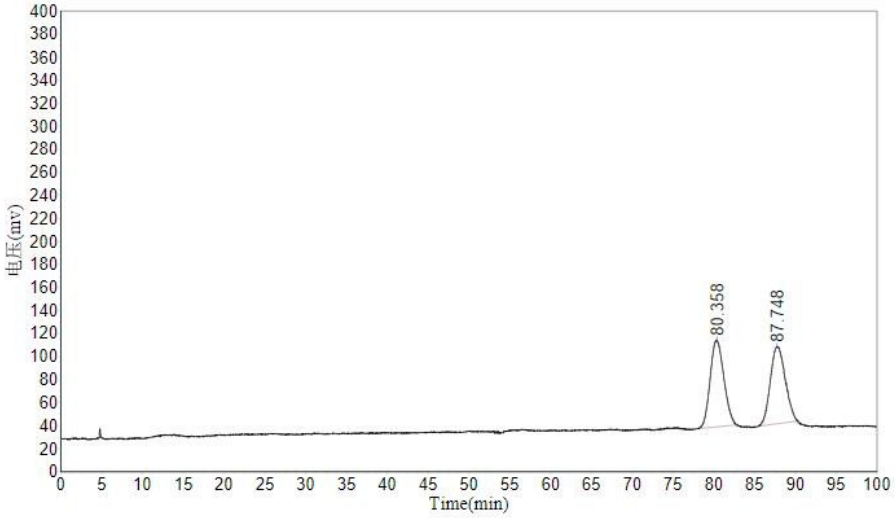
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	21.409	885550	5.17	20100
2	W2489 ChA 254nm	23.220	16241686	94.83	324547

2q

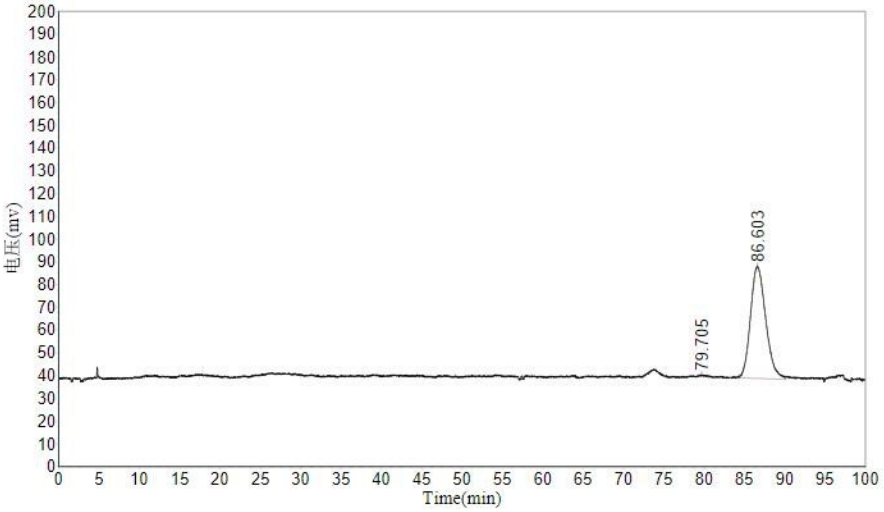

7.754
7.734
7.379
7.359
7.336
7.322
7.312
7.296
7.278
7.265
7.246
7.235
7.215
5.765
4.089
4.050
3.725
3.686
3.259
3.231
2.947
2.914
2.877
2.843
2.769
2.741
2.458
1.530
1.511
1.492
1.474
0.940
0.922
0.903
Ph
Et
Bn
N
Ts
2.03
12.61
1.00
1.03
1.04
1.04
2.07
1.04
3.12
2.10
3.15
5.0
0.0
ppm (t1)


143.704
138.561
137.482
132.875
132.063
131.050
130.747
129.790
128.559
128.004
127.783
126.295
125.325
77.483
77.060
76.636
50.592
46.699
43.273
40.394
29.135
21.588
8.420
200
150
100
50
0
ppm (t1)



Results

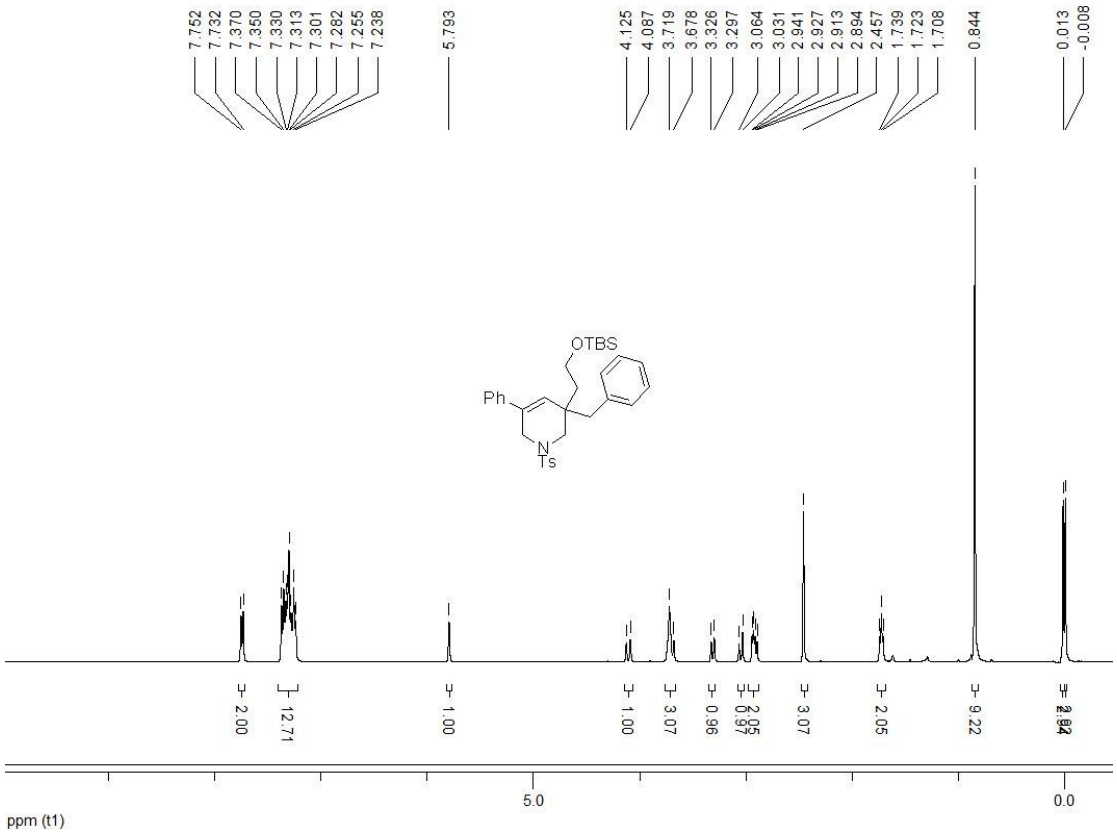
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		80.358	75453.719	8814077.000	50.8892
2		87.748	66999.938	8506042.000	49.1108
Total			142453.656	17320119.000	100.0000

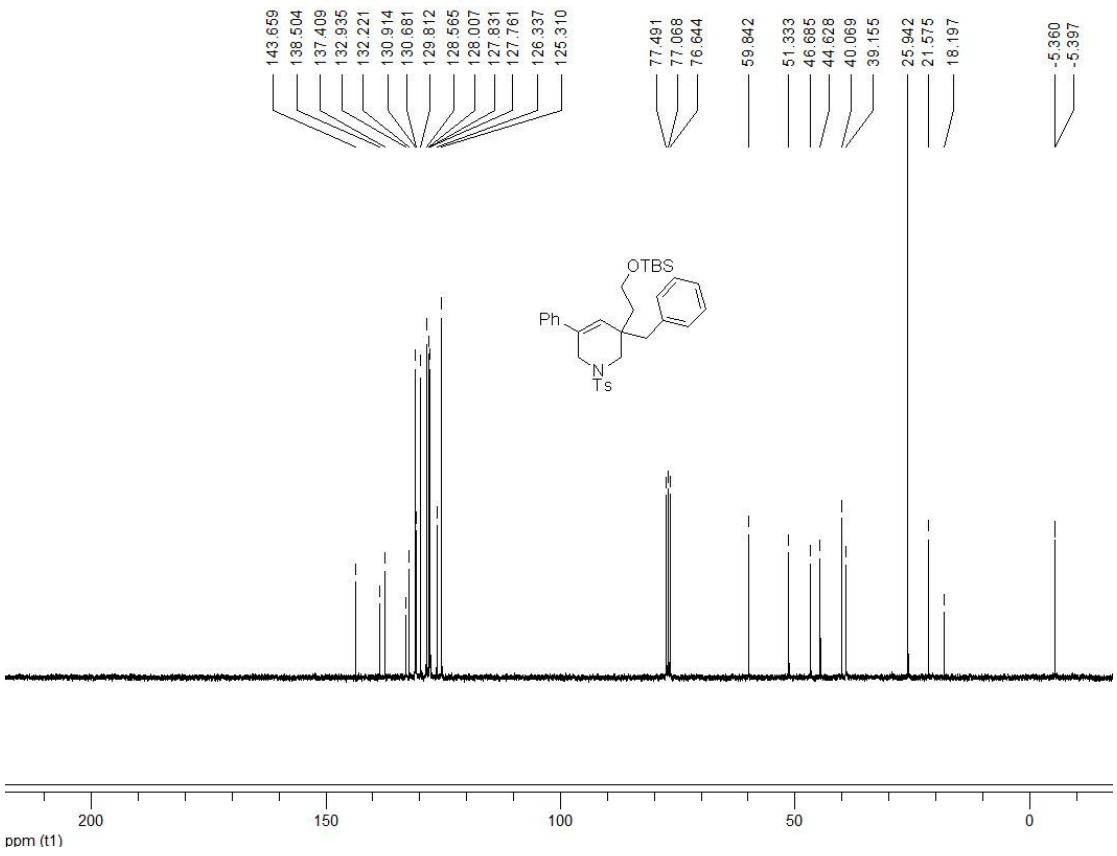


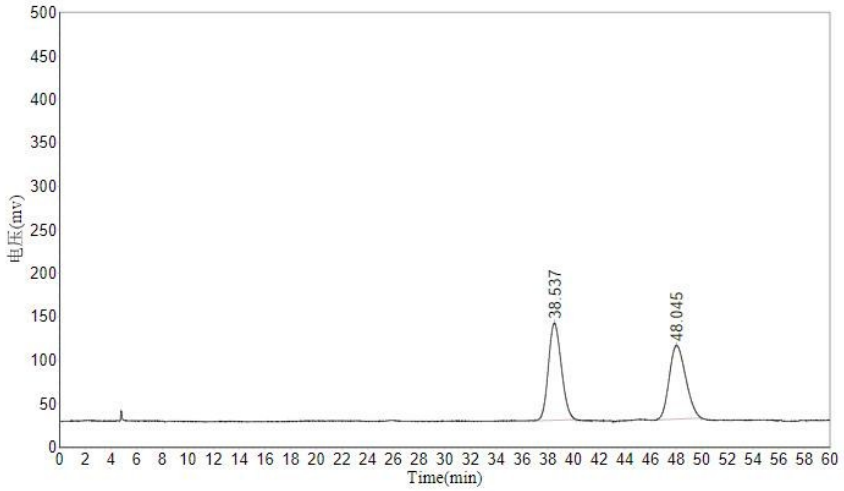
Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		79.705	540.892	18083.471	0.2807
2		86.603	49151.117	6425236.000	99.7193
Total			49692.009	6443319.471	100.0000

