Supporting Information for

Visible Light-Induced Intramolecular Cyclization Reactions of Diamines: A New Strategy to Construct Tetrahydroimidazoles

Jun Xuan, Ying Cheng, Jing An, Liang-Qiu Lu, Xiao-Xiao Zhang and Wen-Jing Xiao*

Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, 152 Luoyu Road, Wuhan, Hubei 430079, China

Fax: (+86)-27-67862041; E-mail: wxiao@mail.ccnu.edu.cn

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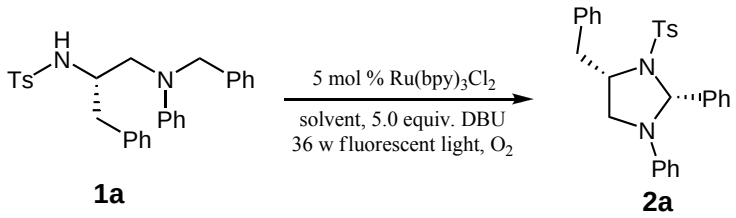
1. General Information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvent were treated according to general methods. Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H NMR spectra were recorded on Varian Mercury 400 / 600 (400 / 600 MHz) spectrophotometers. Chemical shifts (δ) are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = single, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR spectra were recorded on Varian Mercury 400/600 (100/150MHz) with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm). Mass spectra were measured on a Finnigan Trace MS spectrometer. Elementary analysis was taken on a Vario EL III elementary analysis instrument. Optical rotations were measured with JASCO P-1020 polarimeter.

2. The Optimization of Reaction Conditions

SI-Table 1. Solvent effects on the model reaction.[a]

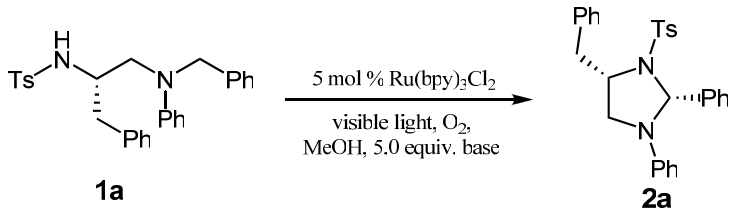


1a **2a**

entry	solvent	time (h)	yield (%)[b]	d.r.[c]
1	CH_3CN	10	27	nd[d]
2	DMSO	24	trace	nd
3	$CHCl_3$	24	16	nd
4	DMF	24	0	-
5	Toluene	24	0	-
6	CH_2Cl_2	24	31	nd
7	THF	24	0	0
8	MeOH	8	89	3:1
9	EtOH	8	72	2:1
10	^{i}PrOH	24	40	-

[a] Unless otherwise specified, all reactions were carried out with **1a** (0.2 mmol), $Ru(bpy)_3Cl_2$ (5.0 mol%), DBU (5.0 equiv.) in the indicated solvent (4 mL) and stirred at a distance of ~10 cm from a 36w fluorescent light at RT. [b] Isolated yield after flash chromatography. [c] Determined by ^{1}HNMR analysis of crude products. [d] nd= not determined.

SI-Table 2. Base effects on the model reaction.[a]



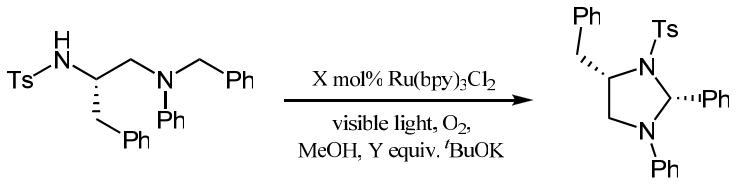
1a **2a**

entry	base	time (h)	yield (%)[b]	d.r.[c]
1	None	24	0	-
2	DBU	8	89	3:1
3	DABCO	24	0	-
4	TMG	8	84	2:1
5	Et_3N	24	23	nd[d]
6	DMAP	24	trace	nd
7	Pyridine	24	0	-
8	DIPEA	24	trace	nd
9	K_2CO_3	16	93	1:1
10	Cs_2CO_3	20	84	1.5:1

11	NaOH	9	84	2.5:1
12	KOH	20	91	1.5:1
13	^{t}BuOK	9	93	4:1
14	tBuONa	23	87	2:1

[a] Unless otherwise specified, all reactions were carried out with **1a** (0.2 mmol), $Ru(bpy)_3Cl_2$ (5.0 mol%), indicated base (5.0 equiv.) in MeOH(4 mL) and stirred at a distance of ~10 cm from a 36w fluorescent light at RT. [b] Isolated yield after flash chromatography. [c] Determined by ^{1}HNMR analysis of crude products. [d] nd= not determined.

SI-Table 3. Effects of base equivalence and catalyst loading on the model reaction.[a]



1a **2a**

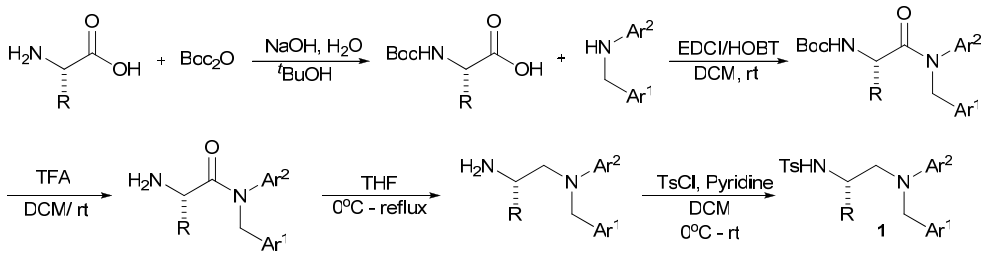
entry	$Ru(bpy)_3Cl_2$ (X mol%)	^{t}BuOK (Y equiv.)	time (h)	yield (%)[b]	d.r.[c]
1	5.0 mol%	5.0 eq.	9	93	4:1
2	5.0 mol%	2.5 eq.	9	94	4:1
3	5.0 mol%	2.0 eq.	9	94	2:1
4	5.0 mol%	1.5 eq.	9	93	2:1
5	5.0 mol%	1.0 eq.	9	93	2:1
6	2.5 mol%	5.0 eq.	9	92	2:1
7	1.0 mol%	5.0 eq.	9	93	4:1
8	0.5 mol%	5.0 eq.	21	93	4:1
9[d]	1.0 mol%	5.0 eq.	9	92	10:1

[a] Unless otherwise specified, all reactions were carried out with **1a** (0.2 mmol), $Ru(bpy)_3Cl_2$ (X mol%), indicated base (Y equiv.) in MeOH (4 mL) and stirred at a distance of ~10 cm from a 36w fluorescent light at RT. [b] Isolated yield after flash chromatography. [c] Determined by ^{1}HNMR analysis of crude products. [d] After reaction completed (TLC moninated), DCM (1.0 mL) was added and continued stirring until 48h.

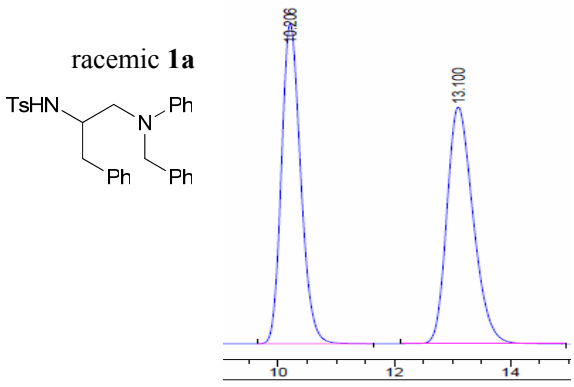
3. Preparation and Spectral Data of Substrates

3.1 Preparation of Substrates

Enantiomerically pure substrates **1** were prepared by following the procedures in references 1, 2 and 3 without racemization.

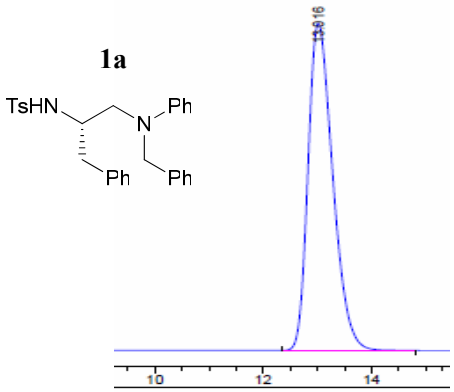


racemic **1a**



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.206	BB	0.3550	1.67519e4	730.15363	49.6953
2	13.100	BB	0.4859	1.69573e4	539.80414	50.3047

1a



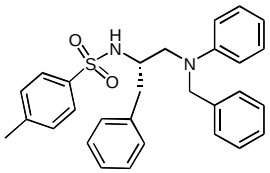
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.016	BB	0.4912	2.80730e4	887.74390	100.0000

References:

1. K. Hofmann, F. M. Finn, Y. Kiso, *J. Am. Chem. Soc*. 1978, **100**, 3585.
2. D. Bhuniya, A. DattaGupta, V. K. Singh, *J. Org. Chem.* 1996, **61**, 6108.
3. K. F. W. Hekking, D. C. J. Waalboer, M. A. H. Moelands, F. L. V. Delft, F. P. J. T. Rutjes, *Adv. Synth. Catal.* 2008, **350**, 95.

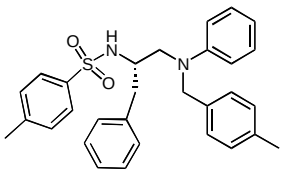
3.2 Spectral Data of Substrates

(*S*)-N-(1-(benzyl(phenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide (1a)



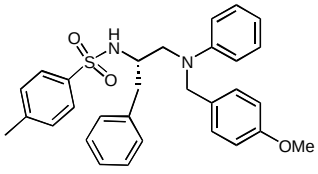
$[\alpha]_D^{22}$ = -47.93 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.40 (d, *J* = 7.8 Hz, 2H), 7.28 – 7.19 (m, 3H), 7.16 – 7.05 (m, 7H), 7.01 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 7.2 Hz, 2H), 6.70 (t, *J* = 7.2 Hz, 1H), 6.57 (d, *J* = 8.5 Hz, 2H), 4.66 (d, *J* = 6.0 Hz, 1H), 4.47 (d, *J* = 17.1 Hz, 1H), 4.30 (d, *J* = 17.0 Hz, 1H), 3.68 – 3.57 (m, 2H), 3.39 (dd, *J* = 14.5, 6.6 Hz, 1H), 2.92 (dd, *J* = 13.8, 5.8 Hz, 1H), 2.68 (dd, *J* = 13.7, 7.1 Hz, 1H), 2.34 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.85, 142.89, 138.12, 136.68, 136.39, 129.38, 129.09, 128.54, 128.49, 126.87, 126.75, 126.68, 126.53, 117.16, 113.17, 55.87, 55.29, 53.33, 39.62, 21.43. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 471.2106, measured 471.2063.

(*S*)-4-methyl-N-(1-((4-methylbenzyl)(phenyl)amino)-3-phenylpropan-2-yl)benzenesulfonamide (1b)



$[\alpha]_D^{22}$ = -48.11 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.40 (d, *J* = 8.1 Hz, 2H), 7.17 – 7.02 (m, 9H), 6.95 (dd, *J* = 16.1, 7.2 Hz, 4H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 2H), 4.59 – 4.33 (m, 2H), 4.24 (d, *J* = 16.7 Hz, 1H), 3.72 – 3.49 (m, 2H), 3.43 – 3.28 (m, 1H), 2.92 (dd, *J* = 13.8, 6.1 Hz, 1H), 2.70 (dd, *J* = 13.8, 6.8 Hz, 1H), 2.35 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.91, 142.86, 136.71, 136.44, 136.34, 134.94, 129.36, 129.21, 129.11, 129.06, 128.46, 126.74, 126.67, 126.50, 117.09, 113.21, 55.67, 55.11, 53.27, 39.61, 21.43, 21.00. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 485.2263, measured 485.2232.

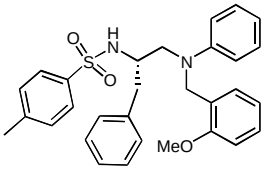
(*S*)-N-(1-((4-methoxybenzyl)(phenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide (1c)



$[\alpha]_D^{23}$ = -42.00 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (600 MHz, $CDCl_3$) δ (ppm) 7.40 (d, *J* = 8.0 Hz, 2H), 7.19 – 7.08 (m, 5H), 7.00 (dd, *J* = 15.3, 8.1 Hz, 4H), 6.93 (d, *J* = 6.8 Hz,

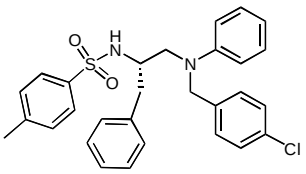
2H), 6.78 (d, *J* = 8.3 Hz, 2H), 6.69 (t, *J* = 7.1 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 2H), 4.69 (s, 1H), 4.39 (d, *J* = 16.6 Hz, 1H), 4.21 (d, *J* = 16.5 Hz, 1H), 3.75 (s, 3H), 3.64 (dd, *J* = 12.8, 6.3 Hz, 1H), 3.52 (dd, *J* = 14.8, 6.8 Hz, 1H), 3.34 (dd, *J* = 14.9, 6.7 Hz, 1H), 2.89 (dd, *J* = 13.7, 5.9 Hz, 1H), 2.69 (dd, *J* = 13.7, 7.1 Hz, 1H), 2.34 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ (ppm) 158.55, 148.02, 142.91, 136.72, 136.40, 129.93, 129.39, 129.12, 128.49, 128.01, 126.81, 126.53, 117.31, 113.95, 113.56, 55.48, 55.17, 54.85, 53.22, 39.59, 21.42. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 501.2212, measured 501.2199.

(*S*)-N-(1-((2-methoxybenzyl)(phenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide (1d)



$[\alpha]_D^{23}$ = -33.72 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.39 (d, *J* = 7.8 Hz, 2H), 7.25 – 7.14 (m, 4H), 7.09 (t, *J* = 7.6 Hz, 2H), 6.99 (d, *J* = 7.9 Hz, 4H), 6.88 (d, *J* = 8.2 Hz, 2H), 6.81 (t, *J* = 7.4 Hz, 1H), 6.67 (t, *J* = 7.0 Hz, 1H), 6.50 (d, *J* = 8.6 Hz, 2H), 4.61 (d, *J* = 5.2 Hz, 1H), 4.40 (d, *J* = 17.3 Hz, 1H), 4.23 (d, *J* = 17.3 Hz, 1H), 3.86 (s, 3H), 3.65 (dd, *J* = 13.0, 6.4 Hz, 1H), 3.52 (dd, *J* = 14.9, 7.3 Hz, 1H), 3.34 (dd, *J* = 14.9, 6.5 Hz, 1H), 2.95 (dd, *J* = 13.8, 6.2 Hz, 1H), 2.75 (dd, *J* = 13.8, 6.8 Hz, 1H), 2.33 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 157.03, 147.83, 142.78, 136.69, 136.17, 129.32, 129.22, 128.98, 128.45, 127.98, 127.82, 126.73, 126.50, 125.35, 120.37, 116.79, 112.81, 110.01, 55.14, 54.76, 52.98, 51.16, 39.69, 21.44. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 501.2212, measured 501.2215.

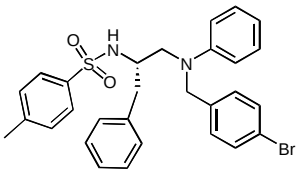
(*S*)-N-(1-((4-chlorobenzyl)(phenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide (1e)



$[\alpha]_D^{23}$ = -41.90 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.39 (dd, *J* = 8.4, 2.6 Hz, 2H), 7.30 – 7.19 (m, 2H), 7.18 – 7.06 (m, 6H), 7.05 – 6.99 (m, 3H), 6.91 (t, *J* = 5.9 Hz, 2H), 6.71 (q, *J* = 7.0 Hz, 1H), 6.57 (t, *J* = 7.7 Hz, 2H), 4.55 (dd, *J* = 17.3, 6.1 Hz, 1H), 4.46 (dd, *J* = 17.0, 10.8 Hz, 1H), 4.29 (dd, *J* = 17.0, 4.7 Hz, 1H), 3.69 – 3.54 (m, 2H), 3.42 – 3.34 (m, 1H), 2.97 – 2.86 (m, 1H), 2.72 – 2.62 (m, 1H), 2.36 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.90, 147.61, 142.98, 136.67, 136.47,

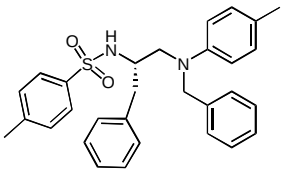
132.52, 129.40, 129.06, 128.63, 128.53, 128.10, 126.74, 126.58, 117.49, 113.32, 55.39, 55.28, 53.44, 39.63, 21.42. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 505.1717, measured 505.1708.

(*S*)-N-(1-((4-bromobenzyl)(phenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzen esulfonamide (1f)



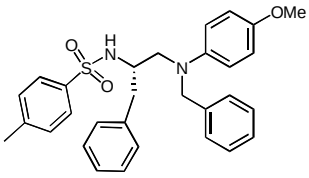
$[\alpha]_D^{23}$ = -48.25 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.40 (d, *J* = 7.8 Hz, 2H), 7.28 (d, *J* = 7.1 Hz, 1H), 7.23 (d, *J* = 6.5 Hz, 1H), 7.17 – 7.06 (m, 7H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 7.6 Hz, 2H), 6.71 (t, *J* = 7.3 Hz, 1H), 6.58 (d, *J* = 8.6 Hz, 2H), 4.54 – 4.39 (m, 2H), 4.29 (d, *J* = 16.9 Hz, 1H), 3.70 – 3.53 (m, 2H), 3.38 (dd, *J* = 14.5, 6.5 Hz, 1H), 2.93 (dd, *J* = 13.7, 5.8 Hz, 1H), 2.68 (dd, *J* = 13.8, 7.0 Hz, 1H), 2.35 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ (ppm) 147.78, 142.93, 138.06, 136.56, 136.20, 129.40, 129.08, 128.52, 126.87, 126.73, 126.64, 117.12, 113.07, 55.83, 55.30, 53.24, 39.58, 21.47. **HRMS:** m/z (ESI) calculated $[(M-Br)+H]^+$ 471.2106, measured 471.2079.

(*S*)-N-(1-(benzyl(p-tolyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonami de (1g)



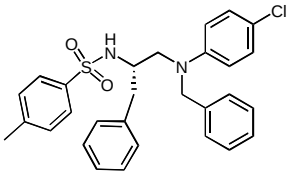
$[\alpha]_D^{23}$ = -45.25 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.41 (d, *J* = 8.3 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.26 – 7.19 (m, 2H), 7.18 – 7.12 (m, 3H), 7.06 (dd, *J* = 15.6, 7.5 Hz, 4H), 6.92 (dd, *J* = 10.7, 5.1 Hz, 4H), 6.50 (d, *J* = 8.6 Hz, 2H), 4.46 (d, *J* = 5.7 Hz, 1H), 4.40 (d, *J* = 16.6 Hz, 1H), 4.24 (d, *J* = 16.7 Hz, 1H), 3.65 – 3.55 (m, 1H), 3.50 (dd, *J* = 14.6, 6.9 Hz, 1H), 3.31 (dd, *J* = 14.6, 6.8 Hz, 1H), 2.91 (dd, *J* = 13.8, 6.1 Hz, 1H), 2.70 (dd, *J* = 13.8, 7.0 Hz, 1H), 2.36 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (pm）145.74, 142.86, 138.27, 136.70, 136.27, 129.61, 129.35, 129.10, 128.50, 128.45, 126.80, 126.77, 126.56, 126.48, 113.70, 56.33, 55.32, 53.24, 39.49, 21.45, 20.21. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 485.2263, measured 485.2248.

(*S*)-N-(1-(benzyl(4-methoxyphenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzen esulfonamide (1h)



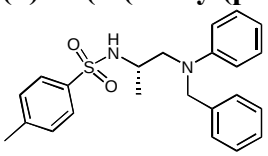
$[\alpha]_D^{23}$ = -38.29 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.43 (d, *J* = 7.5 Hz, 2H), 7.28 (s, 1H), 7.23 (dd, *J* = 12.1, 4.8 Hz, 2H), 7.15 (dd, *J* = 9.5, 5.2 Hz, 3H), 7.09 – 7.02 (m, 4H), 6.95 – 6.89 (m, 2H), 6.71 (d, *J* = 8.2 Hz, 2H), 6.58 (d, *J* = 8.4 Hz, 2H), 4.50 (d, *J* = 4.8 Hz, 1H), 4.27 (d, *J* = 16.0 Hz, 1H), 4.15 (d, *J* = 16.1 Hz, 1H), 3.76 (s, 3H), 3.56 – 3.44 (m, 1H), 3.33 (dd, *J* = 14.1, 7.0 Hz, 1H), 3.19 (dd, *J* = 14.1, 6.6 Hz, 1H), 2.87 (dd, *J* = 13.8, 6.4 Hz, 1H), 2.75 (dd, *J* = 13.8, 6.6 Hz, 1H), 2.36 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 152.68, 142.93, 142.46, 138.16, 136.81, 136.34, 129.38, 129.17, 128.45, 127.36, 126.99, 126.85, 126.48, 116.98, 114.45, 58.01, 55.51, 55.34, 52.99, 39.35, 21.43. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 501.2212, measured 501.2211.

(*S*)-N-(1-(benzyl(4-chlorophenyl)amino)-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide (1i)



$[\alpha]_D^{23}$ = -46.91 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (ppm) (t, *J* = 5.7 Hz, 2H), 7.29 – 7.12 (m, 6H), 7.06 – 6.99 (m, 6H), 6.96 – 6.91 (m, 2H), 6.44 – 6.36 (m, 2H), 4.81 (d, *J* = 6.5 Hz, 1H), 4.38 (dd, *J* = 61.0, 17.1 Hz, 2H), 3.68 – 3.57 (m, 1H), 3.53 (dd, *J* = 14.9, 7.1 Hz, 1H), 3.37 (dd, *J* = 14.9, 6.5 Hz, 1H), 2.86 (dd, *J* = 13.8, 6.4 Hz, 1H), 2.70 (dd, *J* = 13.7, 7.0 Hz, 1H), 2.35 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 146.15, 143.13, 137.56, 136.49, 136.18, 129.42, 129.05, 128.82, 128.64, 128.59, 127.05, 126.70, 126.53, 121.83, 114.16, 56.11, 55.36, 53.04, 39.67, 21.47. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 505.1717, measured 505.1715.

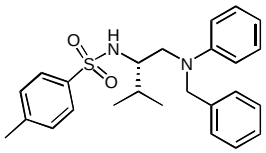
(*S*)-N-(1-(benzyl(phenyl)amino)propan-2-yl)-4-methylbenzenesulfonamide (1j)



$[\alpha]_D^{25}$ = -33.74 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.66 (d, *J* = 8.1 Hz, 2H), 7.31 – 7.09 (m, 7H), 7.06 (d, *J* = 7.6 Hz, 2H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.58 (d, *J* = 8.7 Hz, 2H), 4.85 (d, *J* = 3.9 Hz, 1H), 4.44 (d, *J* = 17.1 Hz, 1H), 4.30 (d, *J* = 17.0 Hz, 1H), 3.62 – 3.56 (m, 1H), 3.50 – 3.40 (m, 1H), 3.21 (dd, *J* = 14.8, 7.0 Hz, 1H), 2.38 (s, 3H), 1.13 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100Hz, $CDCl_3$) δ (ppm) 147.78, 143.27, 137.79,

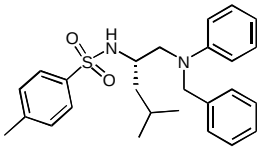
137.01, 129.54, 129.14, 128.56, 126.97, 126.89, 126.61, 117.26, 113.15, 56.77, 55.43, 47.73, 21.50, 19.66. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 395.1793, measured 395.1786.

(*S*)-N-(1-(benzyl(phenyl)amino)-3-methylbutan-2-yl)-4-methylbenzenesulfonamide (1k)



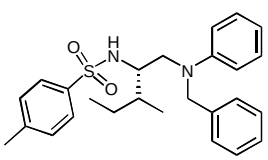
$[\alpha]_D^{25}$ = -16.03 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.66 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.09 (m, 7H), 7.04 (d, *J* = 7.1 Hz, 2H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 8.3 Hz, 2H), 4.94 (t, *J* = 8.4 Hz, 1H), 4.35 (d, *J* = 17.3 Hz, 1H), 4.16 (d, *J* = 17.3 Hz, 1H), 3.62 – 3.45 (m, 1H), 3.43 – 3.25 (m, 2H), 2.36 (s, 3H), 2.03 – 1.86 (m, 1H), 0.88 (d, *J* = 6.9 Hz, 3H), 0.77 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.79, 143.07, 137.91, 137.46, 129.38, 129.10, 128.51, 126.96, 126.79, 126.53, 116.82, 112.64, 56.37, 54.73, 52.36, 29.12, 21.49, 18.96, 16.41. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 423.2106, measured 423.2099.

(*S*)-N-(1-(benzyl(phenyl)amino)-4-methylpentan-2-yl)-4-methylbenzenesulfonamide (1l)



$[\alpha]_D^{23}$ = -29.82 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.67 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.19 (m, 3H), 7.14 (t, *J* = 8.8 Hz, 4H), 7.06 (d, J = 7.3 Hz, 2H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.60 (d, *J* = 8.4 Hz, 2H), 4.95 (d, *J* = 7.8 Hz, 1H), 4.43 (d, *J* = 17.2 Hz, 1H), 4.28 (d, *J* = 17.3 Hz, 1H), 3.64 – 3.42 (m, 2H), 3.27 (dd, *J* = 14.7, 7.4 Hz, 1H), 2.35 (s, 3H), 1.61 – 1.47 (m, 1H), 1.37 – 1.28 (m, 2H), 0.81 (d, *J* = 6.6 Hz, 3H), 0.56 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.97, 143.17, 137.94, 137.42, 129.43, 129.05, 128.48, 126.93, 126.73, 126.52, 116.81, 112.67, 77.32, 77.00, 76.68, 56.36, 55.16, 50.53, 42.95, 24.25, 23.35, 21.46, 21.41. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 437.2263, measured 437.2235.

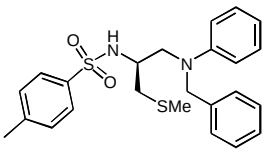
N-((2*S*,3*S*)-1-(benzyl(phenyl)amino)-3-methylpentan-2-yl)-4-methylbenzenesulfonamide (1m)



$[\alpha]_D^{25}$ = -4.19 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$)

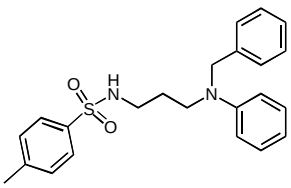
δ (ppm) 7.61 (d, *J* = 8.2 Hz, 2H), 7.28– 7.19 (m, 3H), 7.13 (t, *J* = 7.0 Hz, 4H), 7.03 (d, *J* = 7.2 Hz, 2H), 6.69 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 8.5 Hz, 2H), 4.75 (d, *J* = 7.5 Hz, 1H), 4.31 (d, *J* = 17.2 Hz, 1H), 4.13 (d, *J* = 17.1 Hz, 1H), 3.57 – 3.46 (m, 1H), 3.43 – 3.28 (m, 2H), 2.36 (s, 3H), 1.75 – 1.68 (m, 1H), 1.49 – 1.41 (m, 1H), 1.11 – 1.03 (m, 1H), 0.88 (t, *J* = 7.2 Hz, 3H), 0.77 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.89, 143.08, 137.83, 137.21, 129.38, 129.12, 128.56, 126.97, 126.88, 126.62, 117.04, 112.88, 55.92, 54.85, 51.19, 36.62, 24.23, 21.51, 14.83, 12.11. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 437.2263, measured 437.2266.

(*S*)-N-(1-(benzyl(phenyl)amino)-3-(methylthio)propan-2-yl)-4-methylbenzenesulfonamide (1n)



$[\alpha]_D^{23}$ = -35.48 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.67 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 6.9 Hz, 1H), 7.25 – 7.11 (m, 6H), 7.08 (d, *J* = 7.1 Hz, 2H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.63 (d, *J* = 8.4 Hz, 2H), 4.88 (d, *J* = 6.3 Hz, 1H), 4.46 (d, *J* = 17.0 Hz, 1H), 4.31 (d, *J* = 17.0 Hz, 1H), 3.72 – 3.62 (m, 1H), 3.56 (dd, *J* = 14.9, 6.6 Hz, 1H), 3.46 (dd, *J* = 14.9, 7.4 Hz, 1H), 2.72 (dd, *J* = 13.7, 4.9 Hz, 1H), 2.60 (dd, *J* = 13.7, 5.7 Hz, 1H), 2.39 (s, 3H), 1.92 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 147.59, 143.50, 137.90, 136.53, 129.56, 129.19, 128.58, 127.10, 126.96, 126.62, 117.30, 113.02, 55.61, 54.03, 50.37, 37.59, 21.53, 16.34. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 441.1670, measured 441.1639.

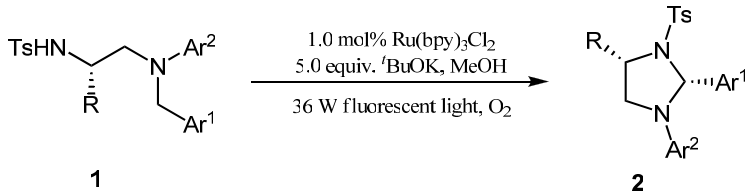
N-(3-(benzyl(phenyl)amino)propyl)-4-methylbenzenesulfonamide (1o)



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.69 (d, *J* = 8.3 Hz, 2H), 7.28 – 7.10 (m, 9H), 6.71 – 6.60 (m, 3H), 4.92 (t, *J* = 6.1 Hz, 1H), 4.44 (s, 2H), 3.46 – 3.30 (m, 2H), 2.94 (q, *J* = 6.5 Hz, 2H), 2.39 (s, 3H), 1.80 – 1.71 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 148.10, 143.40, 138.53, 136.41, 129.67, 129.19, 128.47, 126.98, 126.75, 126.55, 116.63, 112.62, 54.80, 48.19, 41.11, 26.90, 21.48. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 395.1793, measured 395.1756.

4. General Procedure and Spectral Data of Products

4.1 General procedure

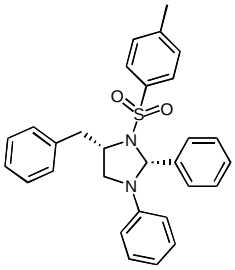


1 2

To a 10 mL flask equipped with a magnetic stir bar was added substrates **1** (0.2 mmol), 1.0 mol % $Ru(bpy)_3Cl_2$ (1.28 mg, 0.002 mmol), ^{t}BuOK (112 mg, 1.00 mmol) and MeOH (4.0 mL). After this solution was stirred under the condition of O_2 balloon at a distance of ～10 cm from a 36w fluorescent lamp at room temperature. Upon the completion of reaction monitored by TLC, 1.0 mL DCM was added to dissolve the generated solid and continued stirring to the mentioned time. Then the solvent was removed under reduced pressure. The crude product was purified by flash chromatography on silica gel (silica: 200~300; eluant: petroleum ether/ ethyl acetate (10:1~5:1)) to provide pure product **2**.

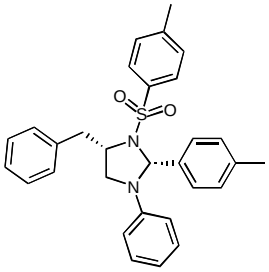
4.2 Spectral Data of Products

(2*R*,4*S*)-4-benzyl-1,2-diphenyl-3-tosylimidazolidine (2a)



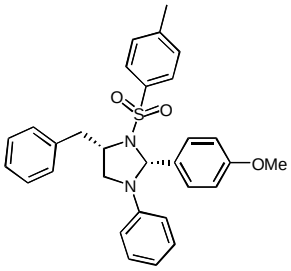
Yield: 92%, white solid, **diastereomer ratio:** 10:1. $[\alpha]_D^{20}$ = -42.23 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (600 MHz, $CDCl_3$) δ (ppm) 7.58 (dd, *J* = 22.5, 7.8 Hz, 4H), 7.42 – 7.33 (m, 3H), 7.25 – 6.93 (m, 9H), 6.74 (t, *J* = 7.2 Hz, 1H), 6.37 – 6.23 (m, 3H), 4.29 (dd, *J* = 16.1, 8.4 Hz, 1H), 3.27 (d, *J* = 9.2 Hz, 1H), 2.99 – 2.82 (m, 2H), 2.53 (dd, *J* = 13.7, 9.8 Hz, 1H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 145.90, 143.97, 139.84, 137.37, 134.45, 129.61, 129.20, 128.94, 128.51, 128.45, 128.18, 127.35, 127.12, 126.57, 117.91, 112.59, 77.32, 60.81, 50.75, 41.55, 21.38. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 469.1950, measured 469.1959.

(2*R*,4*S*)-4-benzyl-1-phenyl-2-p-tolyl-3-tosylimidazolidine (2b)



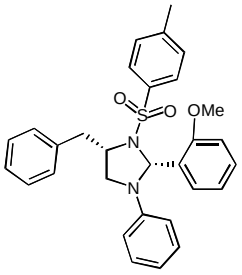
Yield: 93%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -39.11 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (600 MHz, $CDCl_3$) δ (ppm) 7.30 (t, *J* = 7.2 Hz, 2H), 7.26 – 7.19 (m, 5H), 7.08 (t, *J* = 7.4 Hz, 4H), 6.96 (d, *J* = 7.8 Hz, 2H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.65 (t, *J* = 7.2 Hz, 1H), 6.38 (d, *J* = 8.0 Hz, 2H), 6.22 (s, 1H), 4.30 (d, *J* = 4.6 Hz, 1H), 3.67 (d, *J* = 12.3 Hz, 1H), 3.58 – 3.48 (m, 1H), 3.35 (dd, *J* = 8.6, 4.0 Hz, 1H), 2.94 (t, *J* = 12.0 Hz, 1H), 2.32 (s, 3H), 2.25 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ (ppm) 144.54, 142.70, 138.22, 137.97, 134.79, 129.20, 128.94, 128.76, 128.69, 128.42, 126.92, 126.76, 117.43, 112.53, 77.00, 60.58, 51.14, 39.33, 21.39, 21.10. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 483.2106, measured 483.2109.

(2*R*,4*S*)-4-benzyl-2-(4-methoxyphenyl)-1-phenyl-3-tosylimidazolidine (2c)



Yield: 90%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -32.00 (c = 1.0, CH_2Cl_2). **^{1} H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.60 – 7.47 (m, 4H), 7.26 – 7.07 (m, 5H), 7.03 – 6.88 (m, 6H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.29 (d, *J* = 7.9 Hz, 2H), 6.22 (s, 1H), 4.34 – 4.21 (m, 1H), 3.82 (s, 3H), 3.27 (dd, *J* = 9.3, 2.2 Hz, 1H), 2.93 (dd, *J* = 13.6, 5.9 Hz, 1H), 2.84 (dd, *J* = 9.1, 7.7 Hz, 1H), 2.56 (dd, *J* = 13.6, 9.7 Hz, 1H), 2.26 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 159.43, 145.87, 143.92, 137.46, 134.54, 131.81, 129.60, 129.23, 128.92, 128.46, 128.38, 127.32, 126.57, 117.86, 113.80, 112.64, 77.14, 60.72, 55.23, 50.69, 41.61, 21.38. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 499.2055, measured 499.2036.

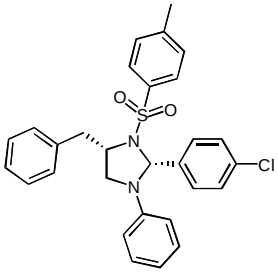
(2*R*,4*S*)-4-benzyl-2-(2-methoxyphenyl)-1-phenyl-3-tosylimidazolidine (2d)



Yield: 92%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -68.64 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.65 (d, *J* = 8.1 Hz, 2H), 7.37 – 7.27 (m, 5H), 7.17 (d, *J* = 7.1 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.91 (t, *J* = 7.2 Hz, 2H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.48 – 6.43 (m, 3H), 4.27 – 4.16 (m, 1H), 3.92

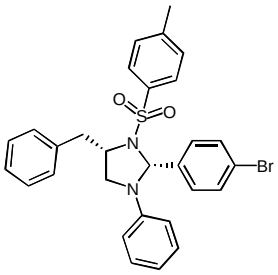
(d, *J* = 0.9 Hz, 3H), 3.45 (dd, *J* = 9.7, 4.5 Hz, 1H), 3.37 (dd, *J* = 13.3, 4.7 Hz, 1H), 3.19 – 3.11 (m, 1H), 2.95 (dd, *J* = 13.2, 10.3 Hz, 1H), 2.33 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 157.58, 145.24, 143.54, 137.80, 134.43, 129.75, 129.44, 129.34, 128.84, 128.71, 128.61, 127.83, 127.61, 126.63, 120.55, 118.23, 113.87, 111.08, 73.73, 60.48, 55.48, 51.38, 41.84, 21.45. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 499.2055, measured 499.2016.