2r

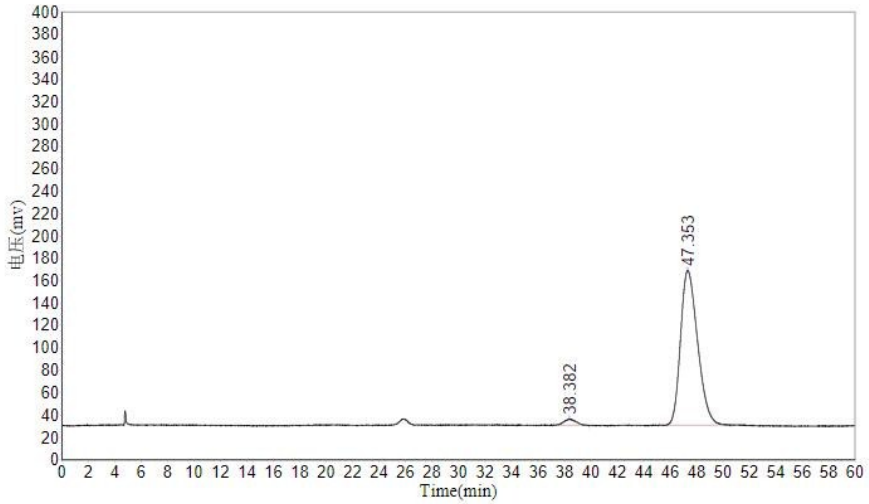

7.752
7.732
7.370
7.350
7.330
7.313
7.301
7.282
7.255
7.238
5.793
4.125
4.087
3.719
3.678
3.326
3.297
3.064
3.031
2.941
2.927
2.913
2.894
2.457
1.739
1.723
1.708
0.844
0.013
-0.008
OTBS
Ph
N
Ts
2.00
12.71
1.00
1.00
3.07
0.96
2.05
3.07
2.05
9.22
5.0
0.0
ppm (t1)


143.659
138.504
137.409
132.935
132.221
130.914
130.681
129.812
128.565
128.007
127.831
127.761
126.337
125.310
77.491
77.068
76.644
59.842
51.333
46.685
44.628
40.069
39.155
25.942
21.575
18.197
-5.360
-5.397
OTBS
Ph
N
Ts
200
150
100
50
0
ppm (t1)



Results

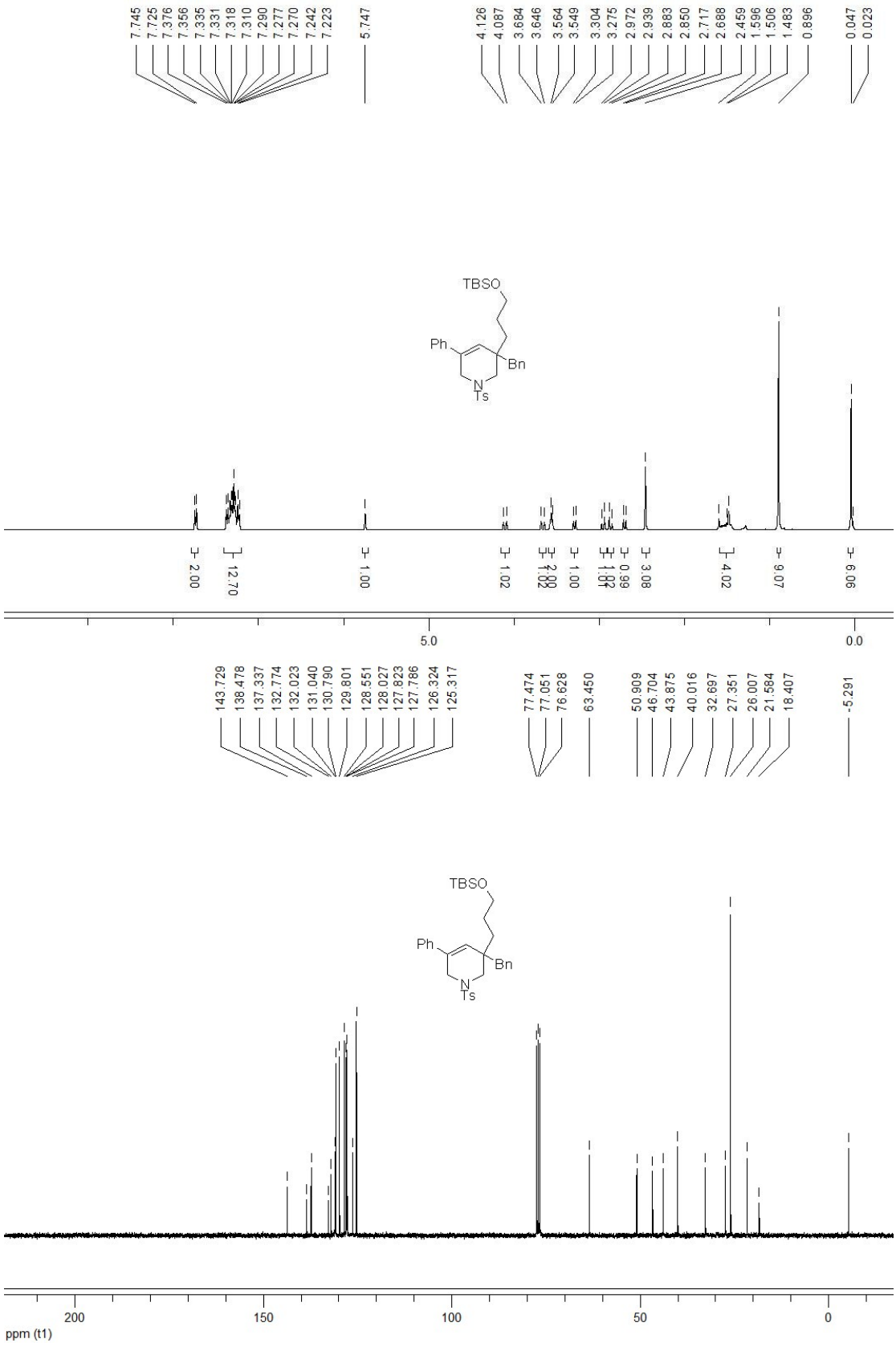
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		38.537	111599.125	7828119.000	50.9268
2		48.045	84537.555	7543199.000	49.0732
Total			196136.680	15371318.000	100.0000

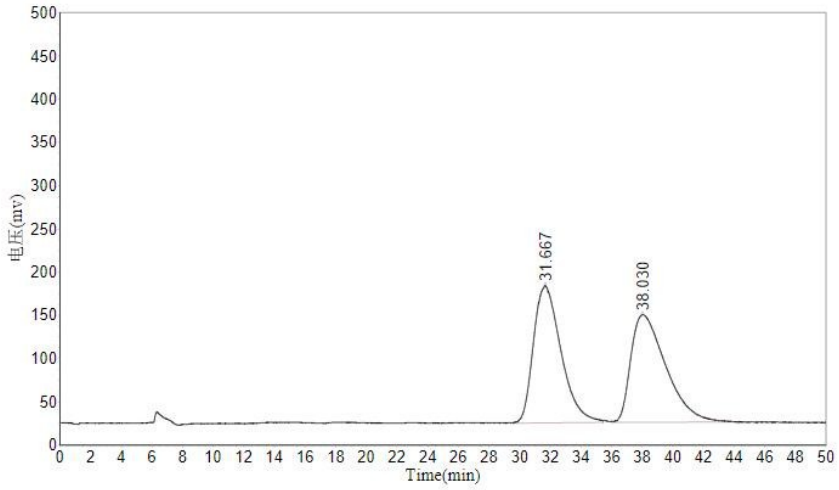


Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		38.382	5565.415	367045.750	2.8879
2		47.353	138102.984	12342545.000	97.1121
Total			143668.399	12709590.750	100.0000

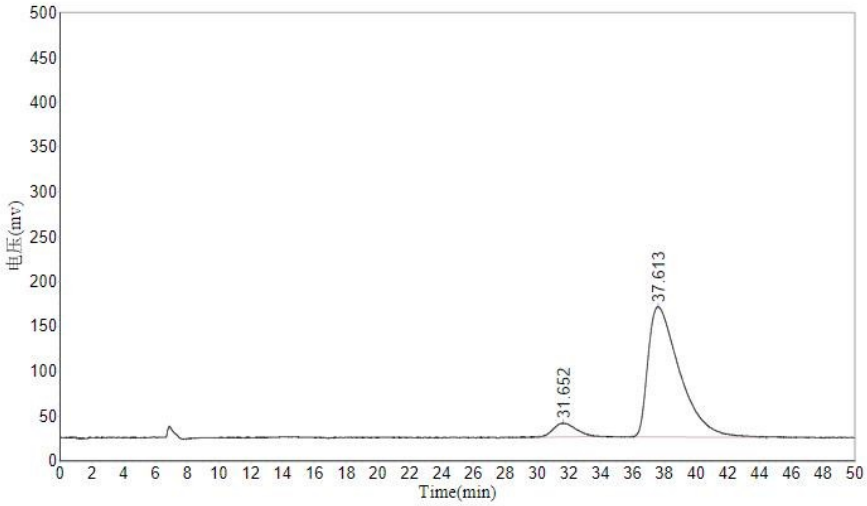
2s


7.745
7.725
7.376
7.356
7.335
7.331
7.318
7.310
7.290
7.277
7.270
7.242
7.223
5.747
4.126
4.087
3.684
3.646
3.564
3.549
3.304
3.275
2.972
2.939
2.883
2.850
2.717
2.688
2.459
1.596
1.506
1.483
0.896
0.047
0.023
TBSO
Ph
Bn
N
Ts
2.00
12.70
1.00
1.02
2.00
1.00
1.01
0.99
3.08
4.02
9.07
6.06
5.0
0.0
143.729
138.478
137.337
132.774
132.023
131.040
130.790
129.801
128.551
128.027
127.823
127.786
126.324
125.317
77.474
77.051
76.628
63.450
50.909
46.704
43.875
40.016
32.697
27.351
26.007
21.584
18.407
-5.291
TBSO
Ph
Bn
N
Ts
200
150
100
50
0
ppm (t1)



Results

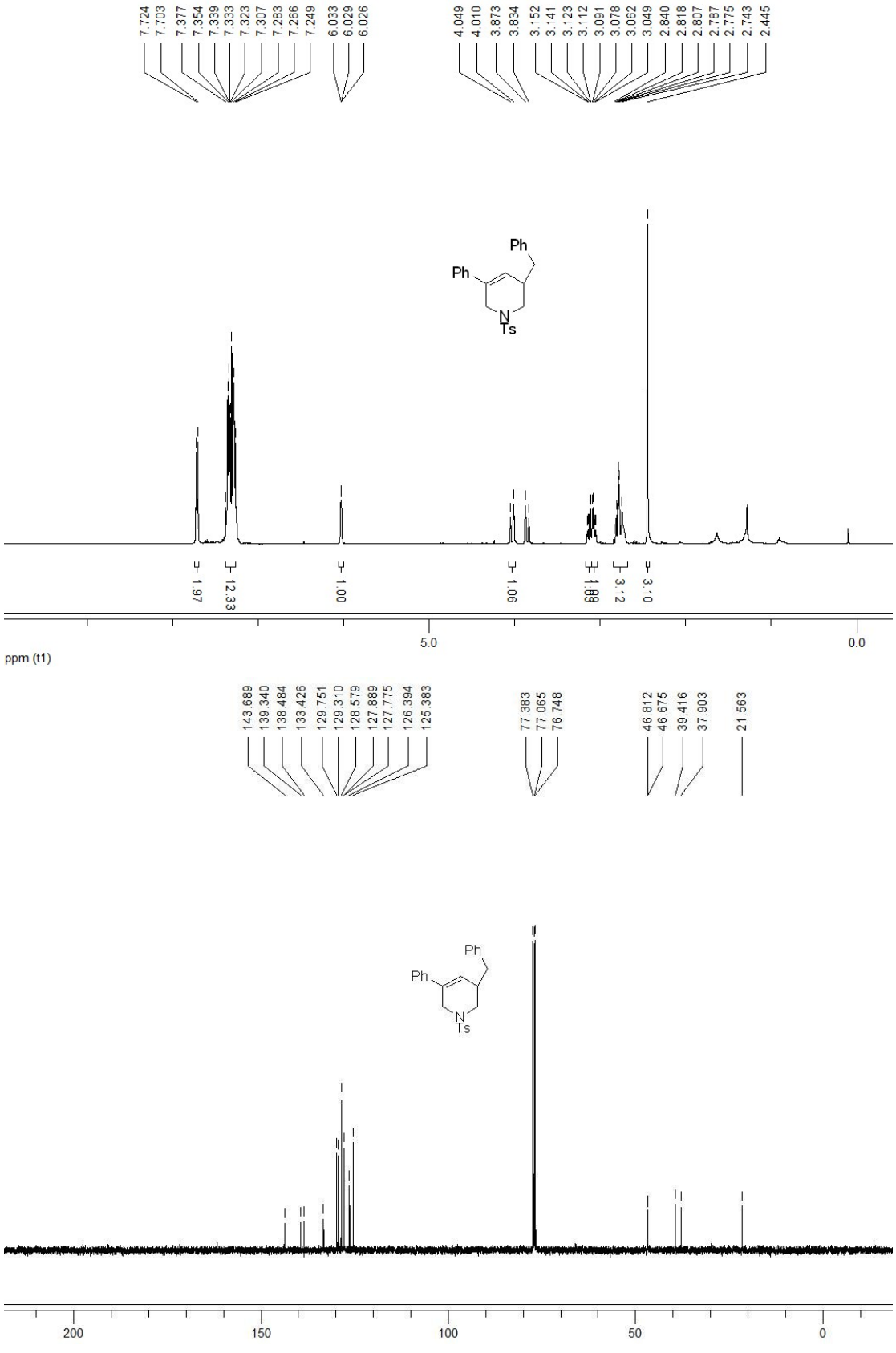
Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		31.667	158576.563	19849586.000	50.1570
2		38.030	124517.281	19725304.000	49.8430
Total			283093.844	39574890.000	100.0000



Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		31.652	15418.680	1574257.375	7.2891
2		37.613	145029.328	20022086.000	92.7061
Total			160759.784	21597388.083	100.0000

2t


7.724
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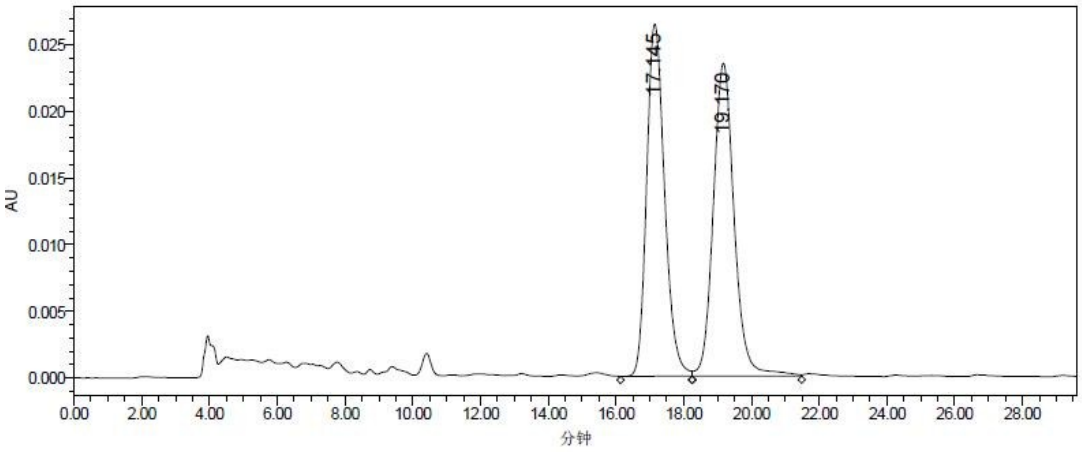
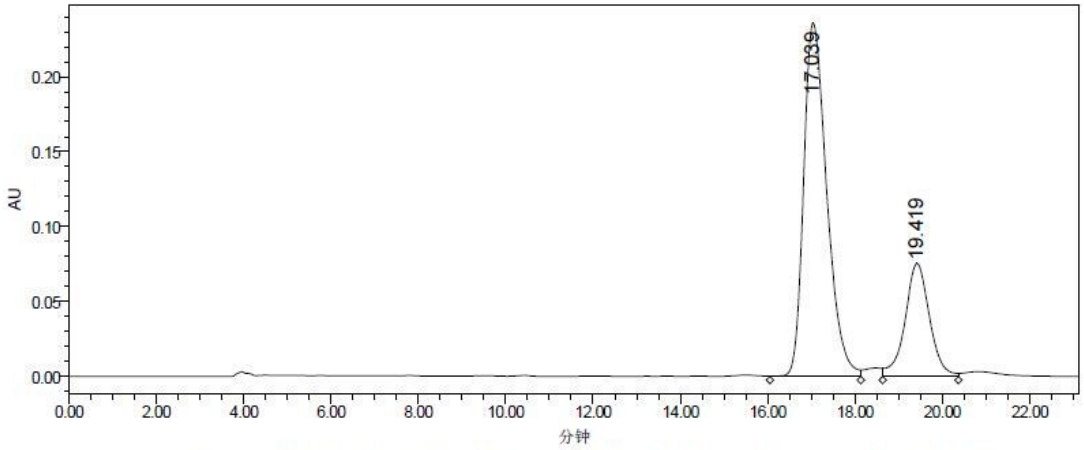
7.354
7.339
7.333
7.323
7.307
7.283
7.266
7.249
6.033
6.029
6.026
4.049
4.010
3.873
3.834
3.152
3.141
3.123
3.112
3.091
3.078
3.062
3.049
2.840
2.818
2.807
2.787
2.775
2.743
2.445
Ph
Ph
N
Ts
1.97
12.33
1.00
1.06
11.88
3.12
3.10
5.0
0.0
ppm (t1)
143.689
139.340
138.484
133.426
129.751
129.310
128.579
127.889
127.775
126.394
125.383
77.383
77.065
76.748
46.812
46.675
39.416
37.903
21.563
Ph
Ph
N
Ts
200
150
100
50
0



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

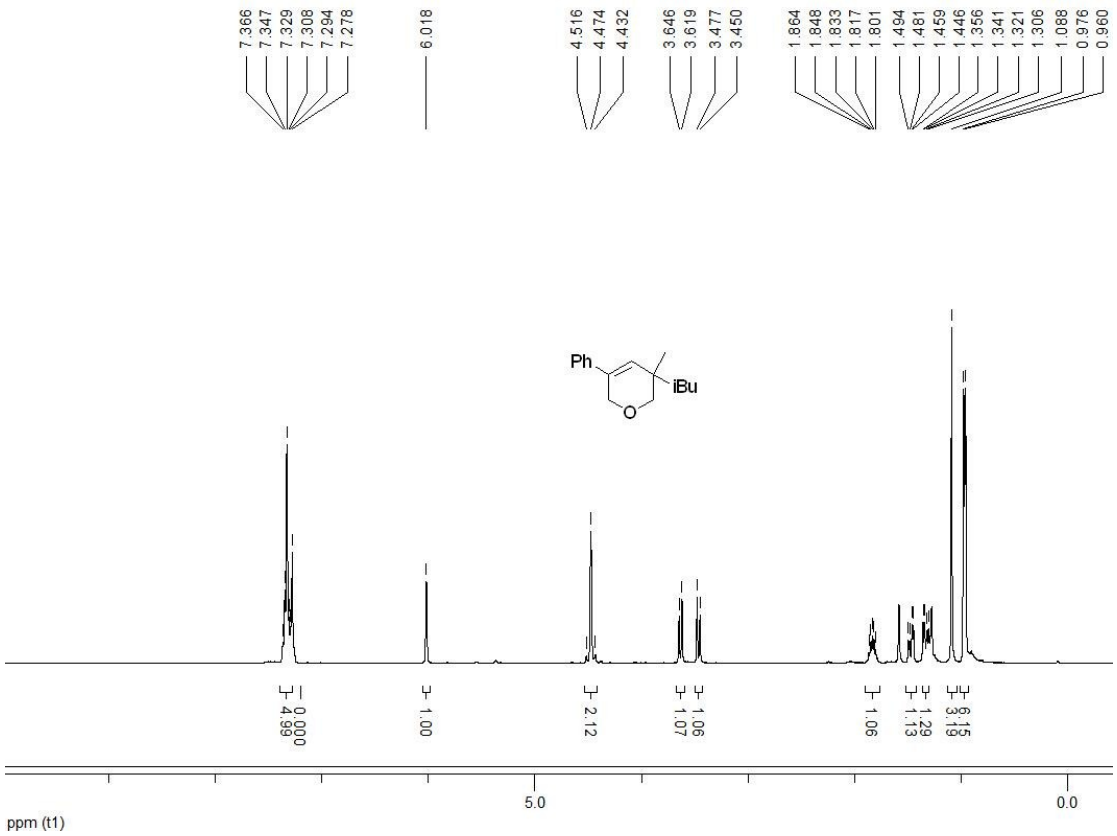
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	17.145	972499	49.12	26440
2	W2489 ChA 254nm	19.170	1007274	50.88	23497