(2*R*,4*S*)-4-benzyl-2-(4-chlorophenyl)-1-phenyl-3-tosylimidazolidine (2e)



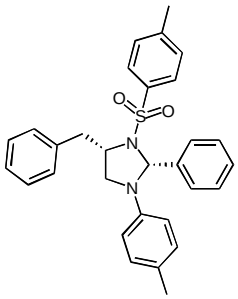
Yield: 92%, white solid, **diastereomer ratio:** >19:1. **$[\alpha]_D^{20}$** = -51.77 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (600 MHz, $CDCl_3$) δ (ppm) 7.30 (t, *J* = 7.2 Hz, 2H), 7.25 – 7.17 (m, 5H), 7.16 – 7.06 (m, 4H), 7.06 – 6.90 (m, 4H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.36 (d, *J* = 8.2 Hz, 2H), 6.19 (s, 1H), 4.39 – 4.23 (m, 1H), 3.67 (t, *J* = 12.6 Hz, 1H), 3.54 (dd, *J* = 16.6, 10.6 Hz, 1H), 3.40 – 3.29 (m, 1H), 2.94 (t, *J* = 11.9 Hz, 1H), 2.33 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ (ppm) 144.13, 143.12, 137.96, 137.66, 136.21, 134.29, 129.82, 129.06, 128.68, 128.42, 128.33, 128.20, 126.67, 117.75, 112.51, 76.23, 60.78, 51.06, 39.30, 21.39. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 503.1560, measured 503.1563.

(2*R*,4*S*)-4-benzyl-2-(4-bromophenyl)-1-phenyl-3-tosylimidazolidine (2f)



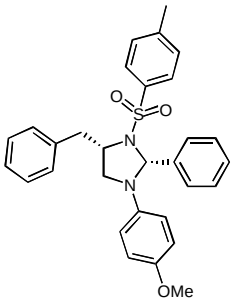
Yield: 92%, white solid, **diastereomer ratio:** 8:1. **$[\alpha]_D^{20}$** = -45.07 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (600 MHz, $CDCl_3$) δ (ppm) 7.31 (t, *J* = 7.4 Hz, 2H), 7.24 – 7.07 (m, 11H), 6.96 (d, *J* = 8.1 Hz, 2H), 6.66 (t, *J* = 7.3 Hz, 1H), 6.38 (d, *J* = 8.1 Hz, 2H), 6.28 (s, 1H), 4.32 – 4.26 (m, 1H), 3.68 (dd, *J* = 13.1, 3.0 Hz, 1H), 3.53 (dd, *J* = 8.9, 6.1 Hz, 1H), 3.34 (dd, *J* = 9.1, 4.7 Hz, 1H), 2.99 – 2.91 (m, 1H), 2.30 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ (ppm) 144.39, 142.83, 137.85, 137.68, 129.13, 129.07, 128.96, 128.67, 128.44, 128.36, 128.13, 126.75, 117.45, 112.41, 77.21, 60.46, 51.16, 39.18, 21.39. **HRMS:** m/z (ESI) calculated $[(M-Br)+H]^+$ 469.1950, measured 469.1915.

(2*R*,4*S*)-4-benzyl-2-phenyl-1-p-tolyl-3-tosylimidazolidine (2g)



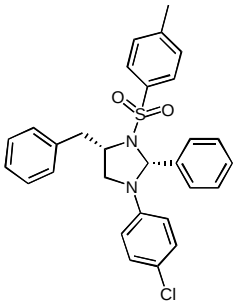
Yield: 94%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -41.55 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.66 – 7.52 (m, 4H), 7.43 – 7.31 (m, 3H), 7.26 – 7.16 (m, 3H), 7.05 – 6.88 (m, 6H), 6.23 (d, *J* = 7.6 Hz, 3H), 4.33 – 4.18 (m, 1H), 3.27 (d, *J* = 9.4 Hz, 1H), 2.94 (dd, *J* = 13.6, 5.7 Hz, 1H), 2.86 (t, *J* = 8.2 Hz, 1H), 2.56 (dd, *J* = 13.6, 9.8 Hz, 1H), 2.28 (s, 3H), 2.22 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 143.88, 140.09, 137.48, 134.56, 129.60, 129.46, 129.22, 128.47, 128.14, 127.39, 127.21, 126.56, 112.89, 77.80, 60.83, 50.99, 41.56, 21.41, 20.28. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 483.2106, measured 483.2094.

(2*R*,4*S*)-4-benzyl-1-(4-methoxyphenyl)-2-phenyl-3-tosylimidazolidine (2h)



Yield: 91%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -38.12 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.68 – 7.53 (m, 4H), 7.43 – 7.18 (m, 6H), 7.08 – 6.95 (m, 4H), 6.68 (d, *J* = 9.0 Hz, 2H), 6.27 (t, *J* = 7.9 Hz, 2H), 6.13 (s, 1H), 4.28 – 4.18 (m, 1H), 3.72 (s, 3H), 3.26 (dd, *J* = 9.4, 2.6 Hz, 1H), 2.98 (dd, *J* = 13.6, 5.7 Hz, 1H), 2.83 (dd, *J* = 9.3, 7.3 Hz, 1H), 2.60 (dd, *J* = 13.5, 9.8 Hz, 1H), 2.29 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 152.40, 143.88, 140.65, 140.16, 137.52, 134.58, 129.58, 129.21, 128.47, 128.17, 127.40, 127.28, 126.56, 114.41, 114.22, 78.64, 60.90, 55.57, 51.48, 41.50, 21.42. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 499.2055, measured 499.1972.

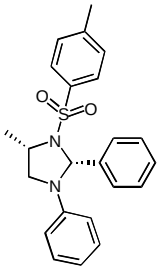
(2*R*,4*S*)-4-benzyl-1-(4-chlorophenyl)-2-phenyl-3-tosylimidazolidine (2i)



Yield: 94%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -34.22 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.31 (dd, *J* = 11.2, 4.3 Hz, 2H), 7.25 – 7.15 (m, 8H), 7.11 (dd, *J* = 8.0, 6.7 Hz, 2H), 7.05 – 7.00 (m, 2H), 6.97 (d, *J* = 8.2 Hz, 2H),

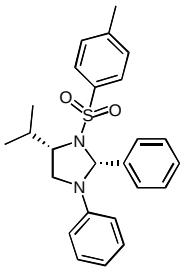
6.30 – 6.25 (m, 2H), 6.19 (s, 1H), 4.32 – 4.26(m, 1H), 3.66 (dd, *J* = 13.2, 3.2 Hz, 1H), 3.51 (dd, *J* = 9.0, 6.0 Hz, 1H), 3.30 (dd, *J* = 9.1, 4.5 Hz, 1H), 2.97 (dd, *J* = 13.1, 10.9 Hz, 1H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 142.94, 142.90, 137.84, 137.64, 137.17, 129.12, 129.09, 128.80, 128.71, 128.54, 128.41, 128.22, 126.84, 126.74, 122.35, 113.50, 77.12, 60.45, 51.28, 39.19, 21.39. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 503.1560, measured 503.1506.

(2*R*,4*S*)-4-methyl-1,2-diphenyl-3-tosylimidazolidine (2j)



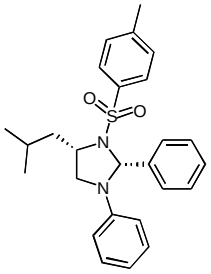
Yield: 92%, white solid, **diastereomer ratio:** >19:1. **$[\alpha]_D^{20}$** = -136.43 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.37 (dd, *J* = 7.4, 1.8 Hz, 2H), 7.30 – 7.18 (m, 5H), 7.13 (t, *J* = 7.9 Hz, 2H), 6.95 (d, *J* = 8.2 Hz, 2H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 8.2 Hz, 2H), 6.33 (s, 1H), 4.13 – 3.99 (m, 1H), 3.71 (dd, *J* = 8.4, 6.1 Hz, 1H), 3.01 (t, *J* = 8.1 Hz, 1H), 2.29 (s, 3H), 1.57 (d, *J* = 6.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 144.98, 142.92, 138.50, 137.69, 129.15, 129.04, 128.37, 128.24, 128.04, 126.94, 117.51, 112.17, 77.91, 54.32, 21.36, 17.38. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 393.1637, measured 393.1600.

(2*R*,4*S*)-4-isopropyl-1,2-diphenyl-3-tosylimidazolidine (2k)



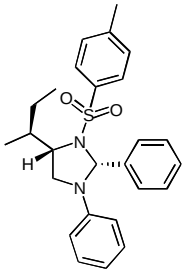
Yield: 89%, white solid, **diastereomer ratio:** 3:1. **$[\alpha]_D^{20}$** = -87.87 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.21 – 7.14 (m, 3H), 7.13 – 7.05 (m, 6H), 6.91 (d, *J* = 8.2 Hz, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 8.2 Hz, 2H), 6.23 (s, 1H), 4.02 – 3.94 (m, 1H), 3.67 (dd, *J* = 9.2, 7.2 Hz, 1H), 3.41 (dd, *J* = 9.2, 4.8 Hz, 1H), 2.85 – 2.69 (m, 1H), 2.29 (s, 3H), 1.06 (d, *J* = 6.8 Hz, 3H), 0.92 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 143.70, 142.51, 137.97, 137.30, 128.96, 128.92, 128.60, 128.24, 128.06, 126.70, 117.28, 112.30, 77.95, 64.30, 47.60, 30.61, 21.36, 20.34, 16.09. HRMS: m/z (ESI) calculated $[M+H]^+$ 421.1950, measured 421.1936.

(2*R*,4*S*)-4-isobutyl-1,2-diphenyl-3-tosylimidazolidine (2l)



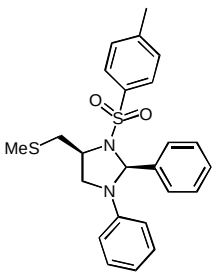
Yield: 94%, white solid, **diastereomer ratio:** >19:1. $[\alpha]_D^{20}$ = -87.09 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.55 (dd, *J* = 15.9, 7.5 Hz, 4H), 7.37 – 7.28 (m, 3H), 7.12 (t, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.1 Hz, 2H), 6.73 (t, *J* = 7.3 Hz, 1H), 6.31 – 6.20 (m, 3H), 4.24 – 4.10 (m, 1H), 3.03 (dd, *J* = 8.7, 1.6 Hz, 1H), 2.79 (t, *J* = 8.1 Hz, 1H), 2.27 (s, 3H), 1.67 – 1.55 (m, 1H), 1.32 – 1.24 (m, 1H), 1.04 – 0.95 (m, 1H), 0.89 (d, *J* = 6.5 Hz, 3H), 0.53 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 146.12, 143.97, 139.85, 134.58, 129.57, 128.90, 128.26, 127.91, 127.31, 126.81, 117.58, 112.02, 77.02, 57.78, 52.14, 44.27, 24.37, 22.65, 21.46, 21.40. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 435.2106, measured 435.2091.

(2*R*,4*S*)-4-sec-butyl-1,2-diphenyl-3-tosylimidazolidine (2m)



Yield: 90%, white solid, **diastereomer ratio:** 2:1. $[\alpha]_D^{20}$ = -69.42 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.17 (t, *J* = 8.7 Hz, 3H), 7.12 – 7.03 (m, 6H), 6.91 (d, *J* = 8.1 Hz, 2H), 6.65 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 8.1 Hz, 2H), 6.23 (s, 1H), 4.14 – 4.04 (m, 1H), 3.68 (dd, *J* = 8.9, 7.4 Hz, 1H), 3.41 (dd, *J* = 9.1, 4.8 Hz, 1H), 2.60 – 2.47 (m, 1H), 2.29 (s, 3H), 1.58 – 1.50 (m, 1H), 1.29 – 1.15 (m, 1H), 1.02 (t, *J* = 7.3 Hz, 3H), 0.92 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 143.68, 142.49, 138.10, 137.19, 128.97, 128.91, 128.66, 128.23, 128.07, 126.74, 117.29, 112.33, 78.03, 62.86, 47.75, 37.41, 27.46, 21.36, 13.19, 12.02. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 435.2106, measured 435.2081.

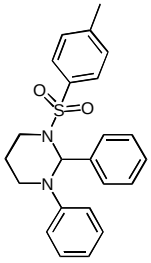
(2*R*,4*R*)-4-(methylthiomethyl)-1,2-diphenyl-3-tosylimidazolidine (2n)



Yield: 45%, white solid, **diastereomer ratio:** 3:1. $[\alpha]_D^{20}$ = -11.21 (c = 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.19 – 7.05 (m, 9H), 6.93 (d, *J* = 7.9 Hz, 2H), 6.67 (t, *J* = 7.1 Hz, 1H), 6.47 (d, *J* = 8.1 Hz, 2H), 6.23 (d, *J* = 1.3 Hz, 1H), 4.36 – 4.23 (m, 1H), 3.94 (dd, J = 9.3, 6.1 Hz, 1H), 3.69 (dd, *J* = 9.4, 1.7 Hz, 1H),

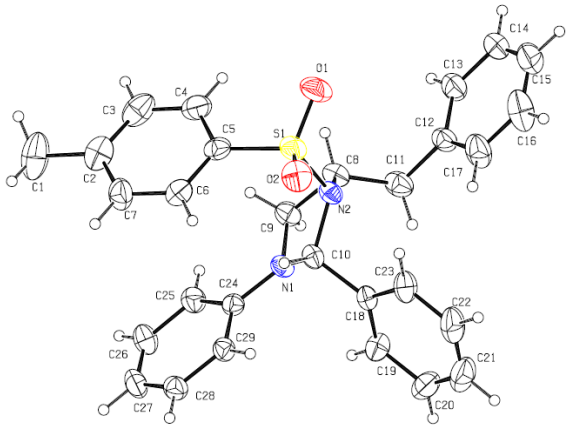
3.40 (d, J = 13.2 Hz, 1H), 2.91 – 2.78 (m, 1H), 2.30 (s, 3H), 2.23 (d, J = 1.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 149.50, 142.76, 137.74, 137.21, 129.37, 129.27, 128.95, 127.97, 127.28, 127.01, 118.82, 114.62, 72.86, 40.68, 40.55, 21.41, 21.29. HRMS: m/z (ESI) calculated $[M+H]^+$ 439.1514, measured 439.1504.

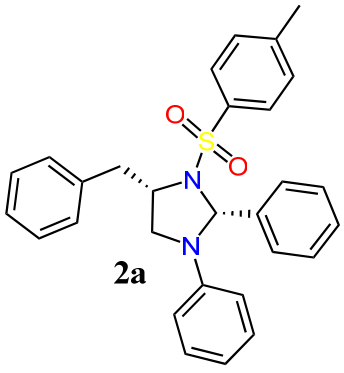
1,2-diphenyl-3-tosylhexahydropyrimidine (2o)



Yield: 61%, white solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.56 (d, J = 8.0 Hz, 2H), 7.39 (m, 5H), 7.25 – 7.19 (m, 2H), 6.99 – 6.83 (m, 4H), 6.71 (d, J = 8.2 Hz, 2H), 3.85 – 3.74 (m, 1H), 3.38 – 3.18 (m, 3H), 2.34 (s, 3H), 1.57 – 1.46 (m, 1H), 1.28 – 1.19 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 149.50, 142.76, 137.74, 137.21, 129.37, 129.27, 128.95, 127.97, 127.28, 127.01, 118.82, 114.62, 72.86, 40.68, 40.55, 21.41, 21.29. **HRMS:** m/z (ESI) calculated $[M+H]^+$ 393.1637, measured 393.1634.

5. X-Ray Structure of Product 2a



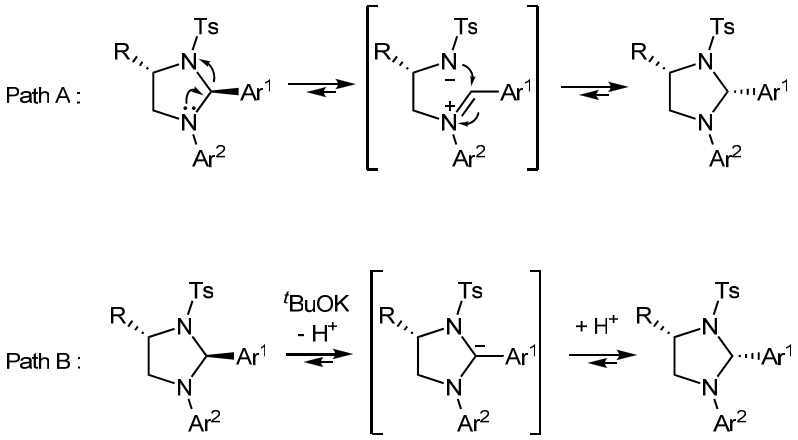


2a

Crystal data for 2a: $C_{29}H_{28}N_2O_2S$, M = 468.59, orthorhombic, $P2(1)2(1)2(1)$, a = 7.9943(10) Å, b = 16.668(2) Å, c = 18.837(2) Å, α = 90°, β = 90°, γ = 90°, V = 2510.0(5) Å3, Z = 4, T = 298(2), $F000$ = 992, final R indices [$I>2\sigma(I)$]: R_1 = 0.0606, wR_2 = 0.0863, R indices (all data): R_1 = 0.0964, wR_2 = 0.0954.

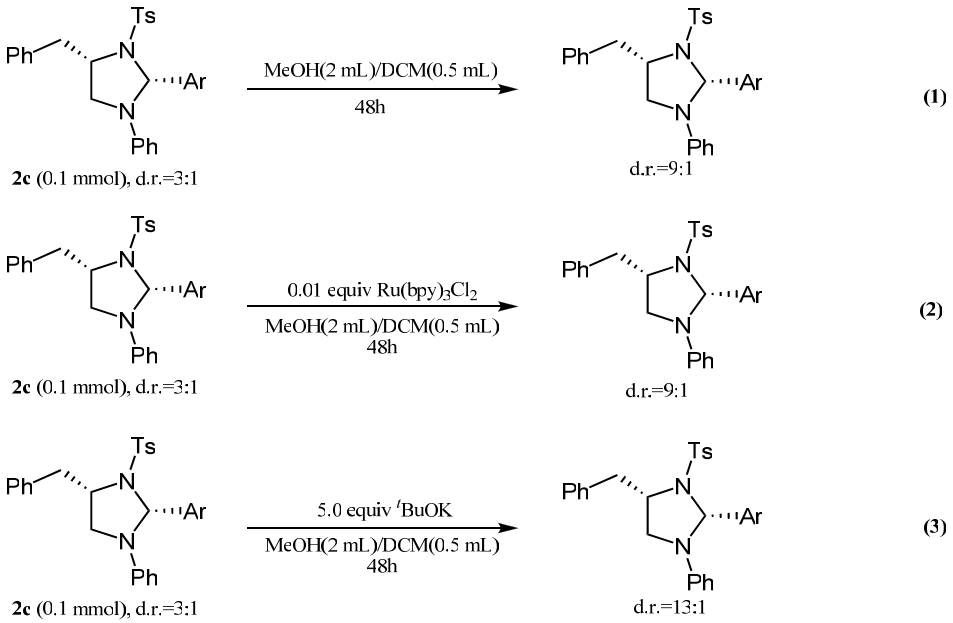
6. Mechanism study of the epimerization of the product

For this photoredox catalytic reaction, the thermodynamically more stable product could be preferentially formed when the reaction time was prolonged. Therefore, we proposed two possible pathways as outlined in scheme 1. In path A, the *anti*-isomer could be transformed into the thermodynamically more stable *syn*-diastereoisomer through the reversibly formed the iminium ion intermediate. On the other hand, the excess of strong base ^{t}BuOK may promote the epimerization of the minor diasteroisomer through deprotonation and protonation process (Path B)..