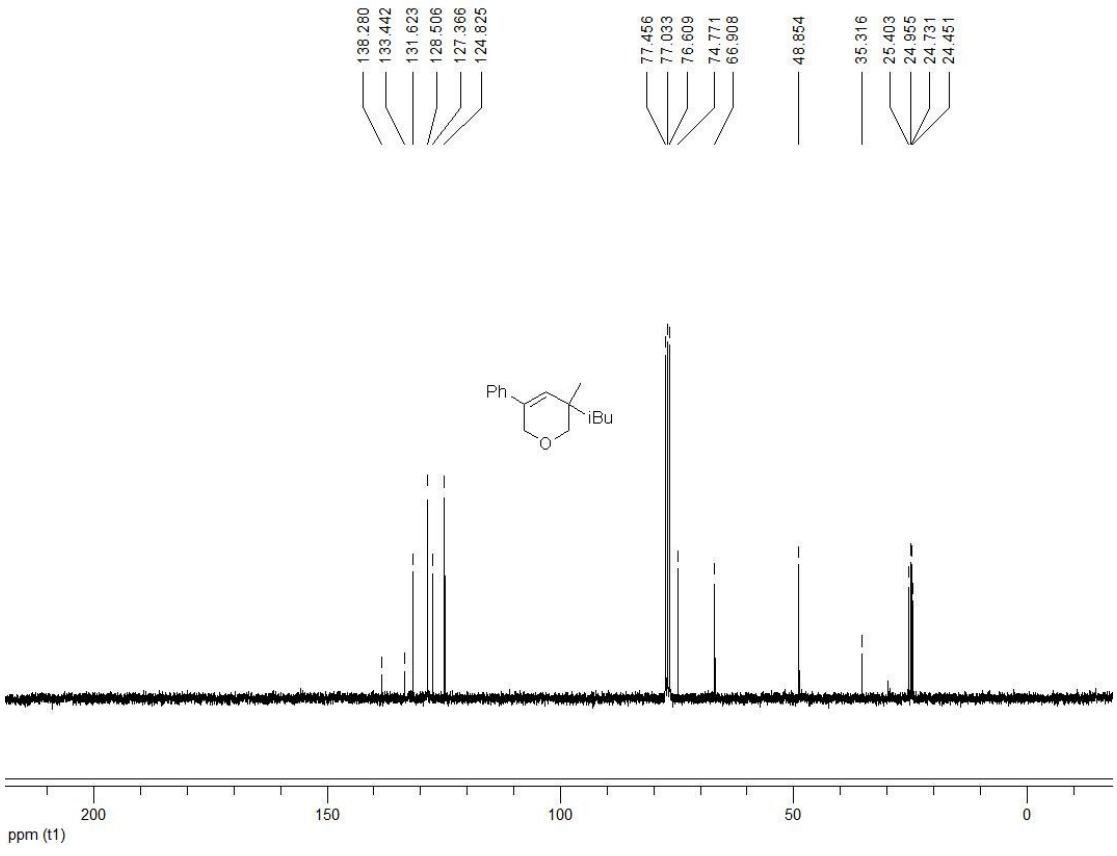


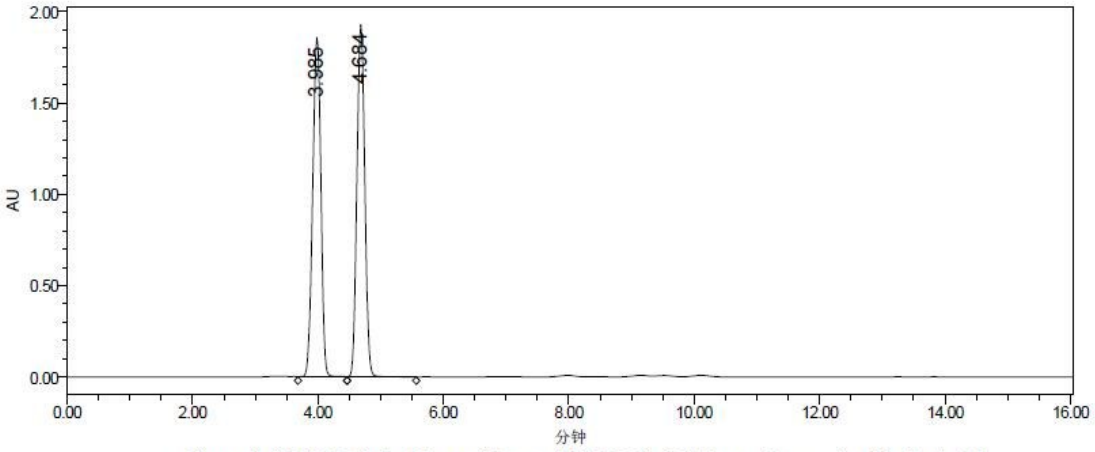
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	17.039	8661235	74.76	236273
2	W2489 ChA 254nm	19.419	2923389	25.24	75396

2v

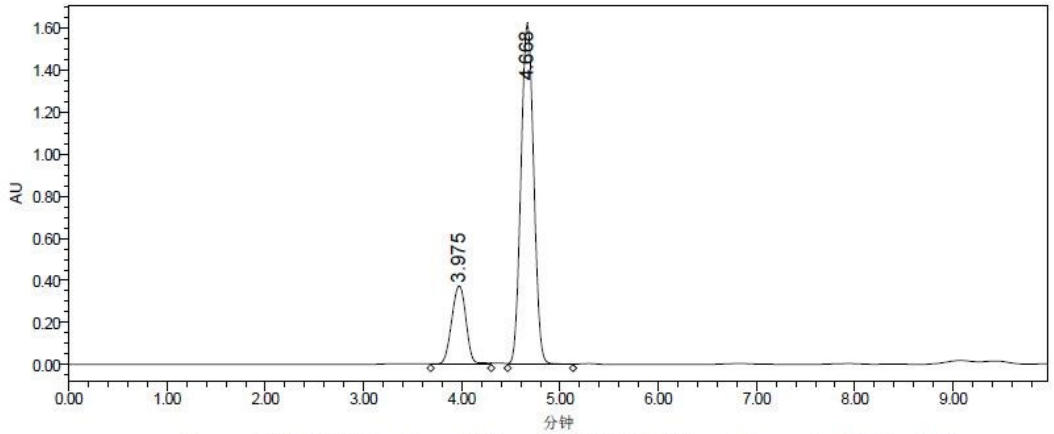

7.366
7.347
7.329
7.308
7.294
7.278
6.018
4.516
4.474
4.432
3.646
3.619
3.477
3.450
1.864
1.848
1.833
1.817
1.801
1.494
1.481
1.459
1.446
1.356
1.341
1.321
1.306
1.088
0.976
0.960
Ph
iBu
O
0.000
4.99
1.00
2.12
1.07
1.06
1.06
1.13
1.29
3.19
6.15
5.0
0.0
ppm (t1)


138.280
133.442
131.623
128.506
127.366
124.825
77.456
77.033
76.609
74.771
66.908
48.854
35.316
25.403
24.955
24.731
24.451
Ph
iBu
O
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

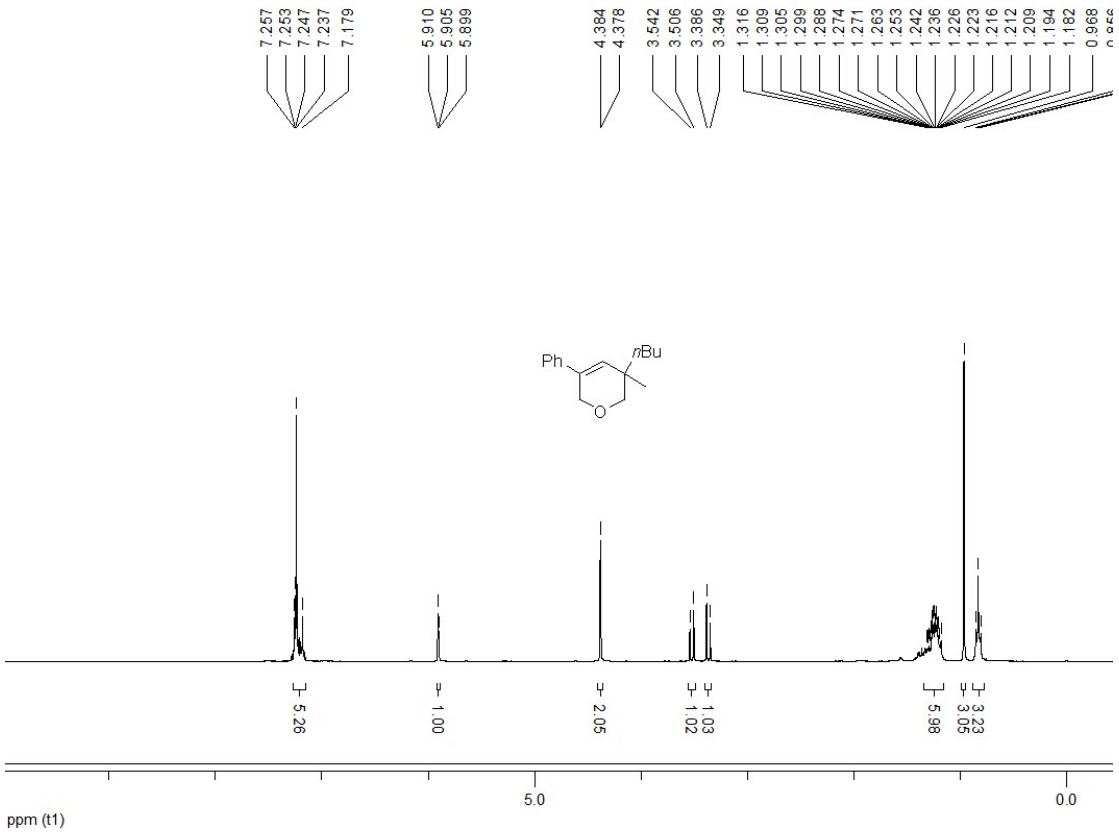
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	3.985	16940633	50.08	1858622
2	W2489 ChA 254nm	4.684	16886352	49.92	1927940

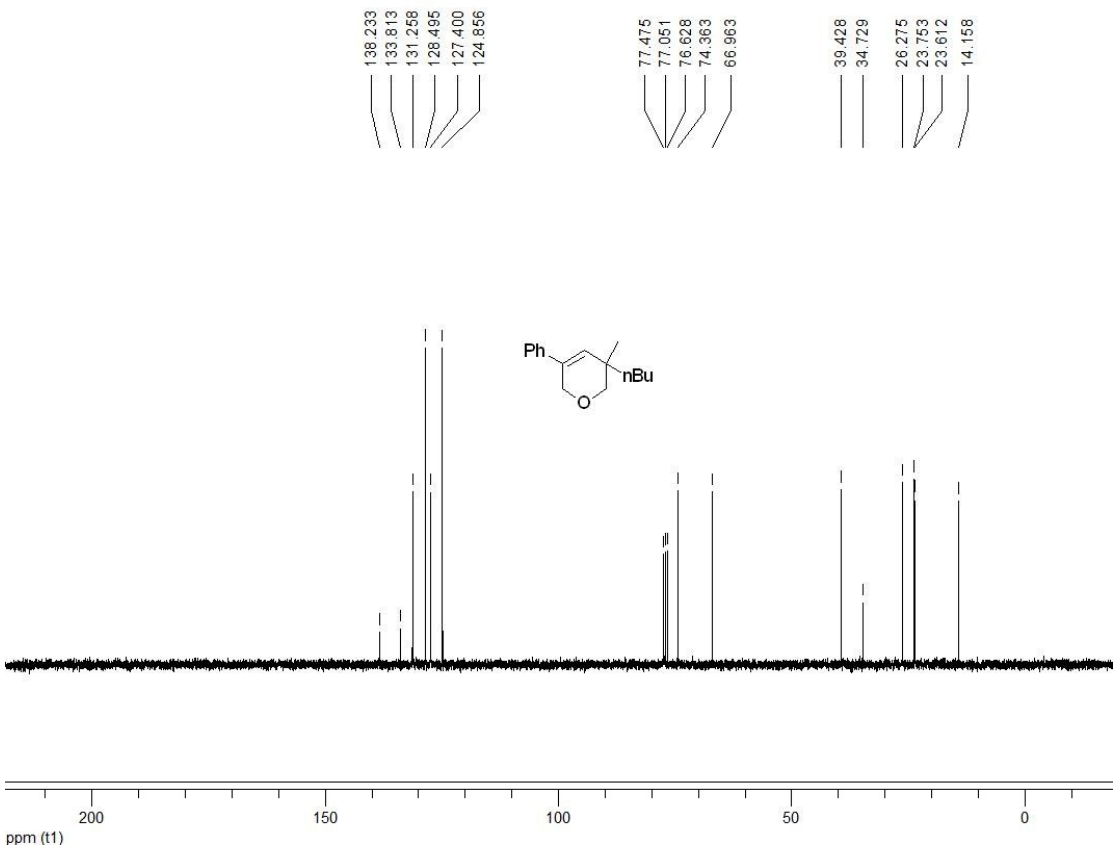


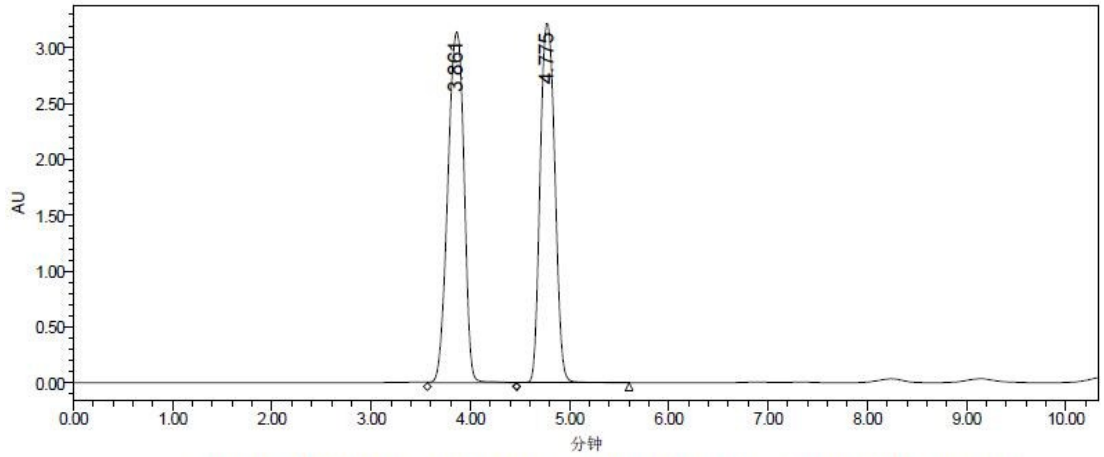
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	3.975	3813712	20.59	375753
2	W2489 ChA 254nm	4.668	14706990	79.41	1625391

2w

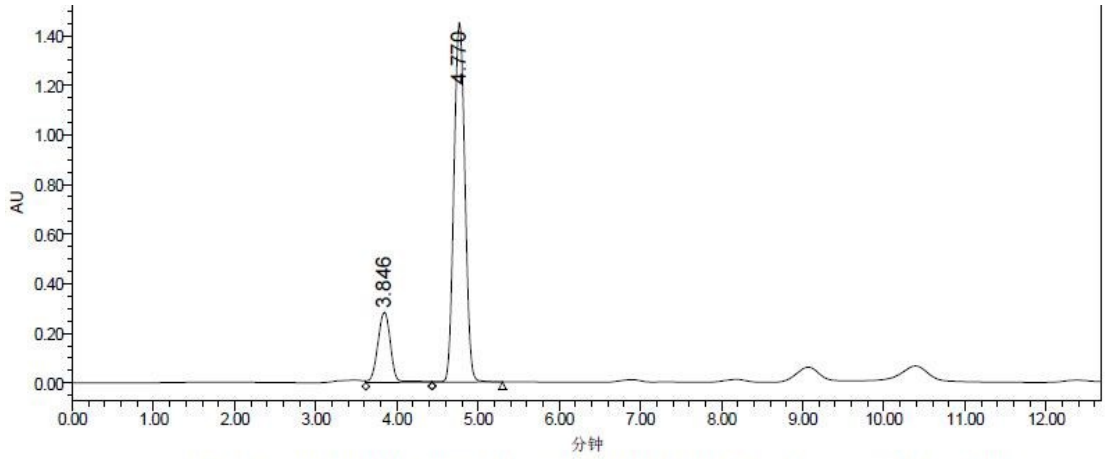

7.257
7.253
7.247
7.237
7.179
5.910
5.905
5.899
4.384
4.378
3.542
3.506
3.386
3.349
1.316
1.309
1.305
1.299
1.288
1.274
1.271
1.263
1.253
1.242
1.236
1.226
1.223
1.216
1.212
1.209
1.194
1.182
0.968
Ph
nBu
O
5.26
1.00
2.05
1.02
1.03
6.98
3.06
3.23
5.0
0.0
ppm (t1)


138.233
133.813
131.258
128.495
127.400
124.856
77.475
77.051
76.628
74.363
66.963
39.428
34.729
26.275
23.753
23.612
14.158
Ph
nBu
O
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

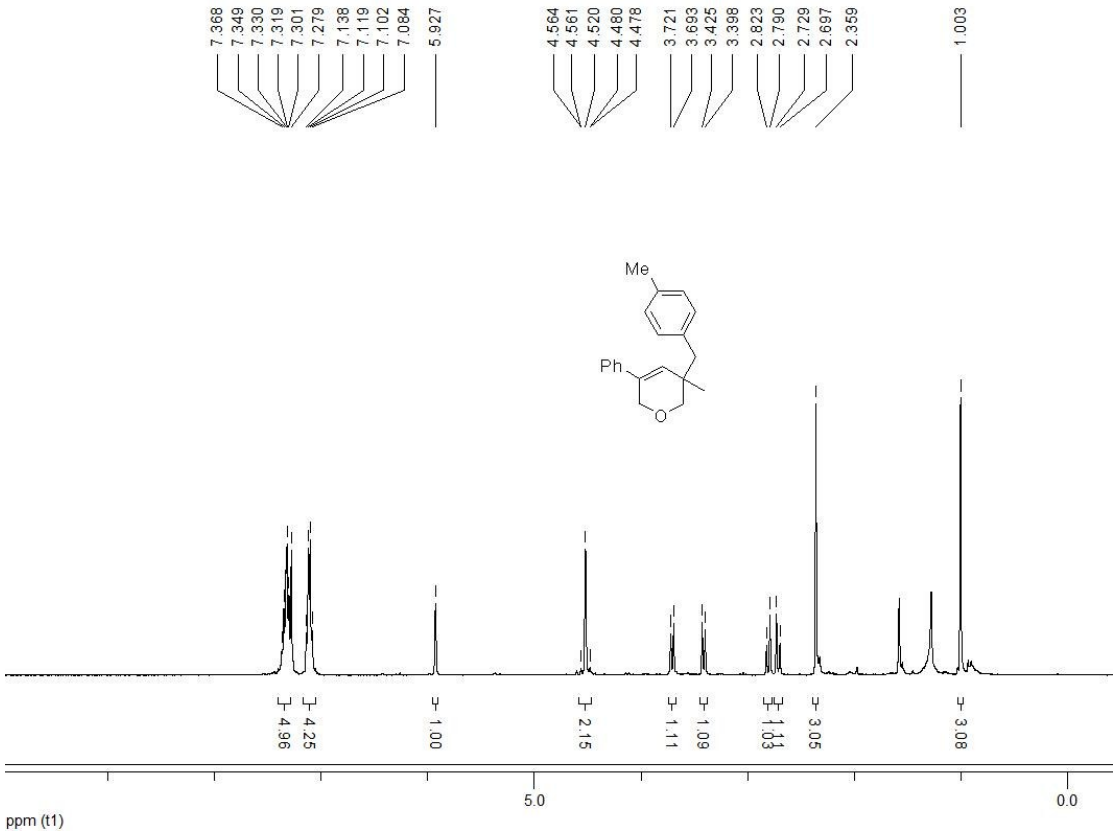
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	3.861	35786439	51.81	3152941
2	W2489 ChA 254nm	4.775	33287033	48.19	3236532