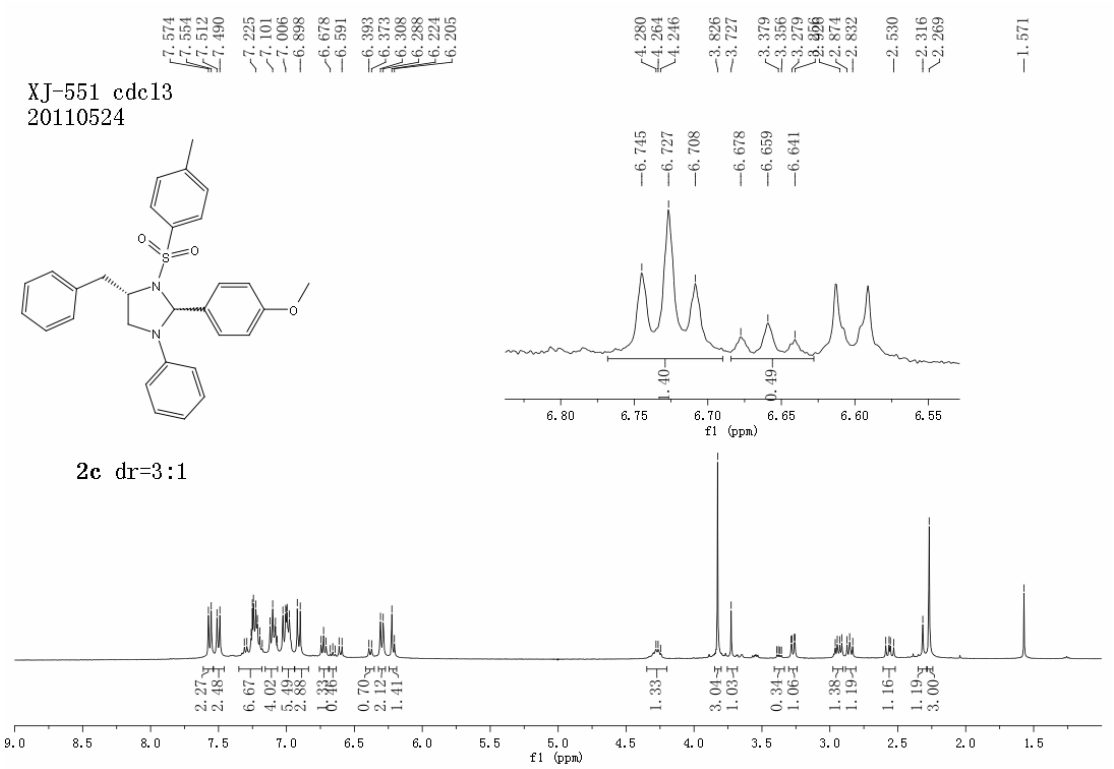


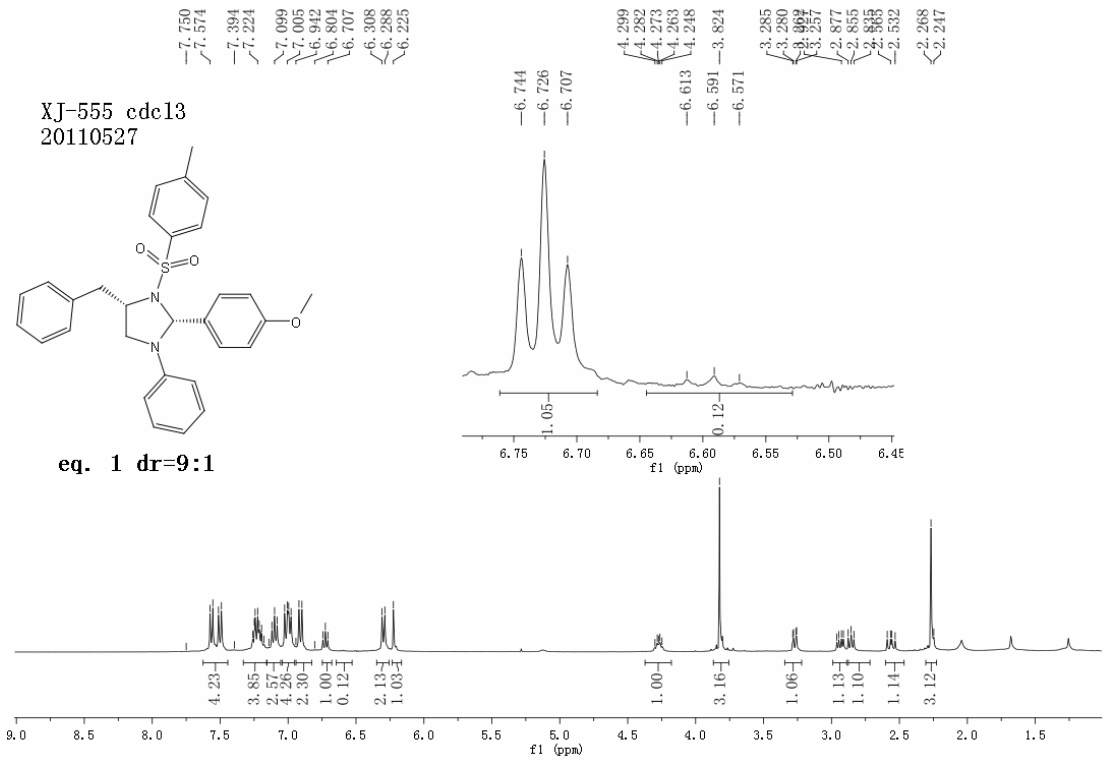
Scheme 1. Two plausible pathway of the epimerization of the product

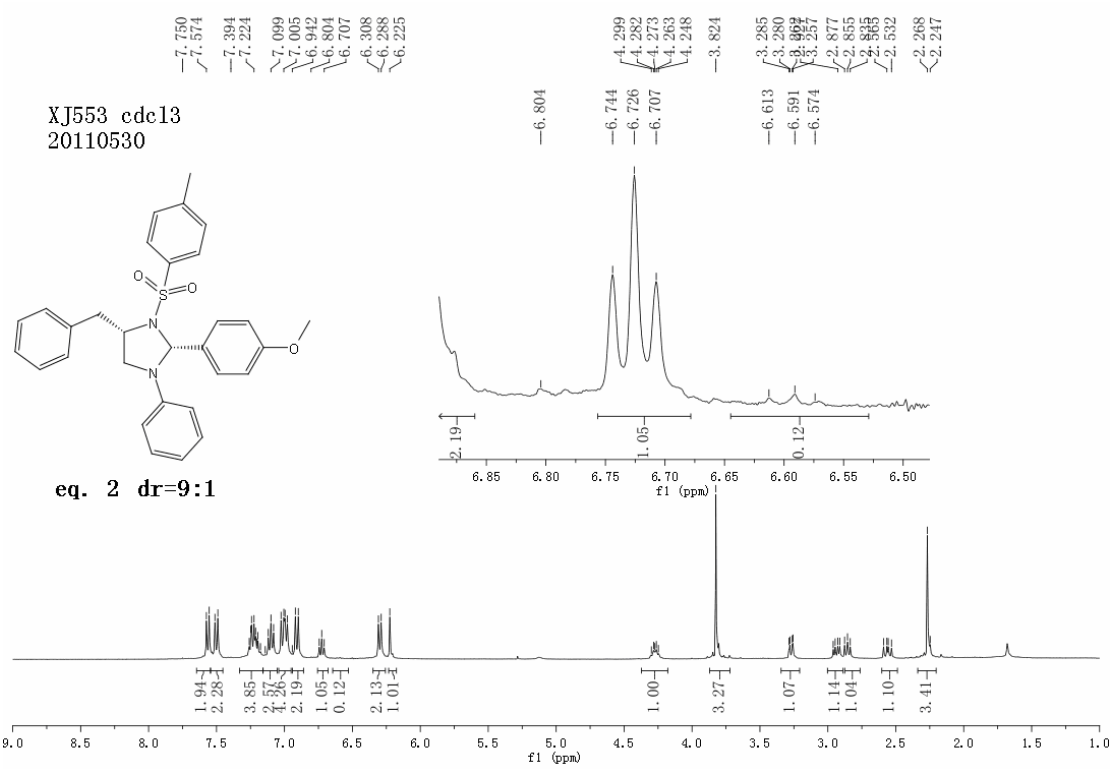
To gain some insights into this process, we carried out some control experiments. As shown in Scheme 2, stirring of **2c** in a mixture solvent of MeOH and CH_2Cl_2 for 48 h increased the dr from 3:1 to 9:1 (eq 1). Treatment of 2c with 1 mol% of photoredox catalyst also gave the same dr value (eq 2). Instead, the use of 5 equivalents of ^{t}BuOK resulted in 13:1 dr, which indicated that the path B was probably more favorable than path A (eq 3).

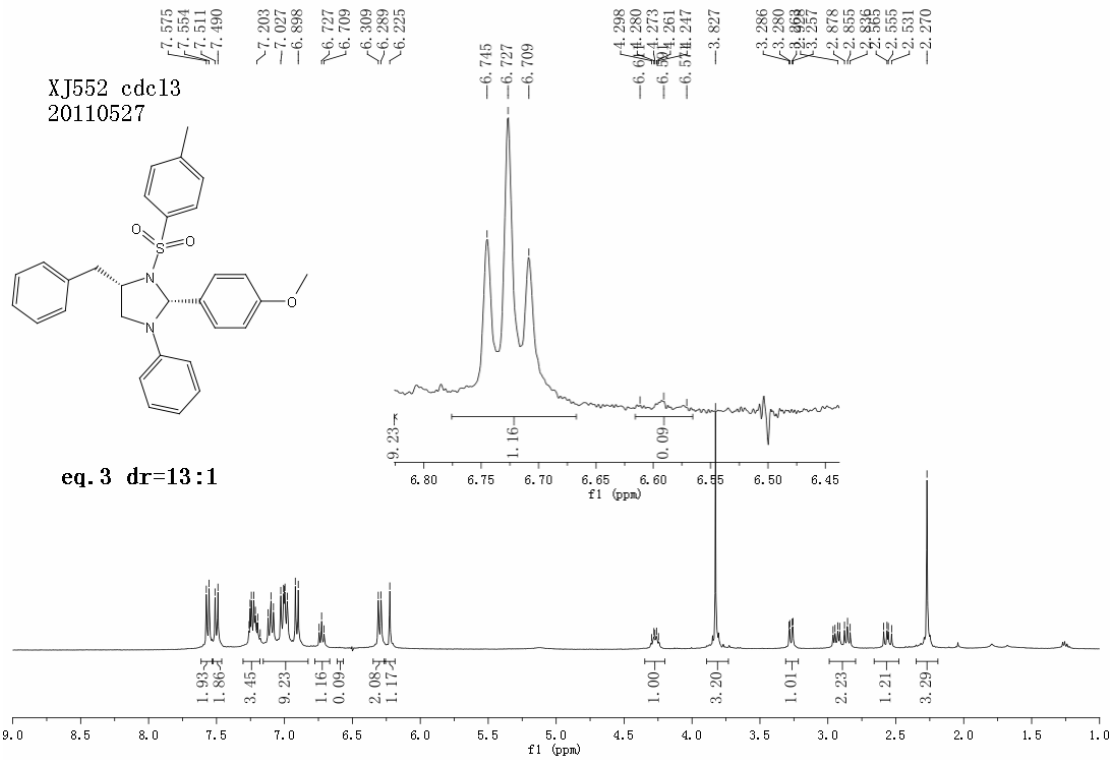


Scheme 2. Control experiments

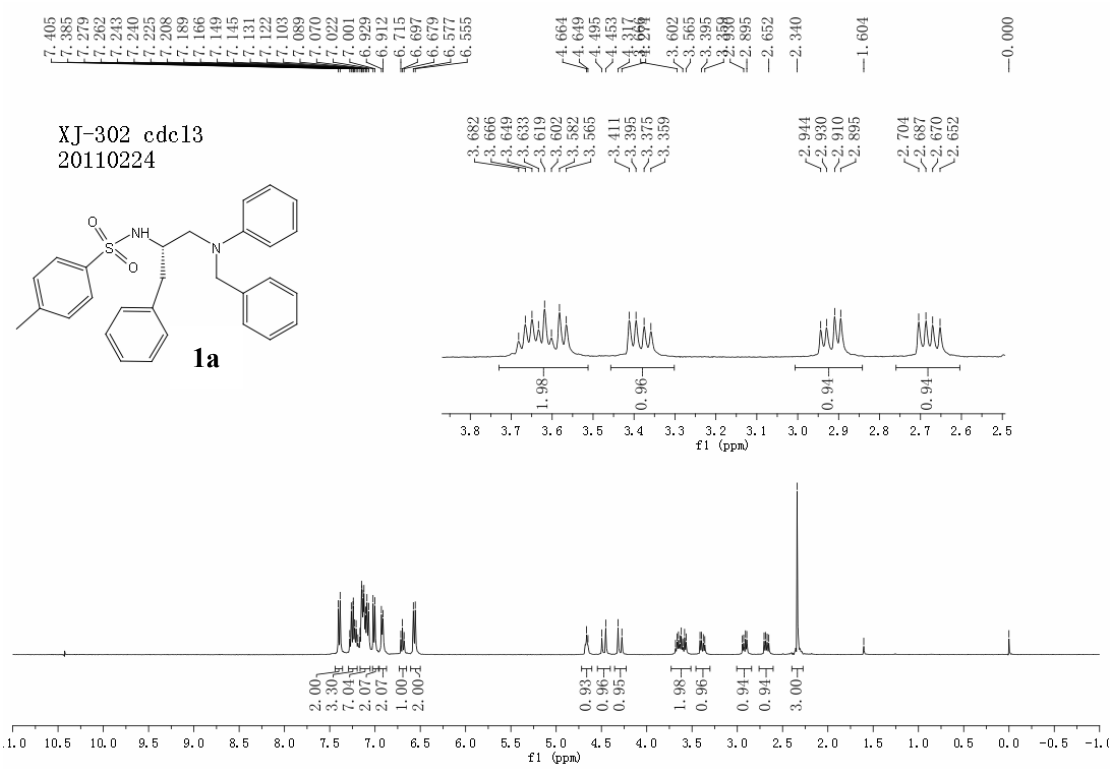

XJ-551 cdcl3
20110524
2c dr=3:1
f1 (ppm)

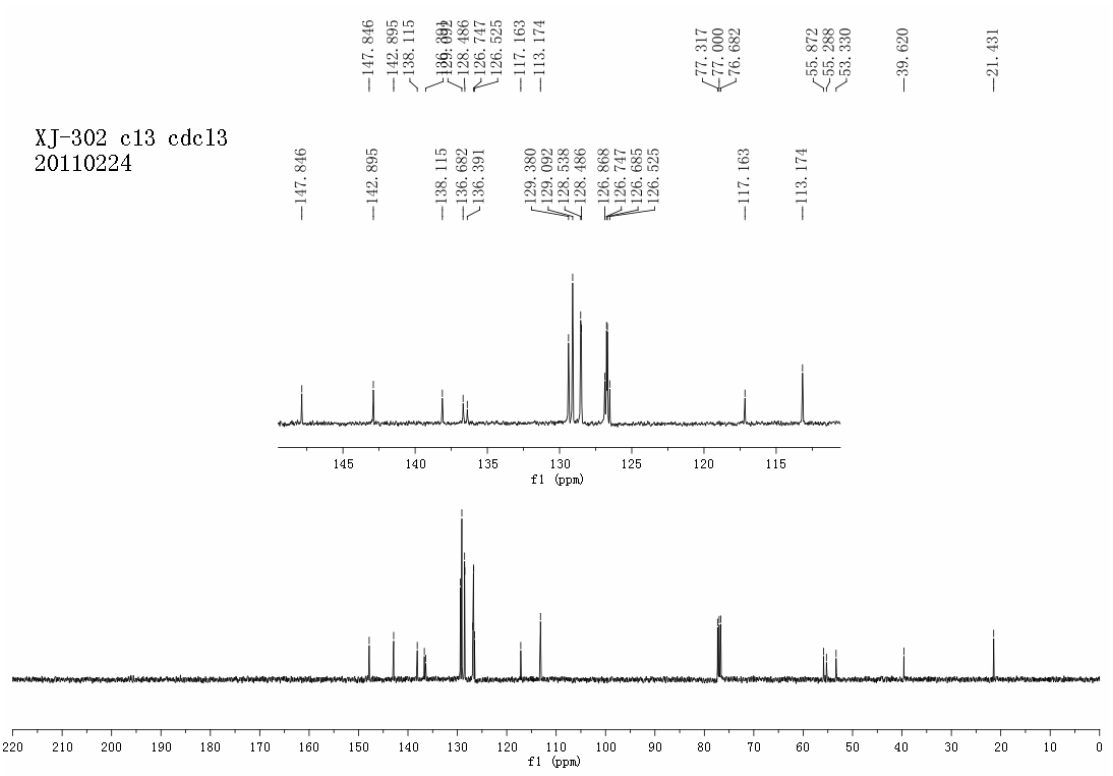

XJ-555 cdcl3
20110527
eq. 1 dr=9:1
f1 (ppm)


XJ553 cdc13
20110530
eq. 2 dr=9:1
f1 (ppm)


XJ552 cdc13
20110527
eq. 3 dr=13:1
f1 (ppm)

7. Copies of ^{1}H NMR, ^{13}C NMR and HRMS Spectrums





Analysis Info

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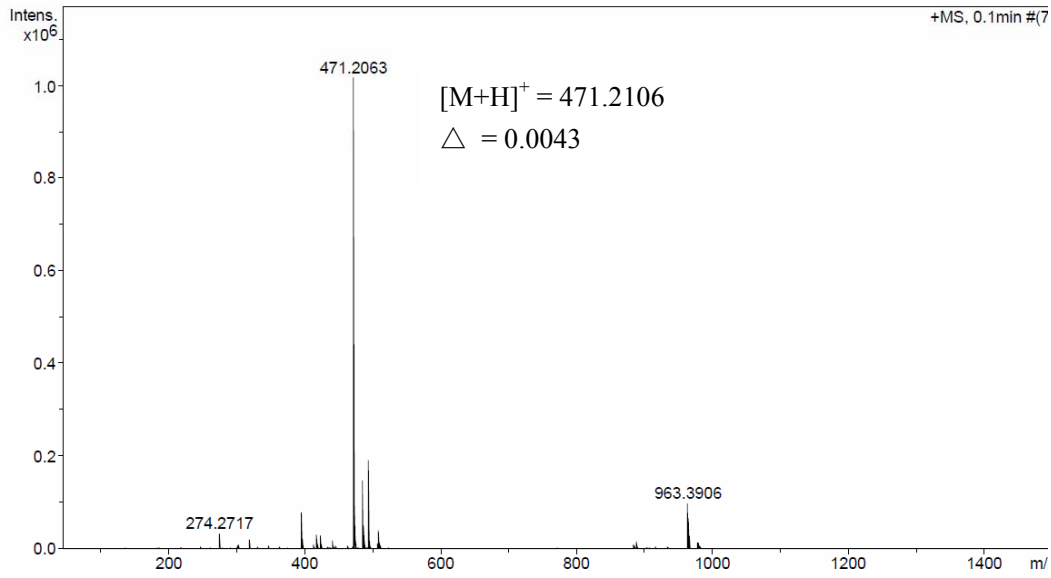
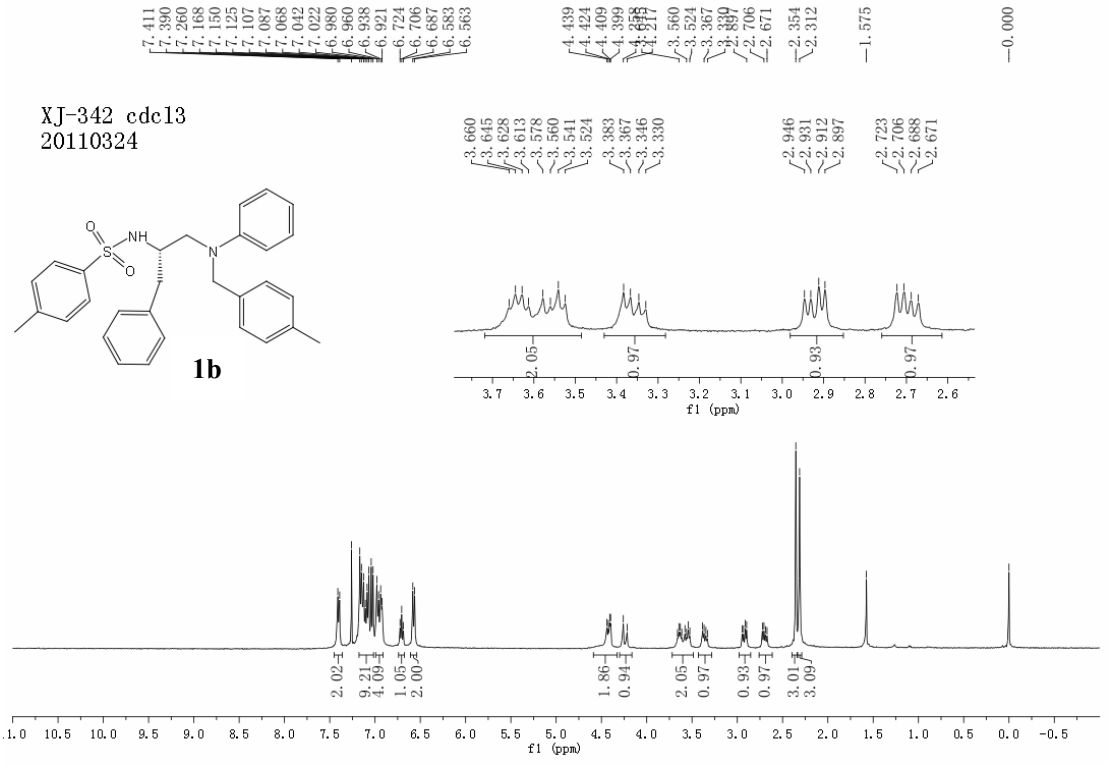
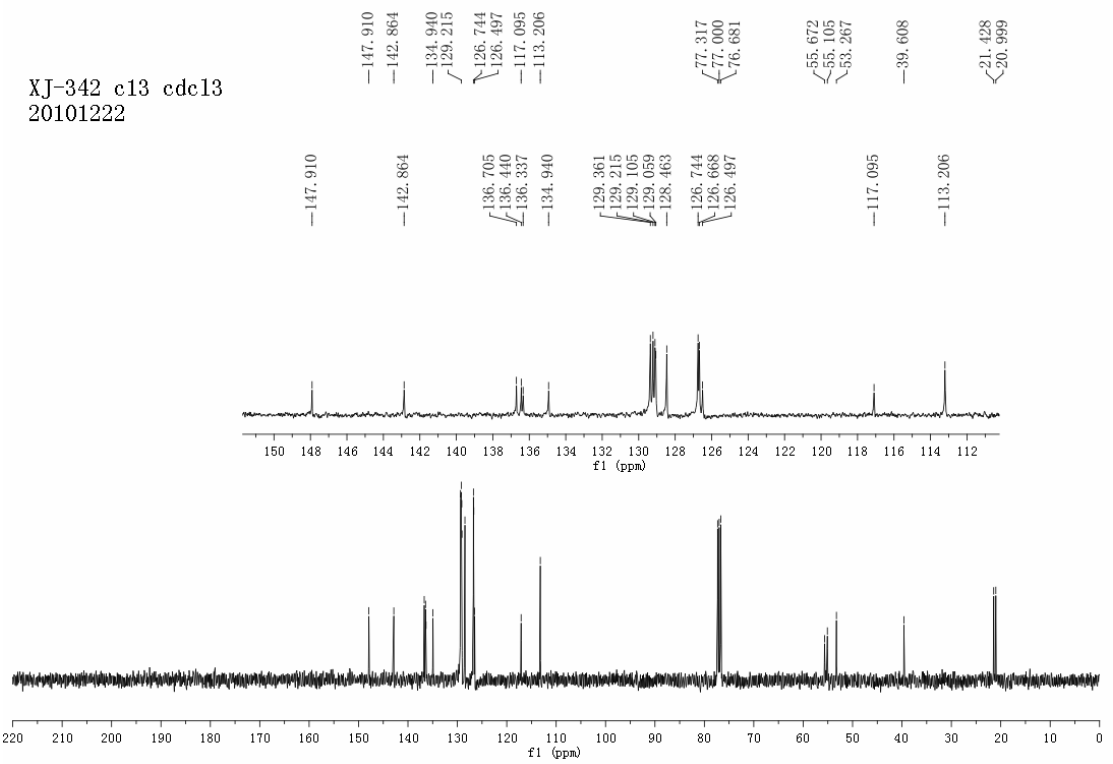
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-302	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste







Analysis Info

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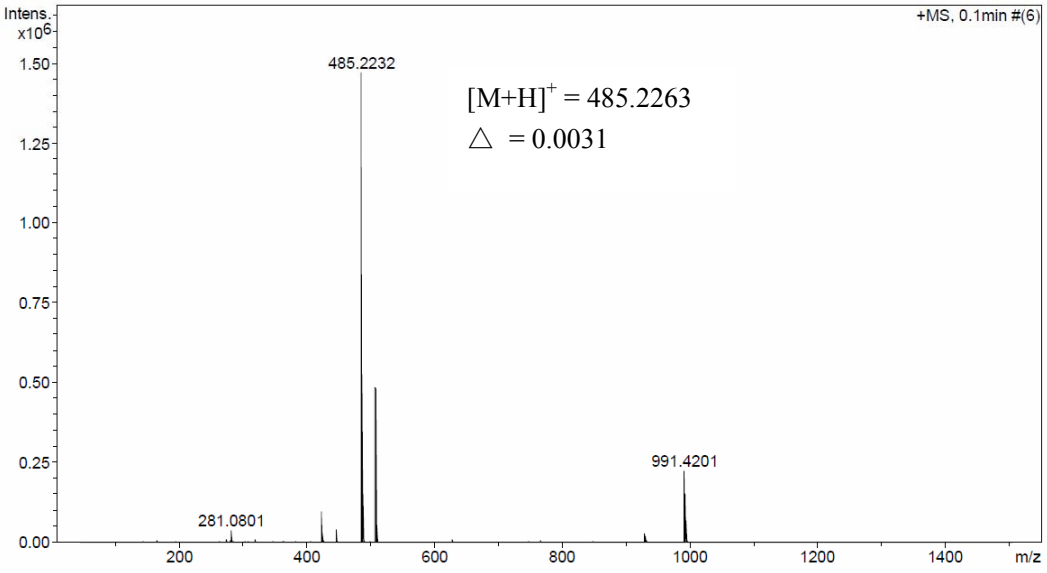
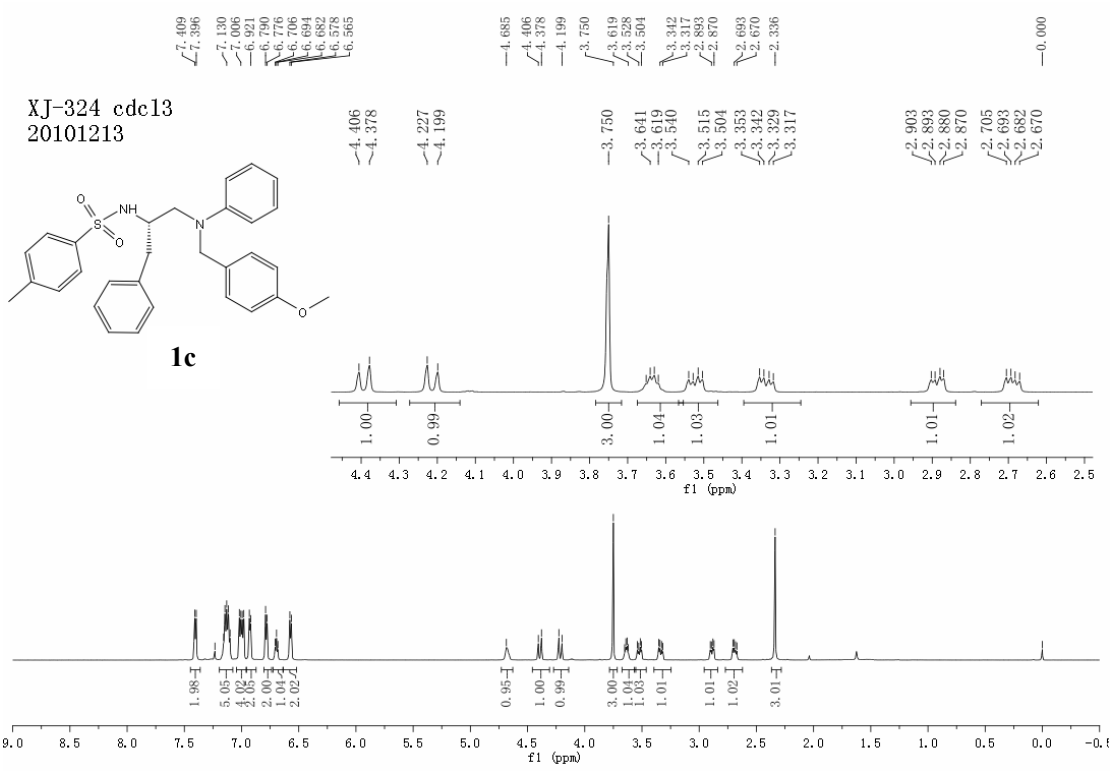
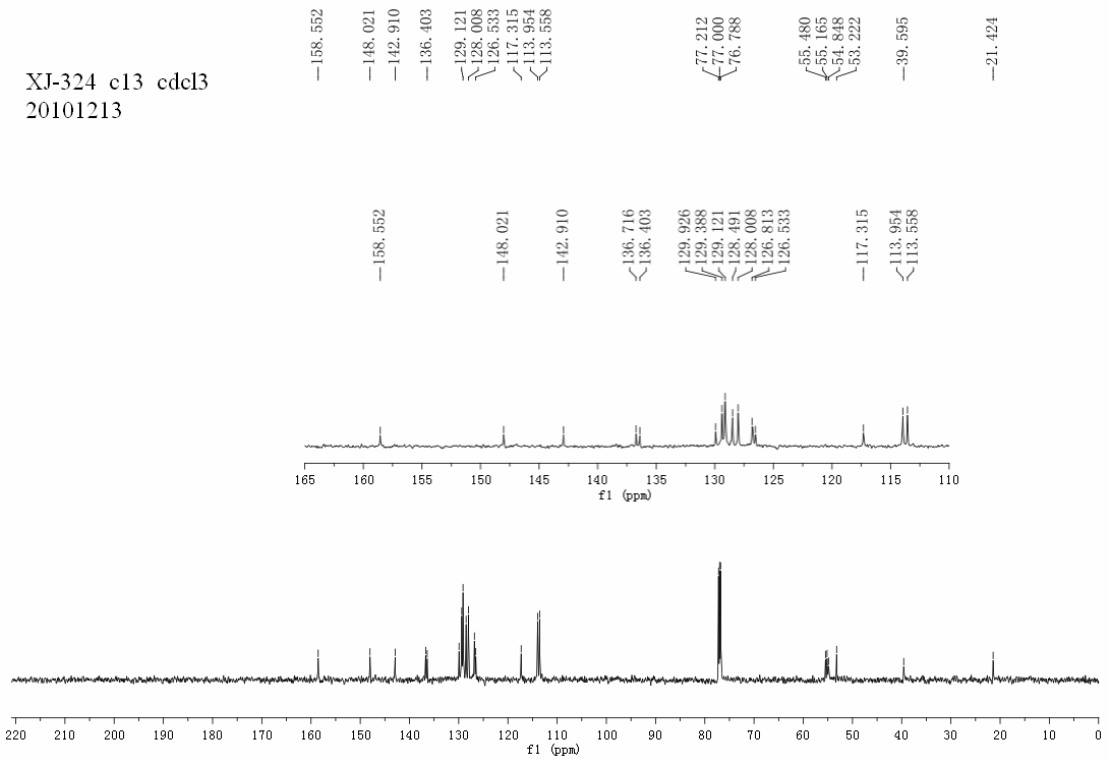
Sample Name	xj-342	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




XJ-324 cdcl3
20101213
1c
f1 (ppm)

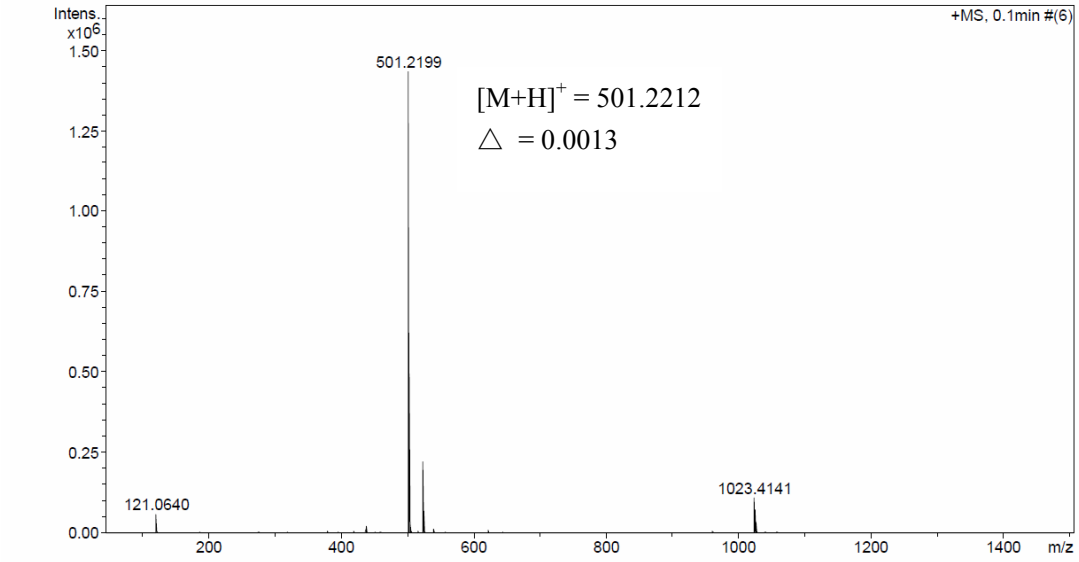

XJ-324 c13 cdcl3
20101213
f1 (ppm)