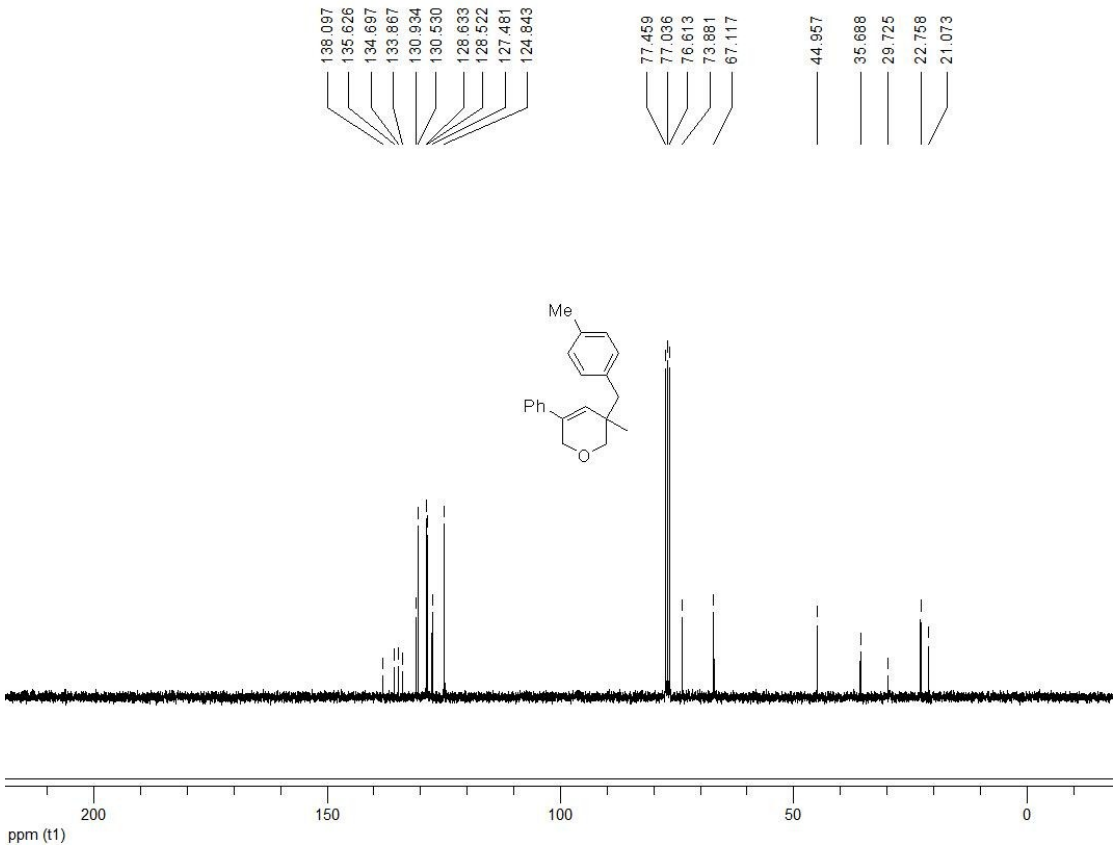


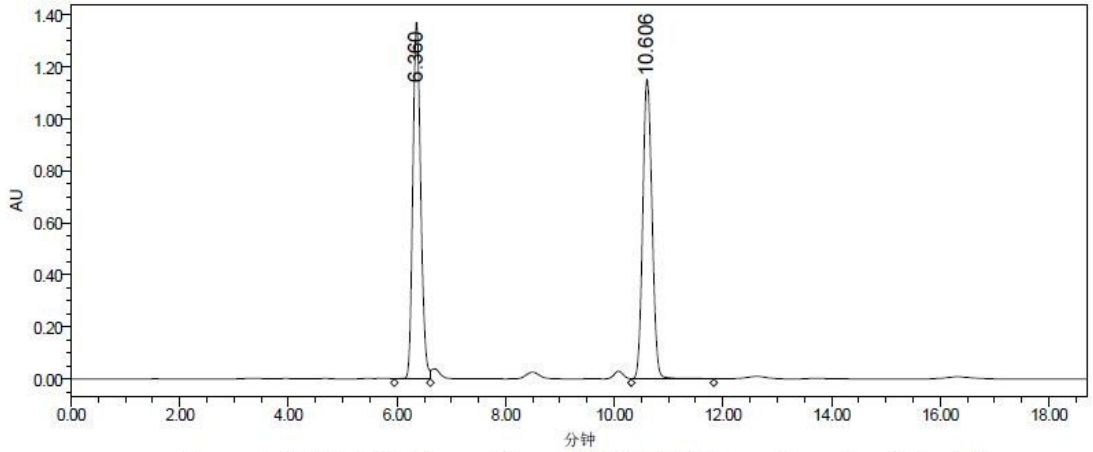
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	3.846	3098025	18.50	283964
2	W2489 ChA 254nm	4.770	13649570	81.50	1450973

2x

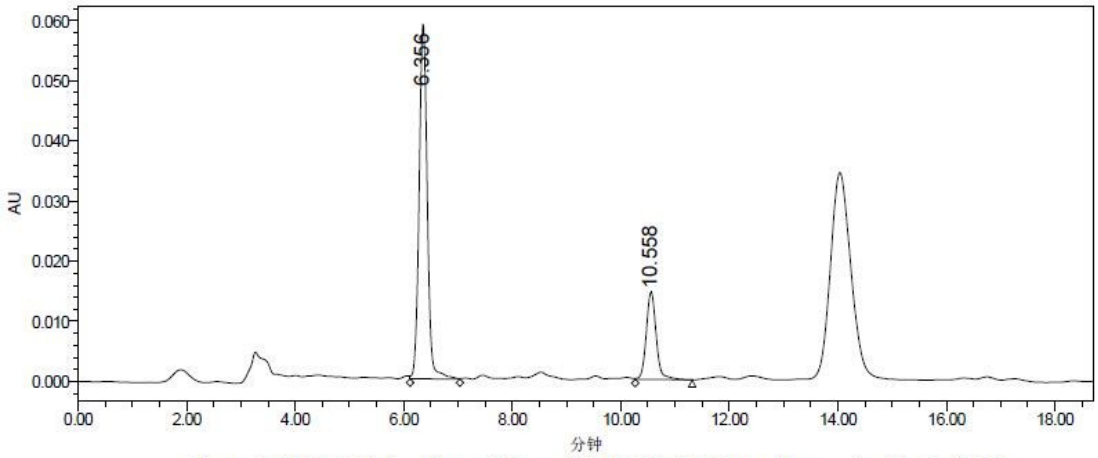

7.368
7.349
7.330
7.319
7.301
7.279
7.138
7.119
7.102
7.084
5.927
4.564
4.561
4.520
4.480
4.478
3.721
3.693
3.425
3.398
2.823
2.790
2.729
2.697
2.359
1.003
Me
Ph
O
4.96
4.25
1.00
2.15
1.11
1.09
1.03
3.05
3.08
5.0
0.0
ppm (t1)


138.097
135.626
134.697
133.867
130.934
130.530
128.633
128.522
127.481
124.843
77.459
77.036
76.613
73.881
67.117
44.957
35.688
29.725
22.758
21.073
Me
Ph
O
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

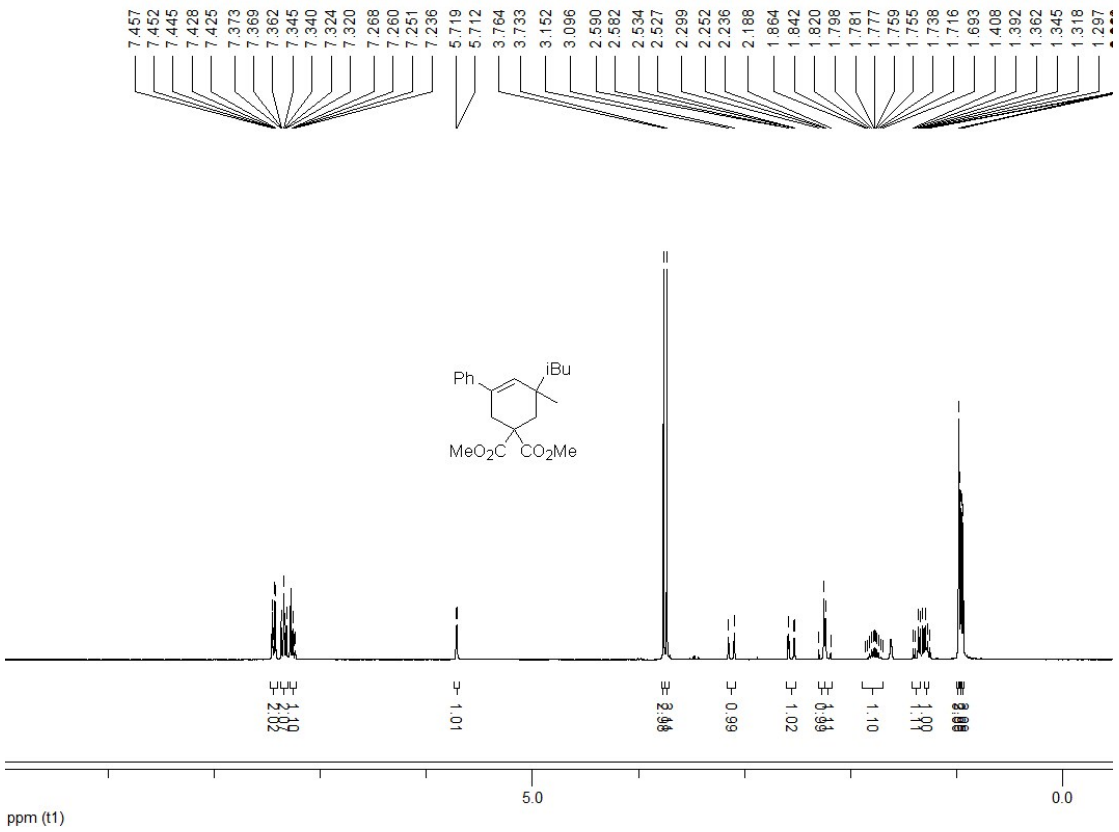
	Channel Description	RT (min)	Area (碘*sec)	% Area	Height (碘)
1	W2489 ChA 254nm	6.360	13885173	50.11	1377434
2	W2489 ChA 254nm	10.606	13824765	49.89	1156977