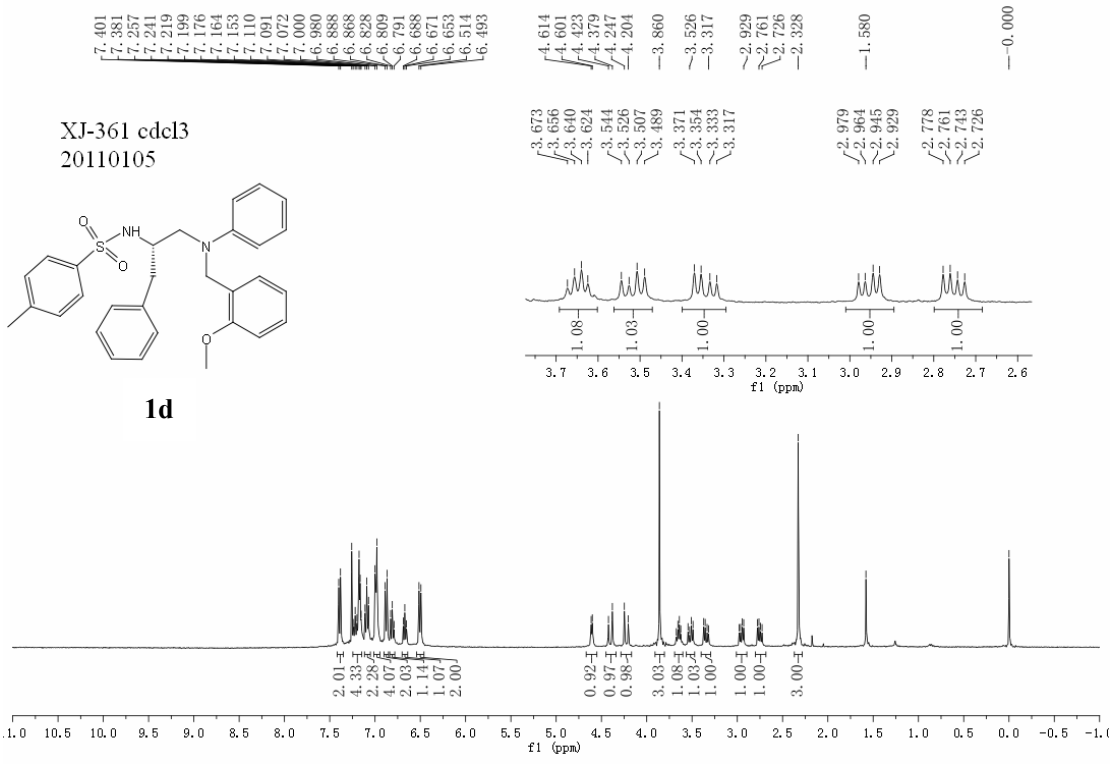
Analysis Info

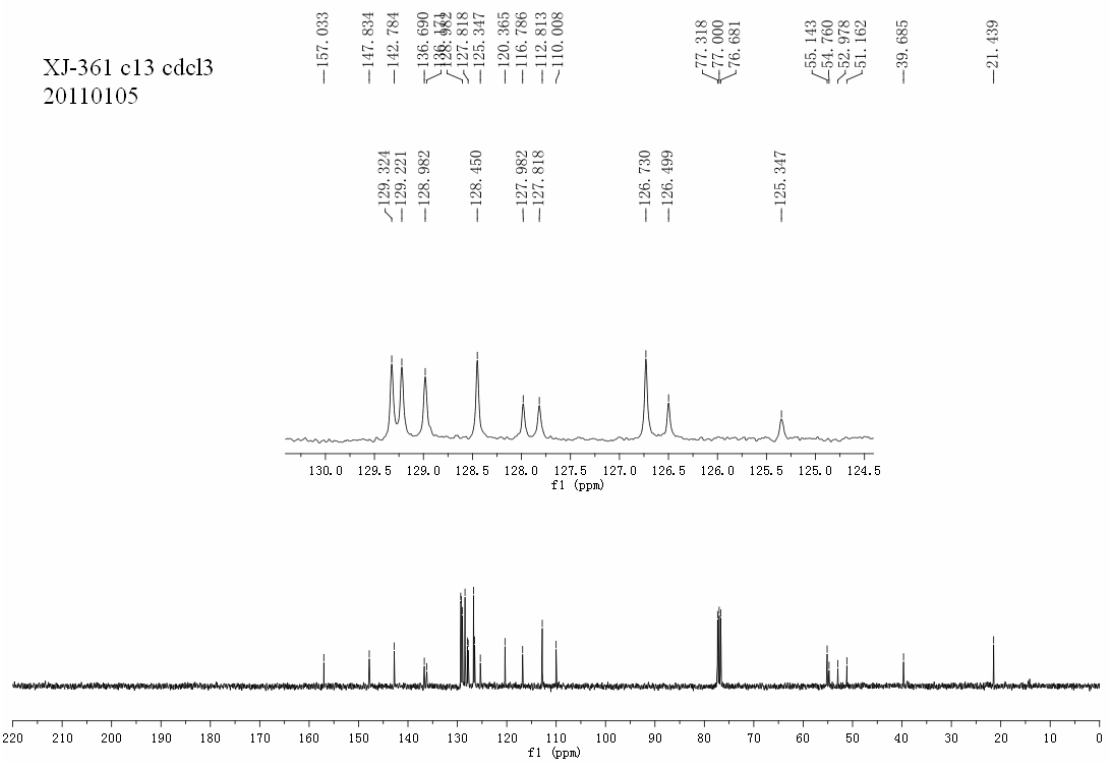
Analysis Name	D:\Data\MS\wj\0607\ysq000014.d	Acquisition Date	6/7/2011 10:50:49 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-324	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





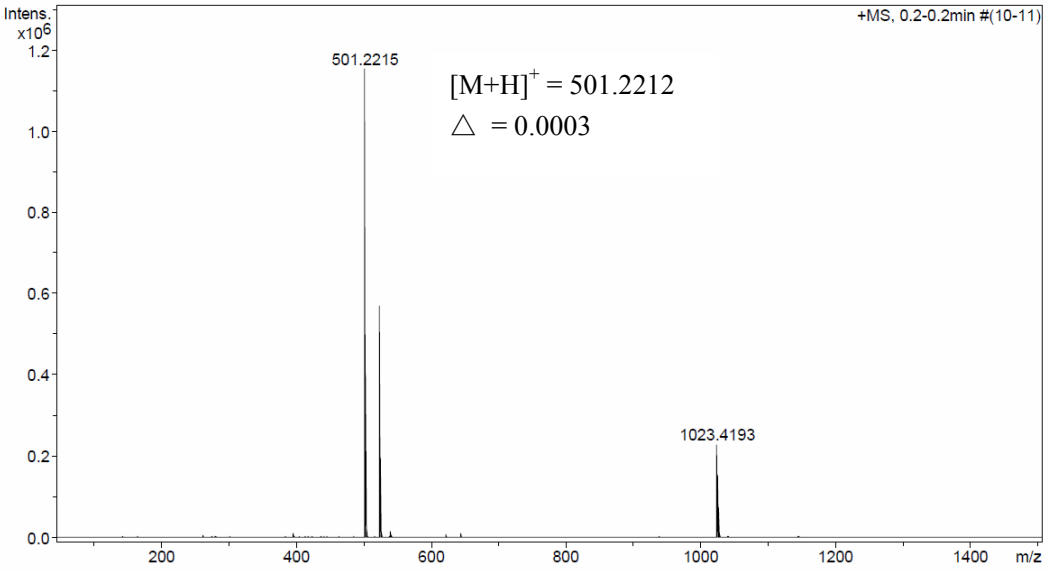


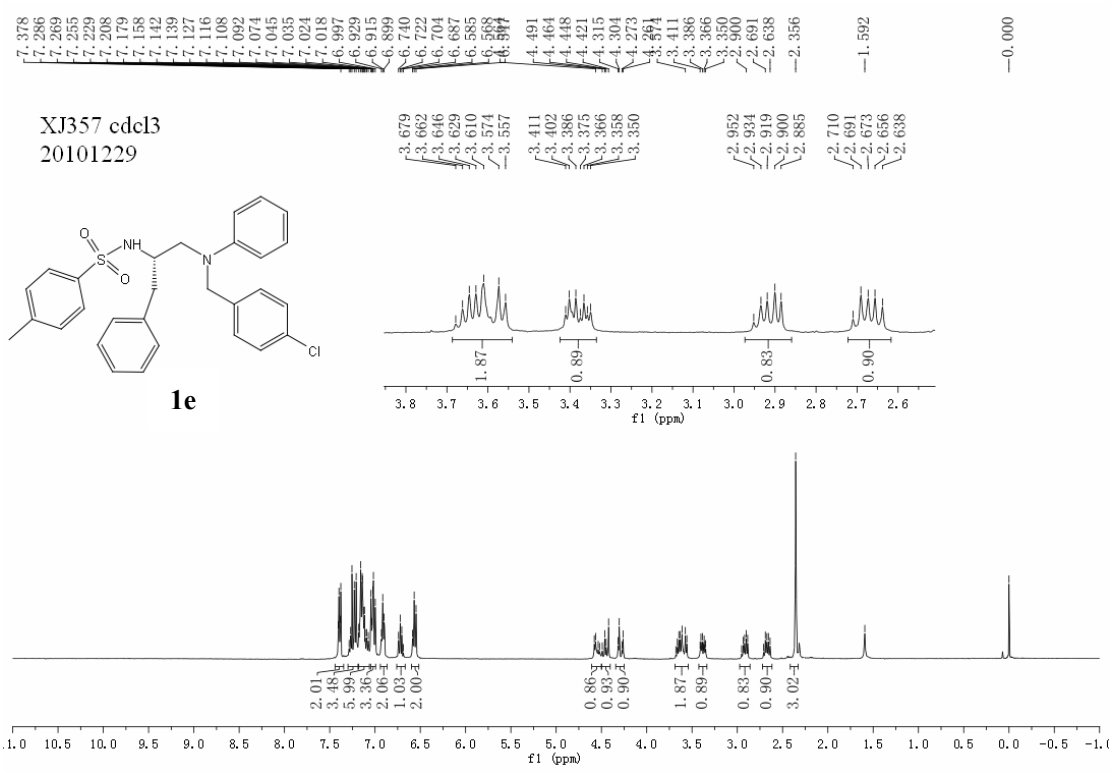
Analysis Info

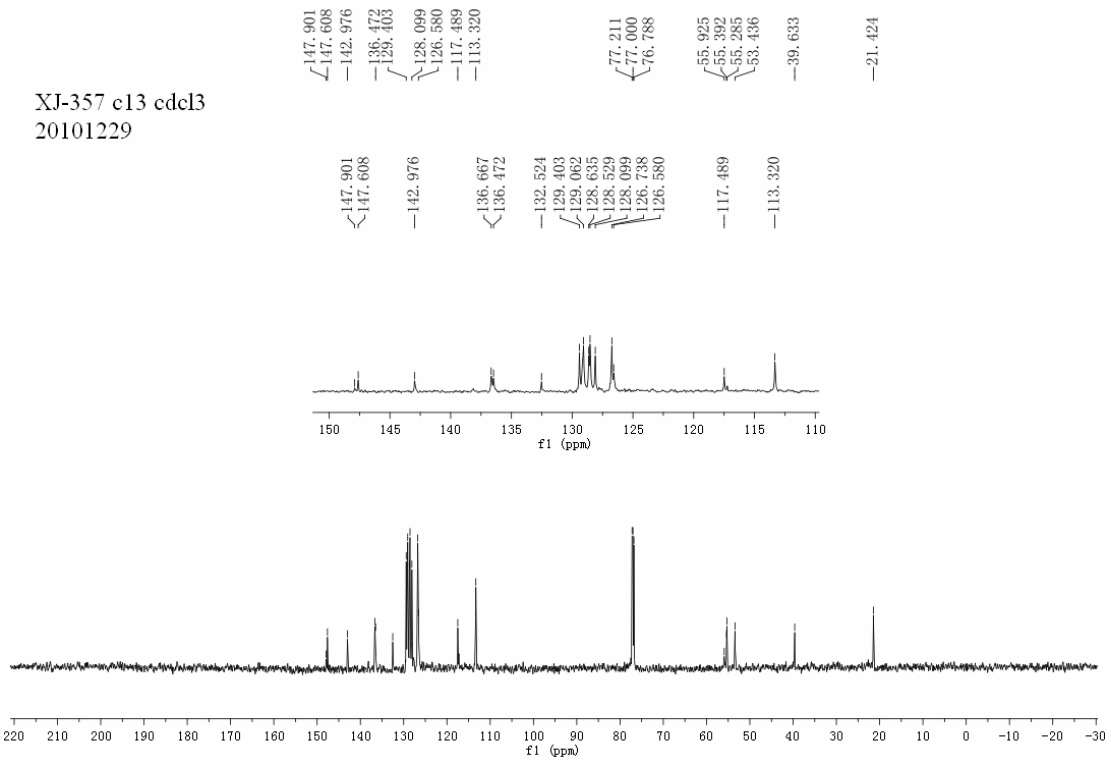
Analysis Name	D:\Data\MS\wj\0607\ysq000010.d	Acquisition Date	6/7/2011 10:25:05 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-361	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




XJ357 cdcl3
20101229
1e
f1 (ppm)

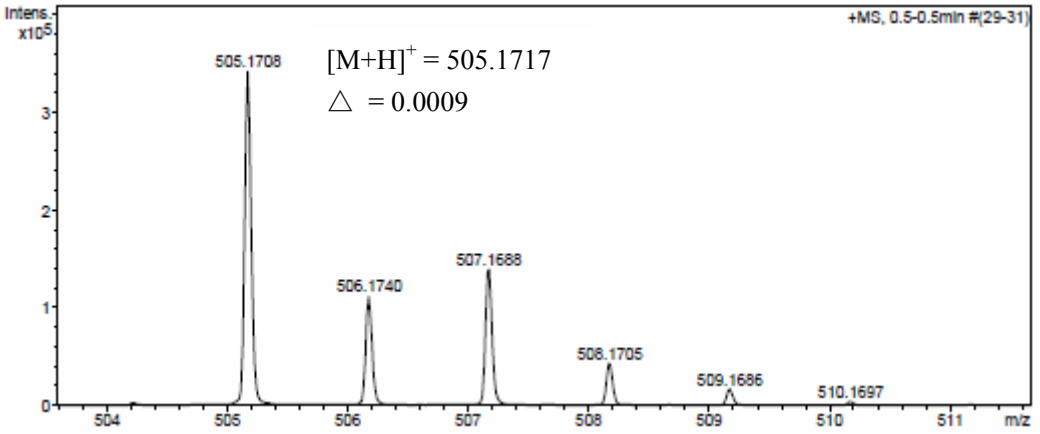

XJ-357 c13 cdcl3
20101229
f1 (ppm)

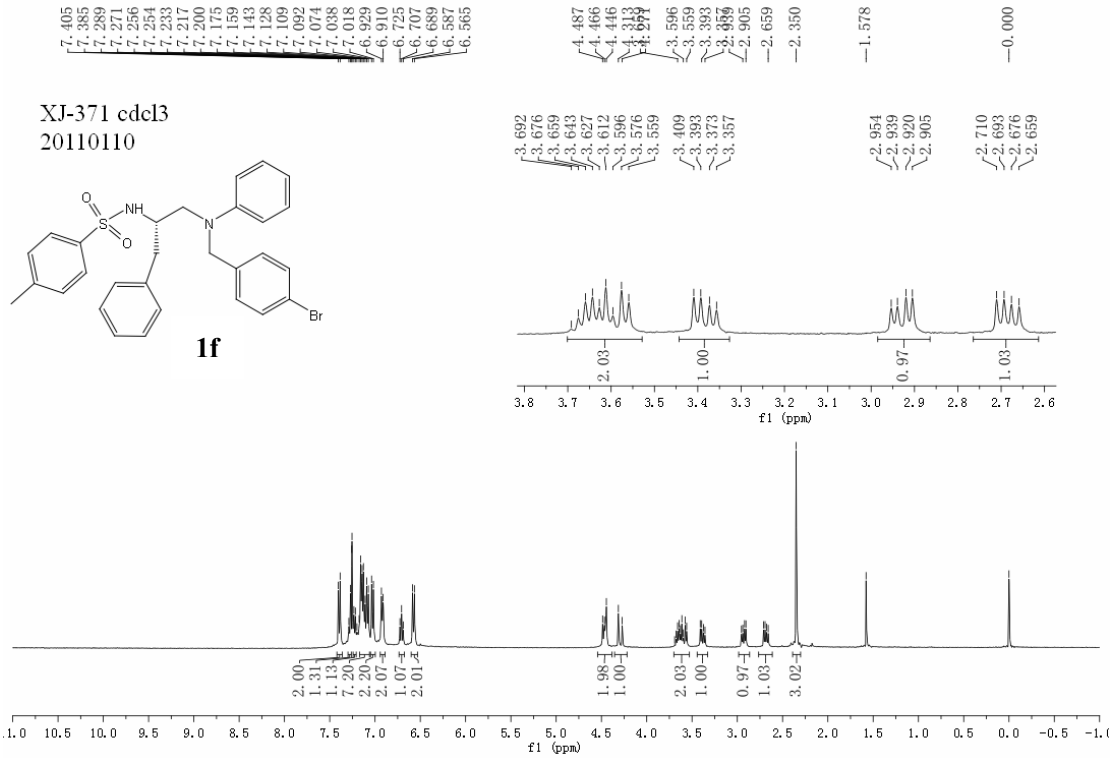
Analysis Info

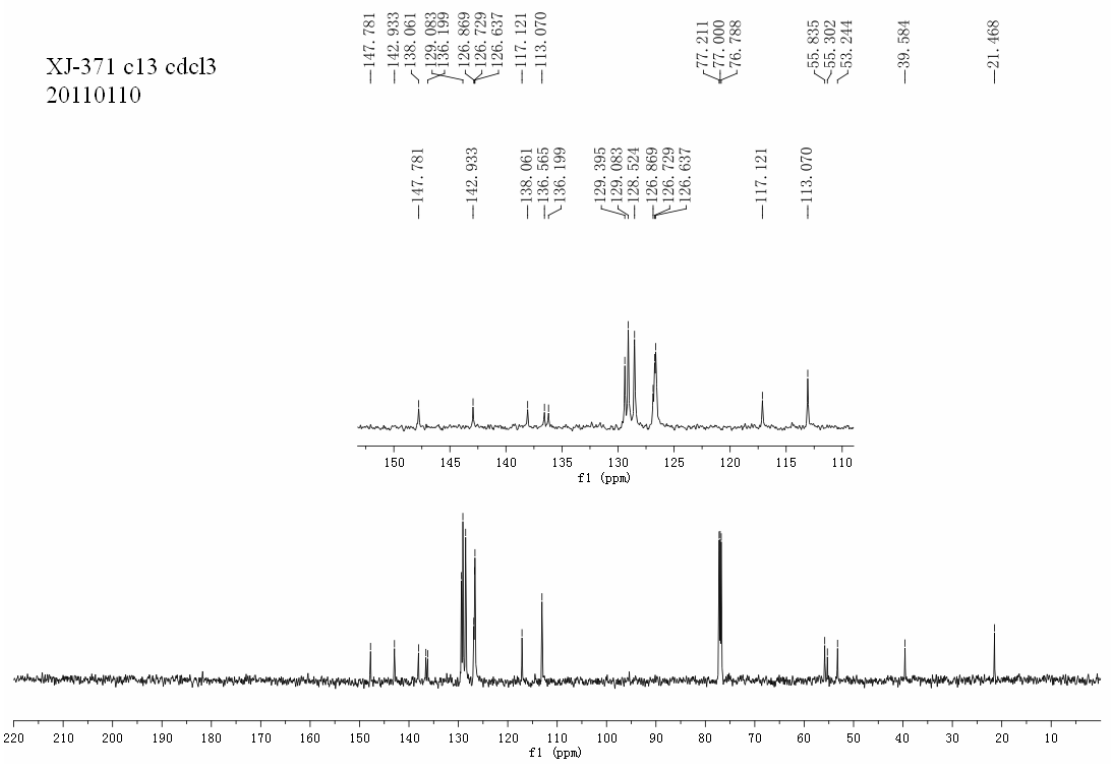
Analysis Name	D:\Data\MS\wj\0607\ysq000015.d	Acquisition Date	6/7/2011 10:53:22 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-357	Instrument / Ser#	micrOTOF II 10257
Comment			