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (碘*sec)	% Area	Height (碘)
1	W2489 ChA 254nm	6.356	613321	76.88	59099
2	W2489 ChA 254nm	10.558	184442	23.12	14576

2y


7.457
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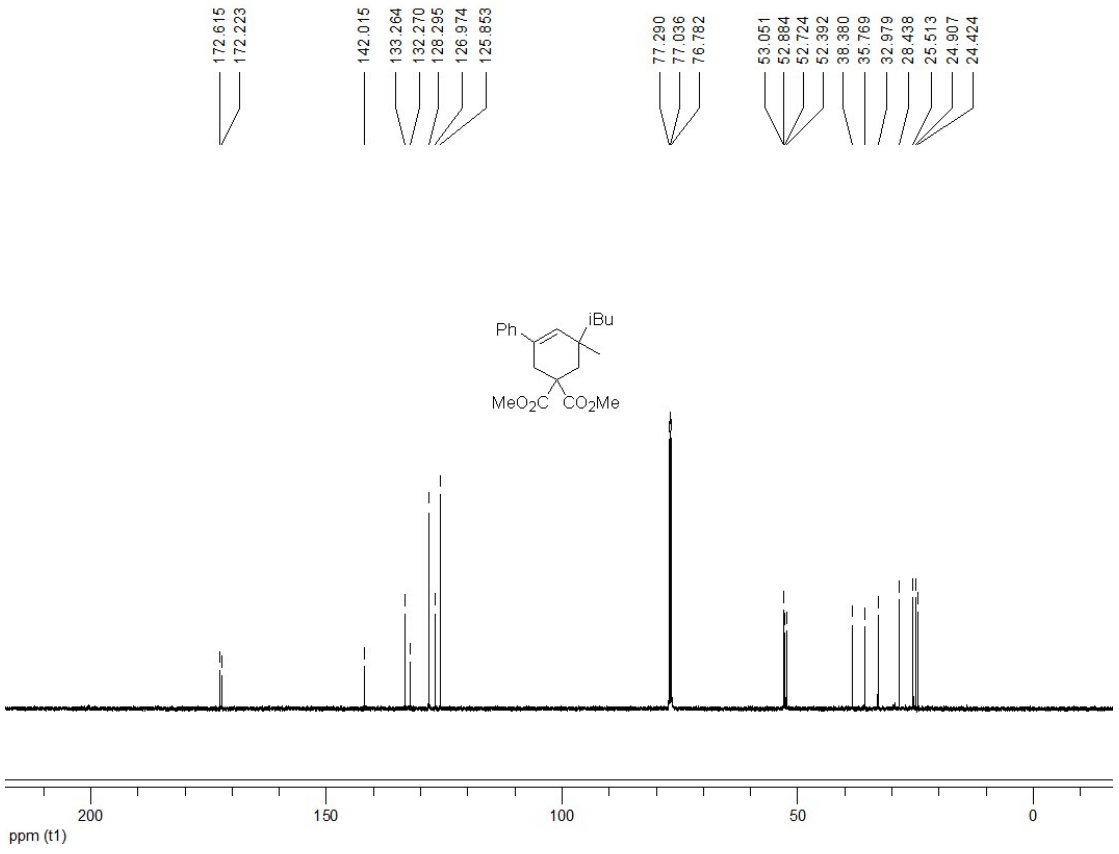
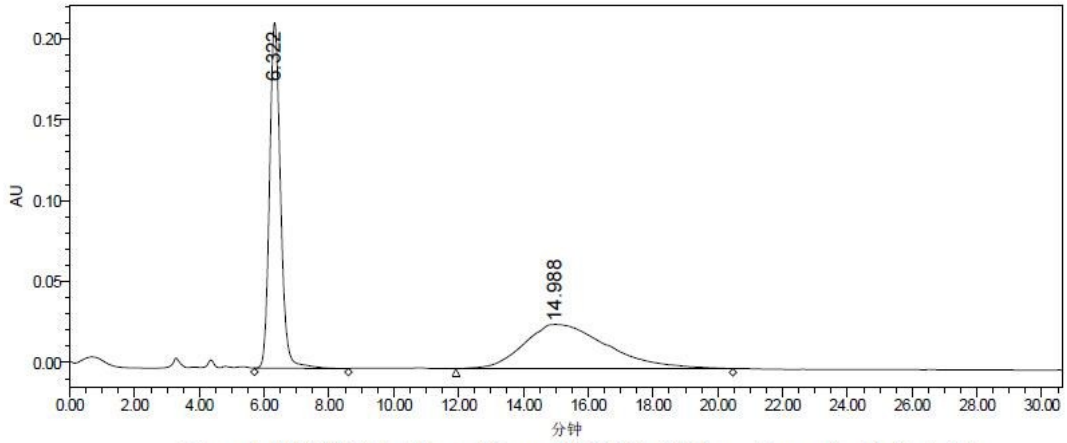
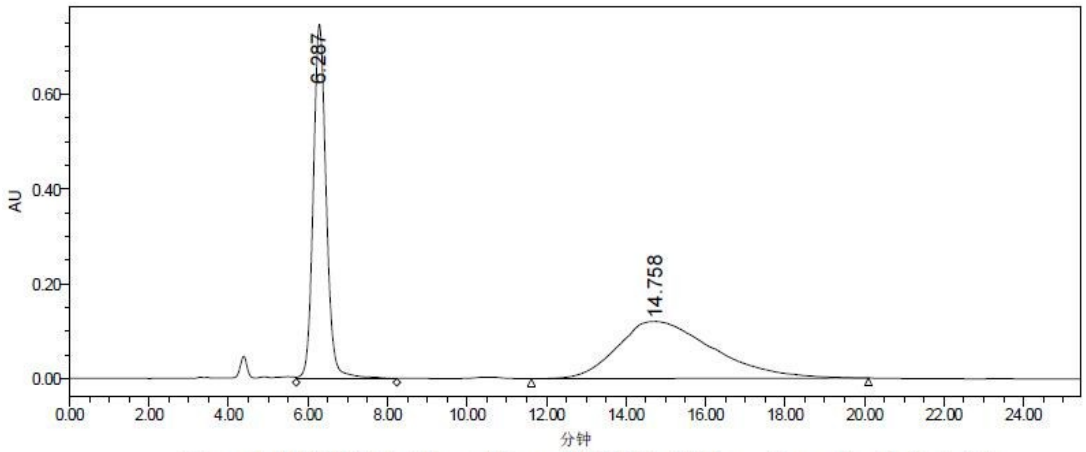
7.445
7.428
7.425
7.373
7.369
7.362
7.345
7.340
7.324
7.320
7.268
7.260
7.251
7.236
5.719
5.712
3.764
3.733
3.152
3.096
2.590
2.582
2.534
2.527
2.299
2.252
2.236
2.188
1.864
1.842
1.820
1.798
1.781
1.777
1.759
1.755
1.738
1.716
1.693
1.408
1.392
1.362
1.345
1.318
1.297
Ph
iBu
MeO2C
CO2Me
2.02
2.10
1.01
2.98
0.99
1.02
0.99
1.10
1.11
1.90
5.0
0.0
ppm (t1)


172.615
172.223
142.015
133.264
132.270
128.295
126.974
125.853
77.290
77.036
76.782
53.051
52.884
52.724
52.392
38.380
35.769
32.979
28.438
25.513
24.907
24.424
Ph
iBu
MeO2C
CO2Me
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

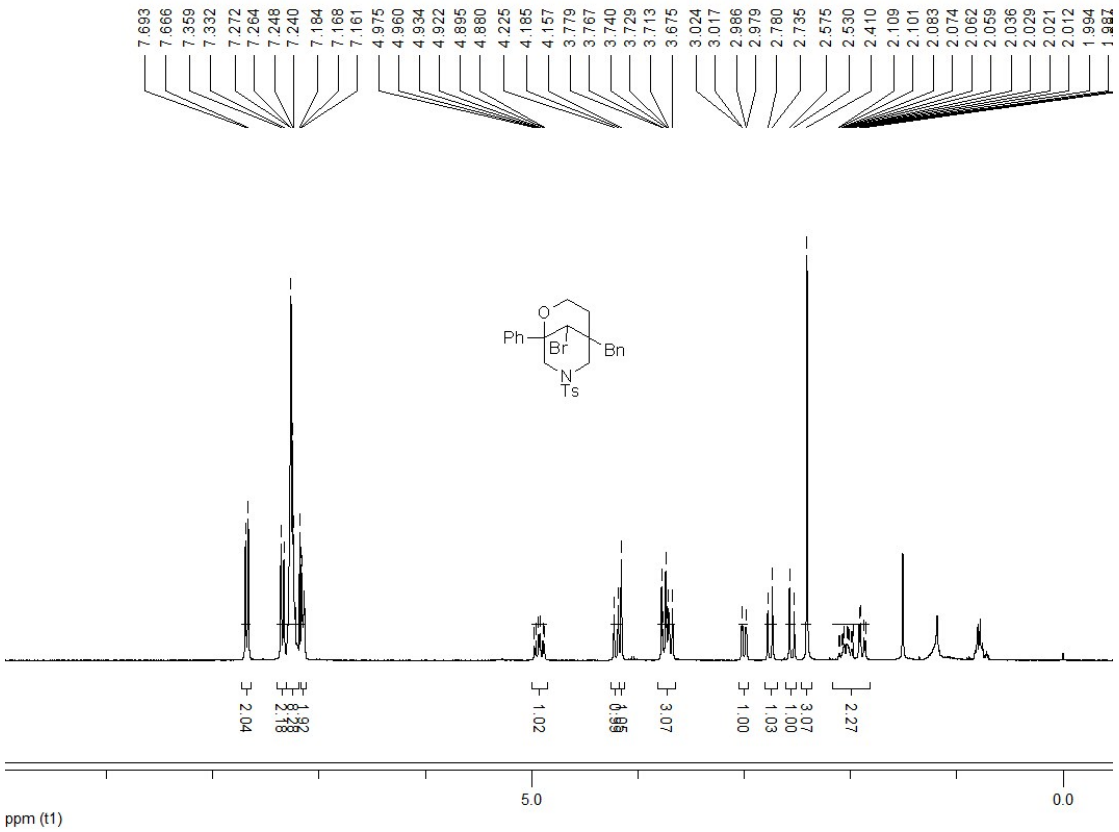
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	6.322	5033903	50.58	213637
2	W2489 ChA 254nm	14.988	4919241	49.42	27354