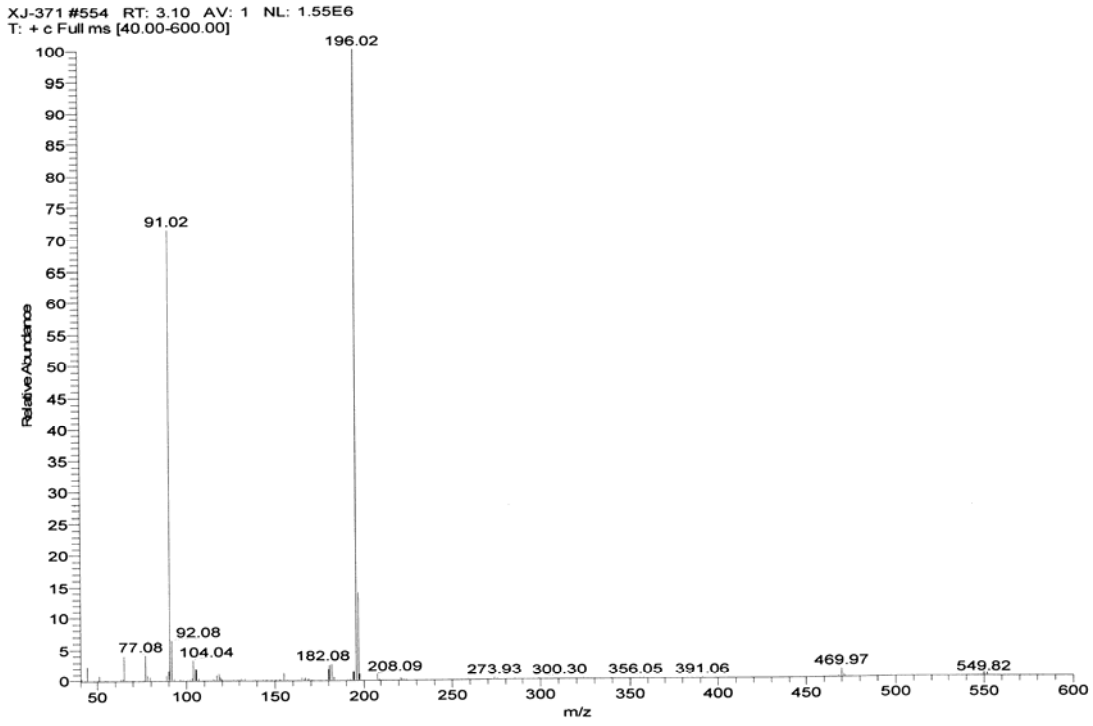
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste






XJ-371 c13 cdcl3
20110110
147.781
142.933
138.061
129.083
136.199
126.869
126.729
126.637
117.121
113.070
77.211
77.000
76.788
55.835
55.302
53.244
39.584
21.468
f1 (ppm)
f1 (ppm)

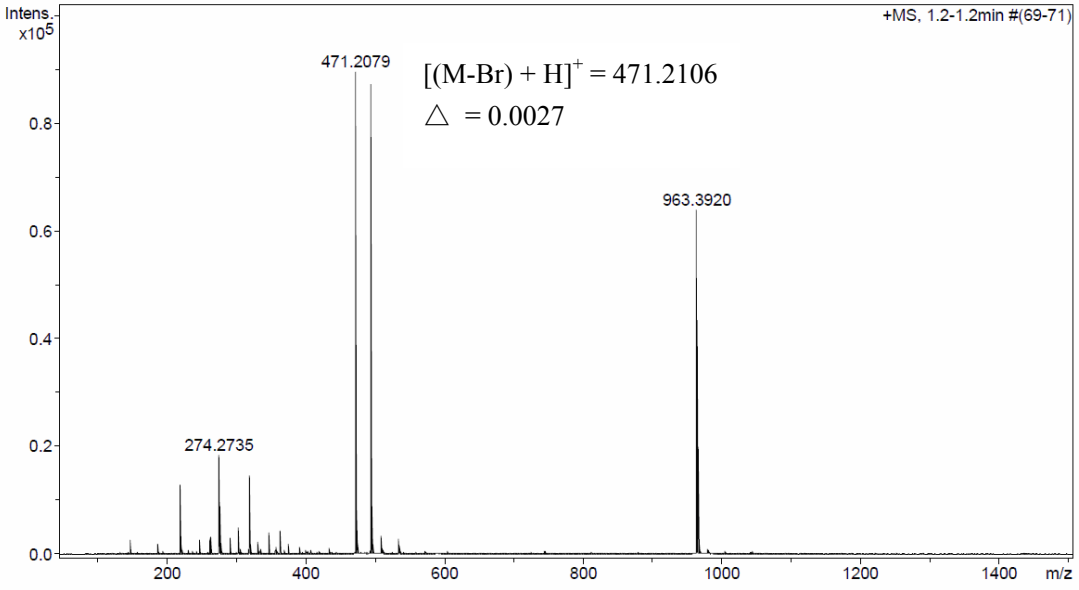

XJ-371 #554 RT: 3.10 AV: 1 NL: 1.55E6
T: + c Full ms [40.00-600.00]
196.02
91.02
92.08
104.04
77.08
182.08
208.09
273.93
300.30
356.05
391.06
469.97
549.82
Relative Abundance
m/z

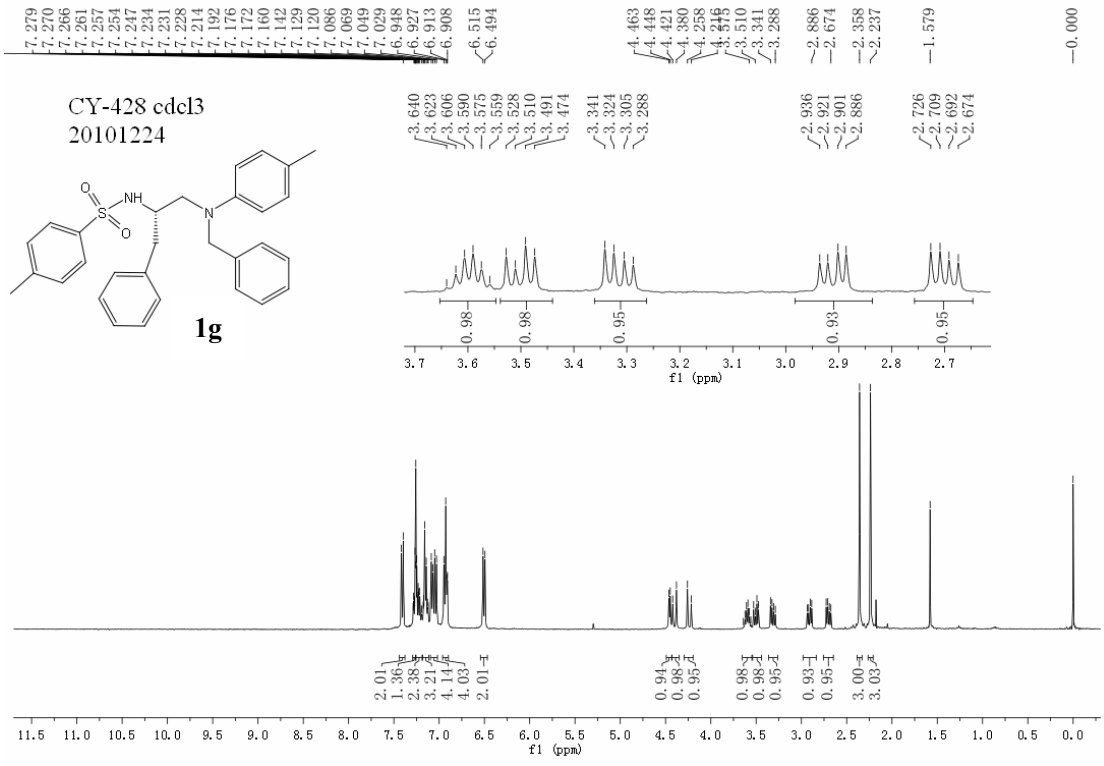
Analysis Info

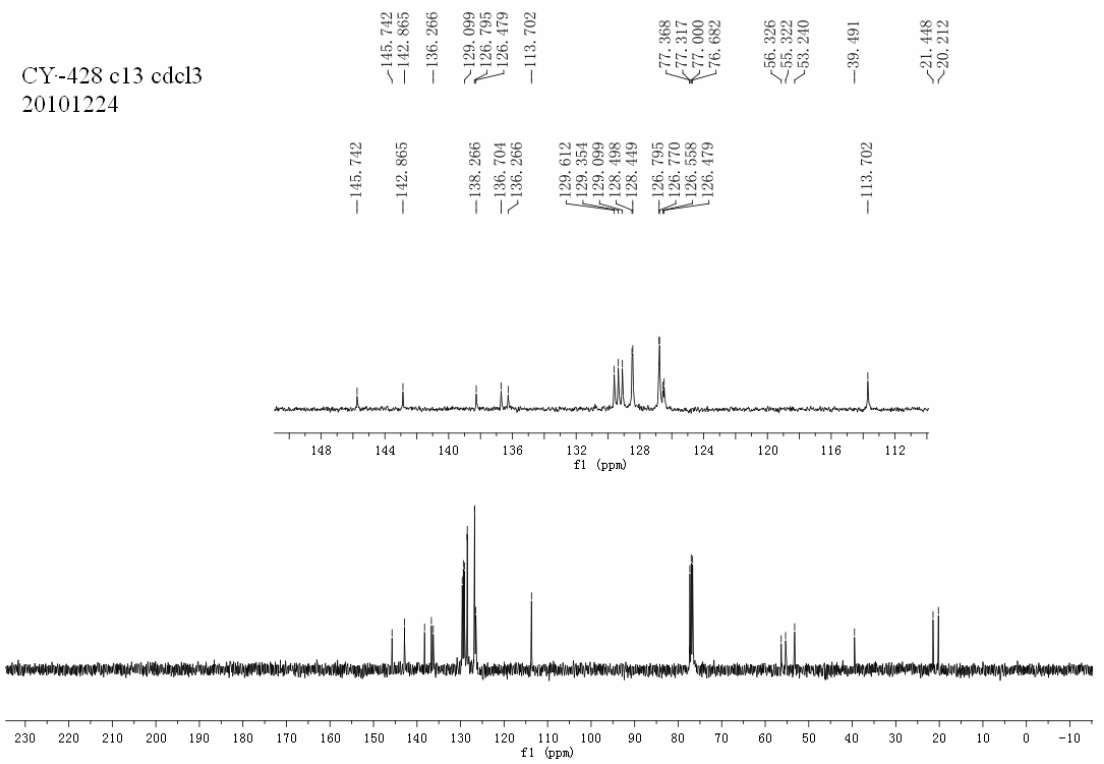
Analysis Name	D:\Data\MS\wj\0607\ysq000016.d	Acquisition Date	6/7/2011 11:03:03 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-371	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





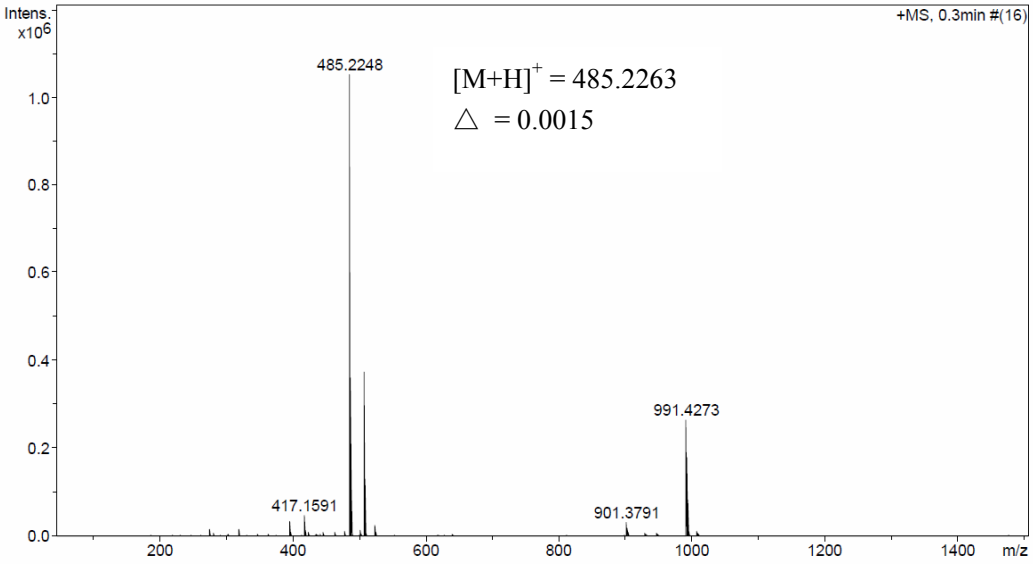


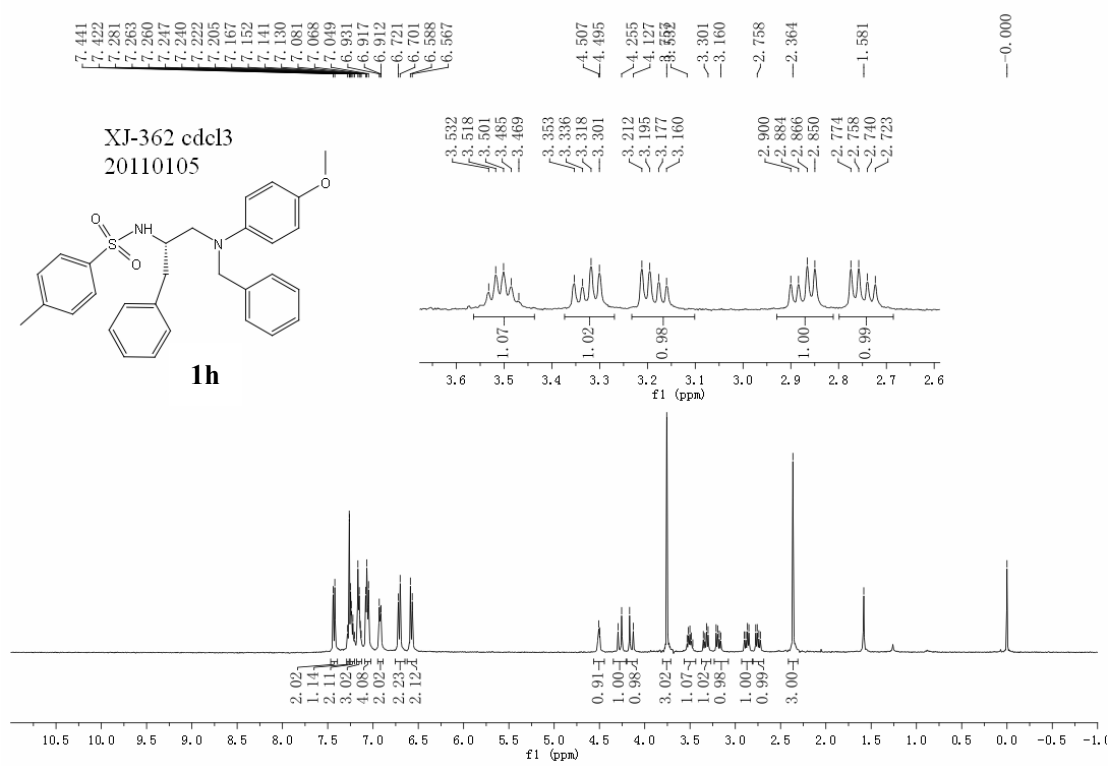
Analysis Info

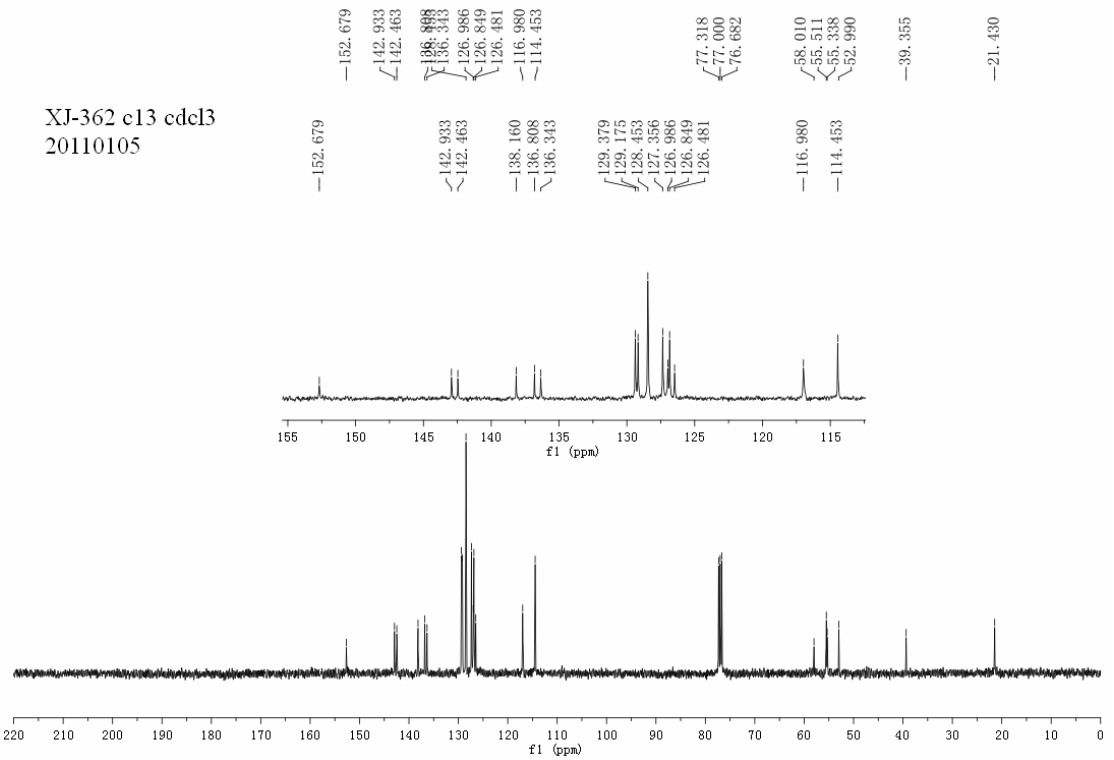
Analysis Name	D:\Data\MS\wj\0607\ysq000006.d	Acquisition Date	6/7/2011 10:13:13 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	cy-428	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




XJ-362 cdcl3
20110105
1h
f1 (ppm)