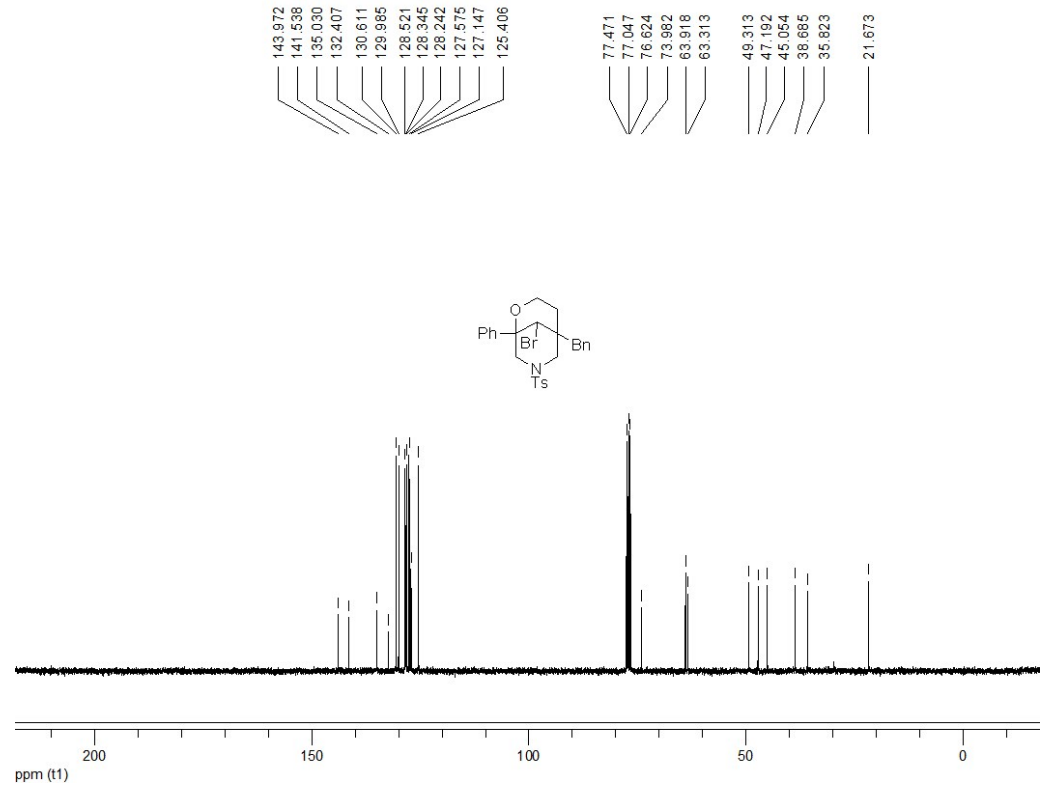


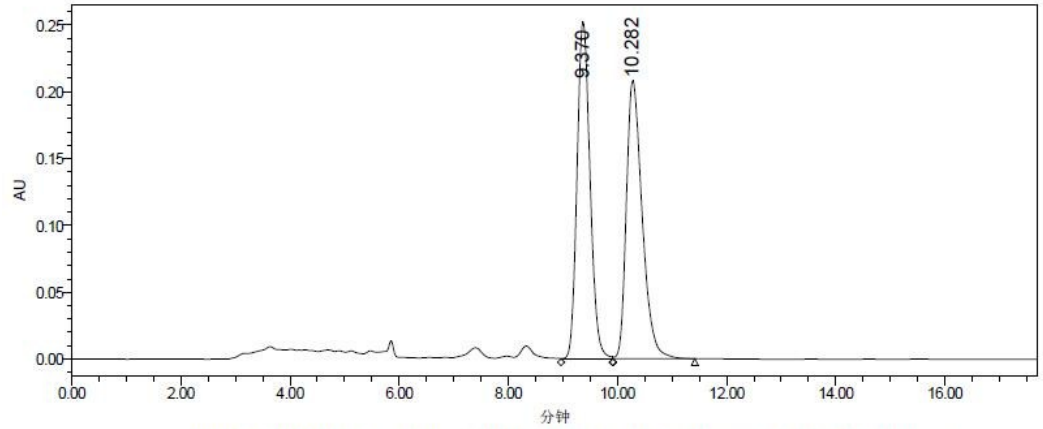
Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 01

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	6.287	16966742	45.71	748379
2	W2489 ChA 254nm	14.758	20149068	54.29	120398

3

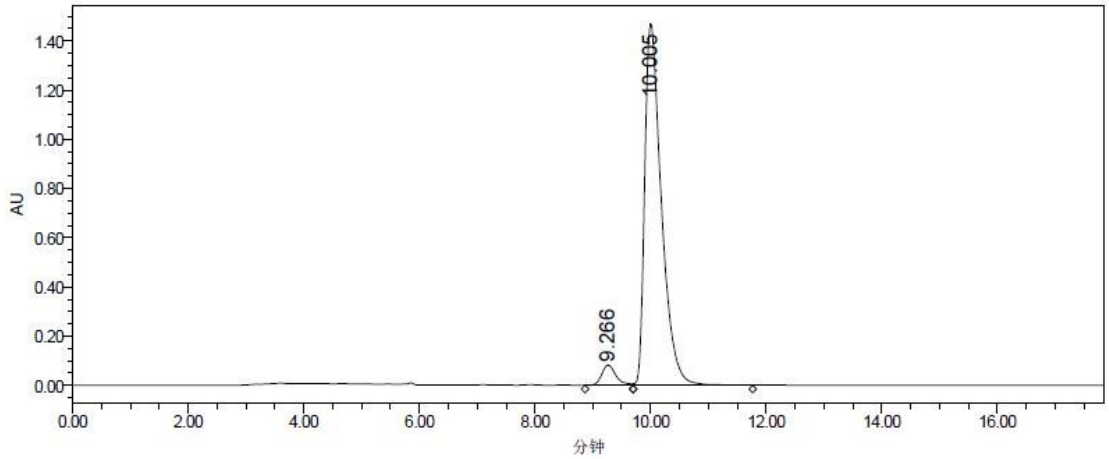

7.693
7.666
7.359
7.332
7.272
7.264
7.248
7.240
7.184
7.168
7.161
4.975
4.960
4.934
4.922
4.895
4.880
4.225
4.185
4.157
3.779
3.767
3.740
3.729
3.713
3.675
3.024
3.017
2.986
2.979
2.780
2.735
2.575
2.530
2.410
2.109
2.101
2.083
2.074
2.062
2.059
2.036
2.029
2.021
2.012
1.994
O
Ph
Br
Bn
N
Ts
2.04
1.02
3.07
1.00
1.03
3.07
2.27
5.0
0.0
ppm (t1)


143.972
141.538
135.030
132.407
130.611
129.985
128.521
128.345
128.242
127.575
127.147
125.406
77.471
77.047
76.624
73.982
63.918
63.313
49.313
47.192
45.054
38.685
35.823
21.673
O
Ph
Br
Bn
N
Ts
200
150
100
50
0
ppm (t1)



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 02

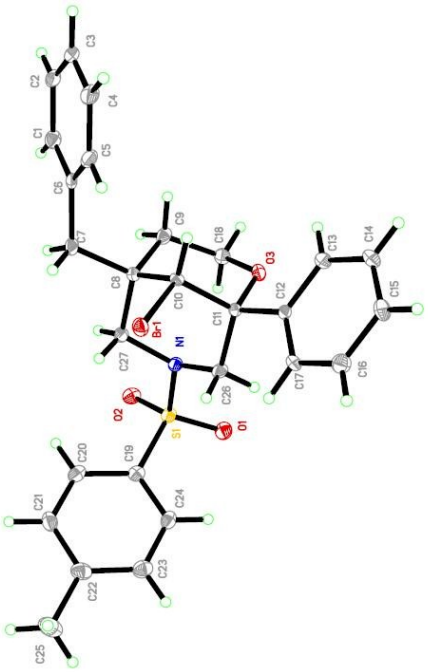
	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	9.370	4168872	49.93	252176
2	W2489 ChA 254nm	10.282	4180487	50.07	207975



Channel: W2489 ChA; Channel Desc.: W2489 ChA 254nm; Processing Method: 02

	Channel Description	RT (min)	Area (礦*sec)	% Area	Height (礦)
1	W2489 ChA 254nm	9.266	1397771	4.54	82740
2	W2489 ChA 254nm	10.005	29413227	95.46	1471356

6.X-ray Analysis



Identification code	20170314cz_0m_b
Empirical formula	$C_{27}H_{28}BrNO_3S$
Formula weight	526.47
Temperature	296 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space_group_IT_number	4
Space_group_name_H-M_alt	'P 21'
Space_group_name_Hall	'P 2yb
Unit cell dimensions	a = 10.207(9) Å= 90°.
	b = 10.425(3) Å= 97.286°.
	c = 11.403(2) Å= 90°.
Volume	1203.7(3) $Å^3$
Z	2
Density (calculated)	1.453 Mg/m^3
Absorption coefficient	1.824 mm^{-1}

F(000)	544
Crystal size	0.26 x 0.24 x 0.22 mm^3
Theta range for data collection	2.52 to 27.40°.
Index ranges	-8<=h<=12, -12<=k<=12, -13<=l<=13
Reflections collected	8311
Independent reflections	3751 [R(int) = 0.0512]
Completeness to theta =25.003°	99.8 %
Max. and min. transmission	0.648 and 0.690
Refinement method	\f and \w scans
Data / restraints / parameters	4132 / 1 / 299
Final R indices [I>2sigma(I)]	R1 = 0.0592, wR2 = 0.1217
R indices (all data)	R1 = 0.1601, wR2 = 0.1545
Absolute structure parameter	0.092(9)
Extinction coefficient	MoK/a
Largest diff. peak and hole	0.356and -0.445 e.$Å^{-3}$