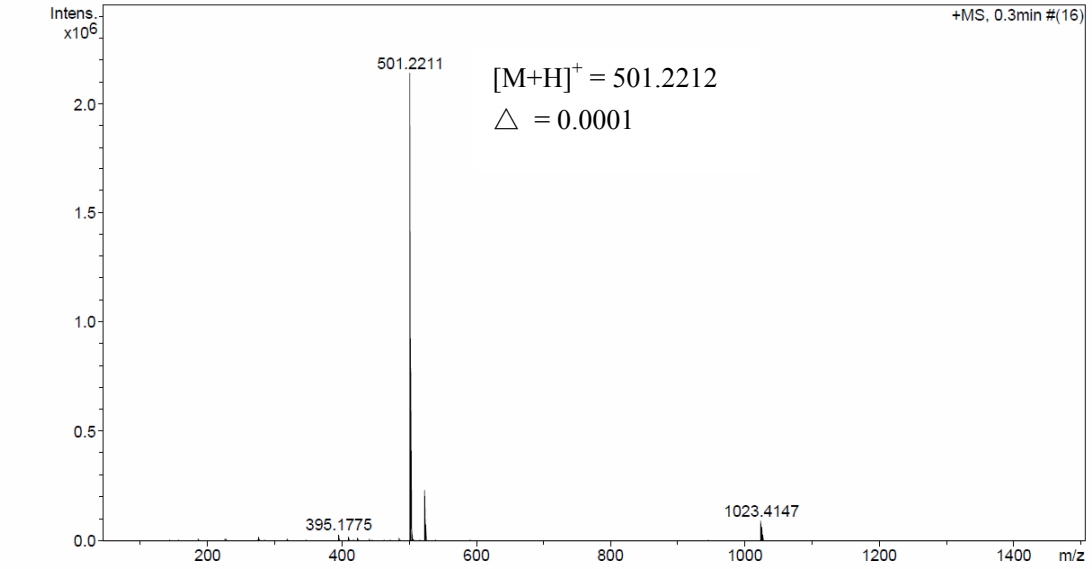

XJ-362 c13 cdcl3
20110105
f1 (ppm)

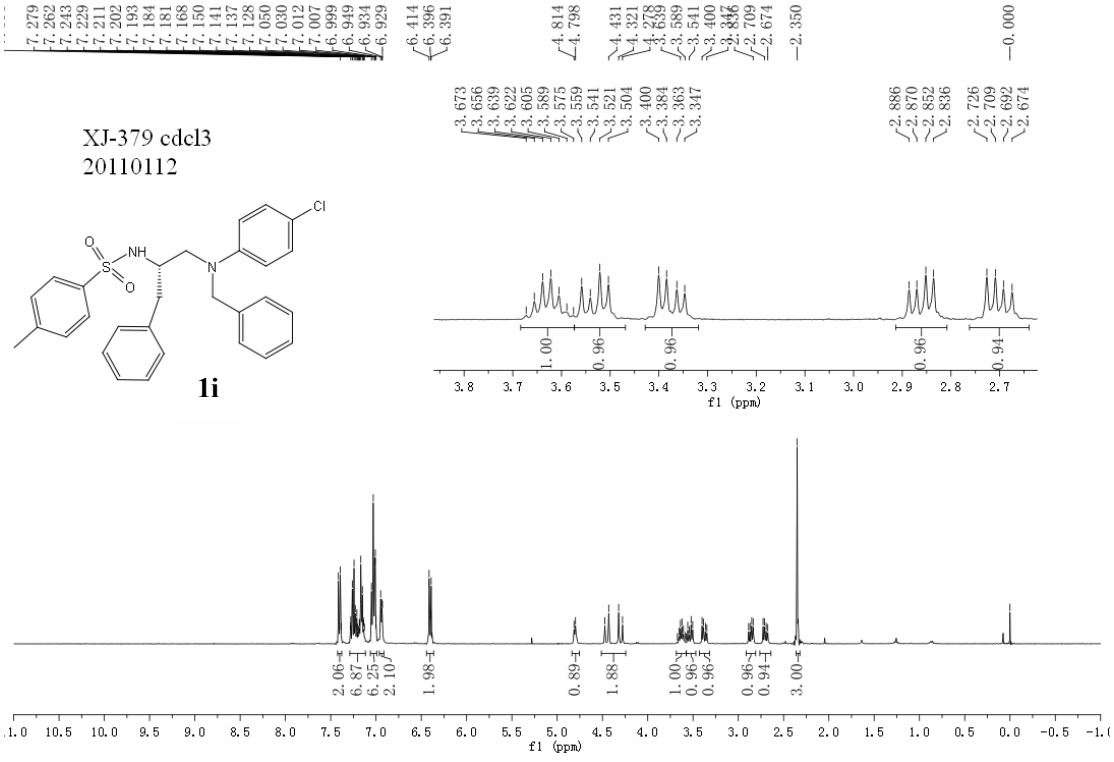
Analysis Info

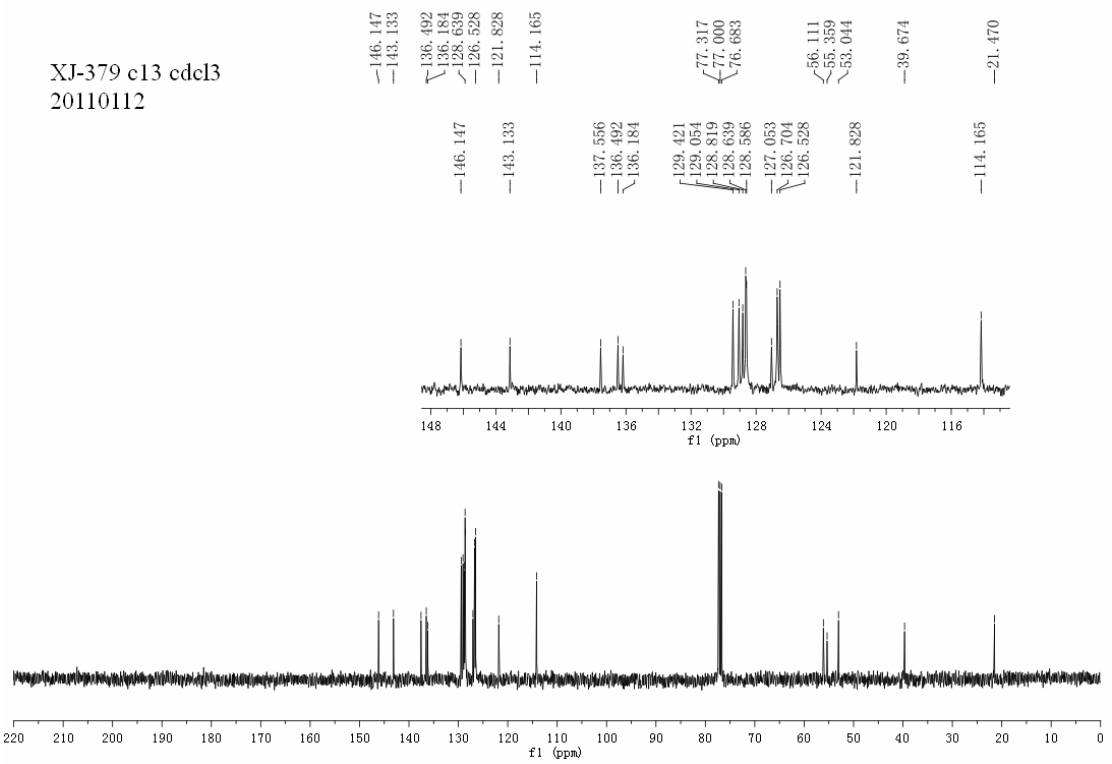
Analysis Name	D:\Data\MS\wj\0607\ysq000011.d	Acquisition Date	6/7/2011 10:30:06 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-362	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





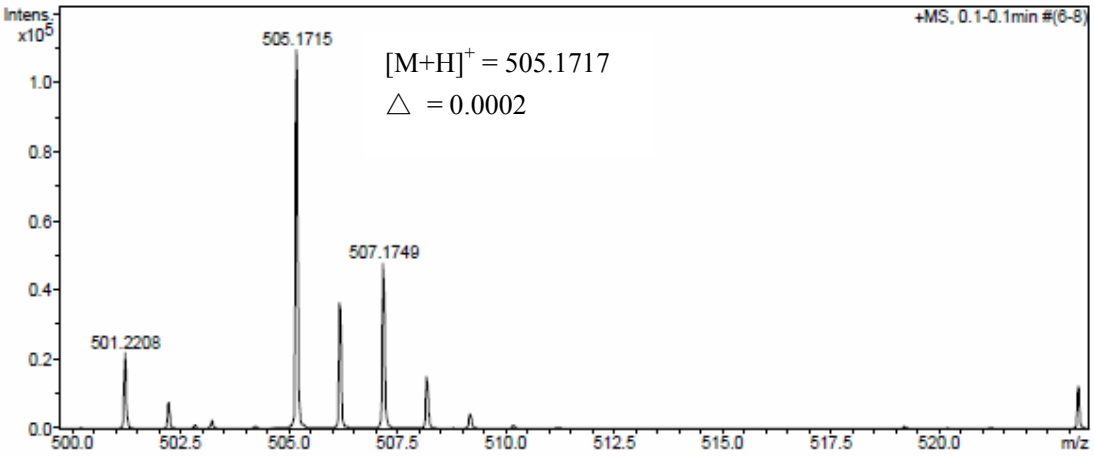


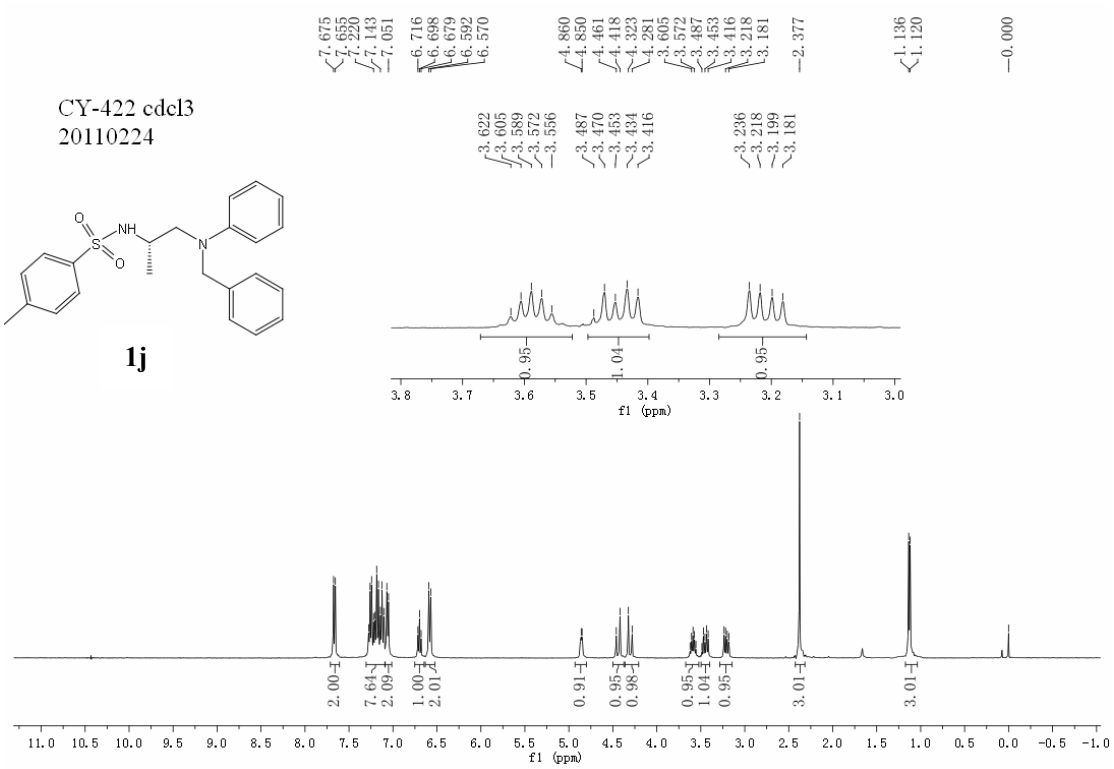
Analysis Info

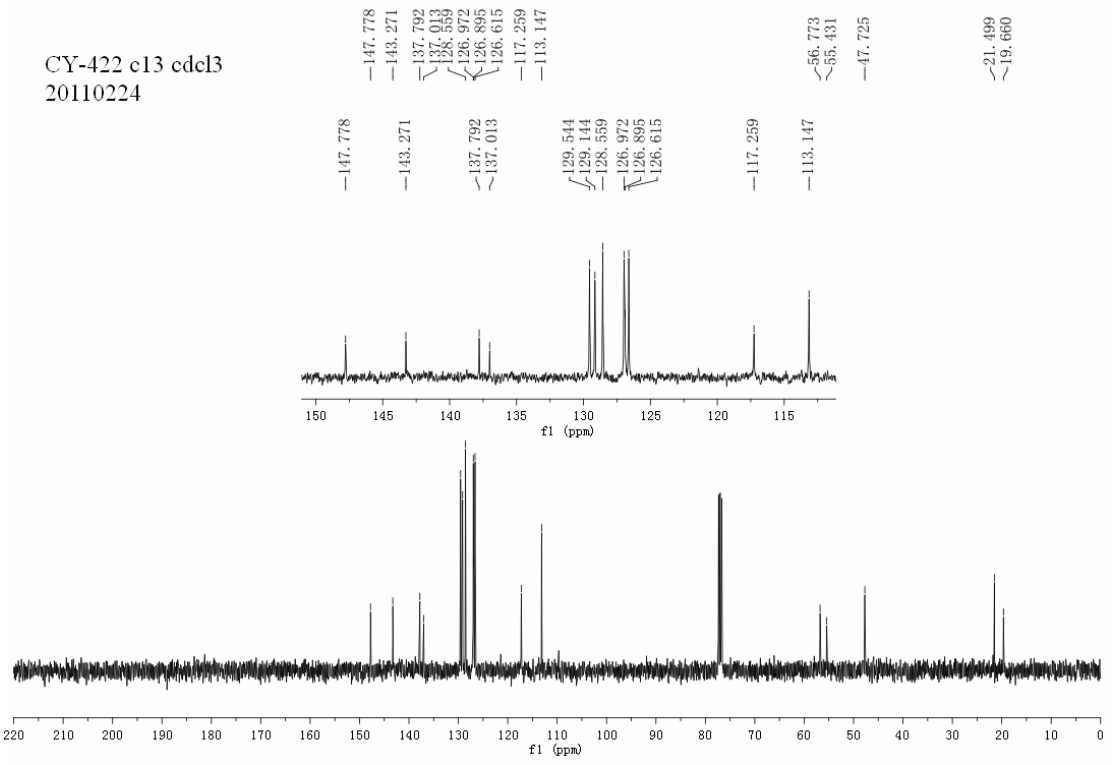
Analysis Name	D:\Data\MS\wj\0607\ysq000012.d	Acquisition Date	6/7/2011 10:38:31 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-379	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




CY-422 cdcl3
20110224
1j

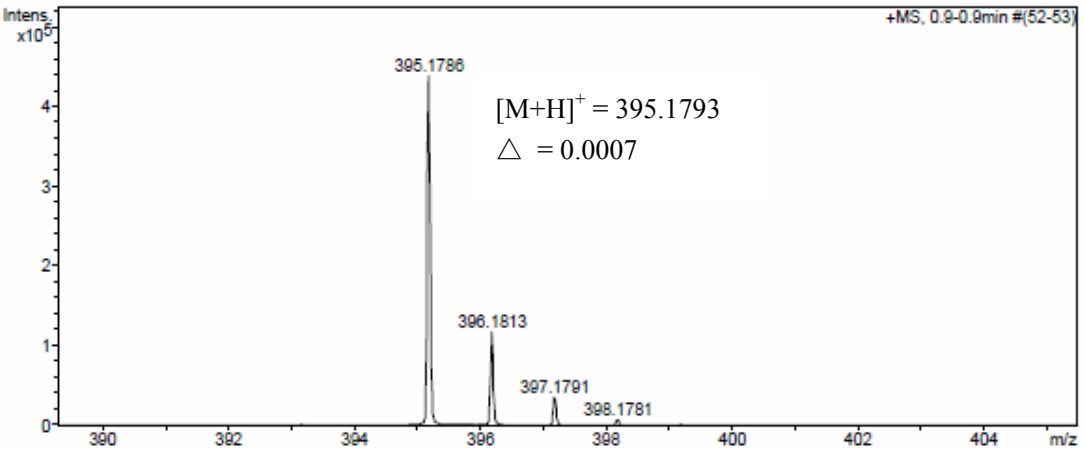

CY-422 c13 cdcl3
20110224

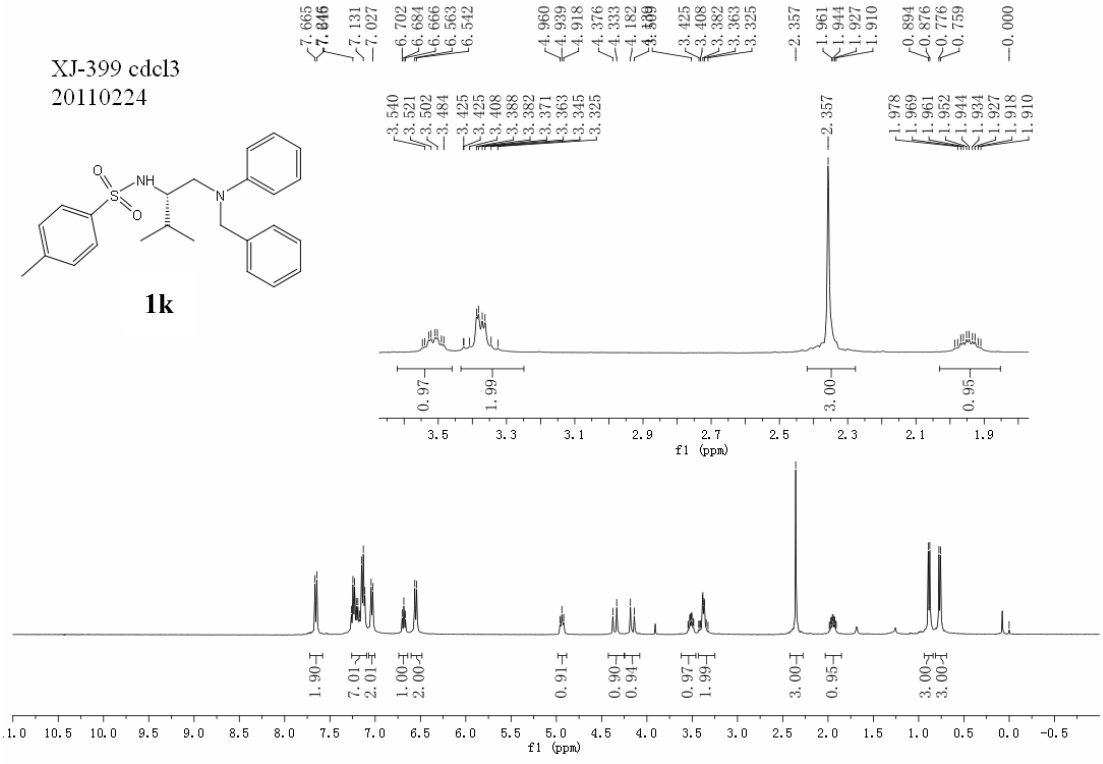
Analysis Info

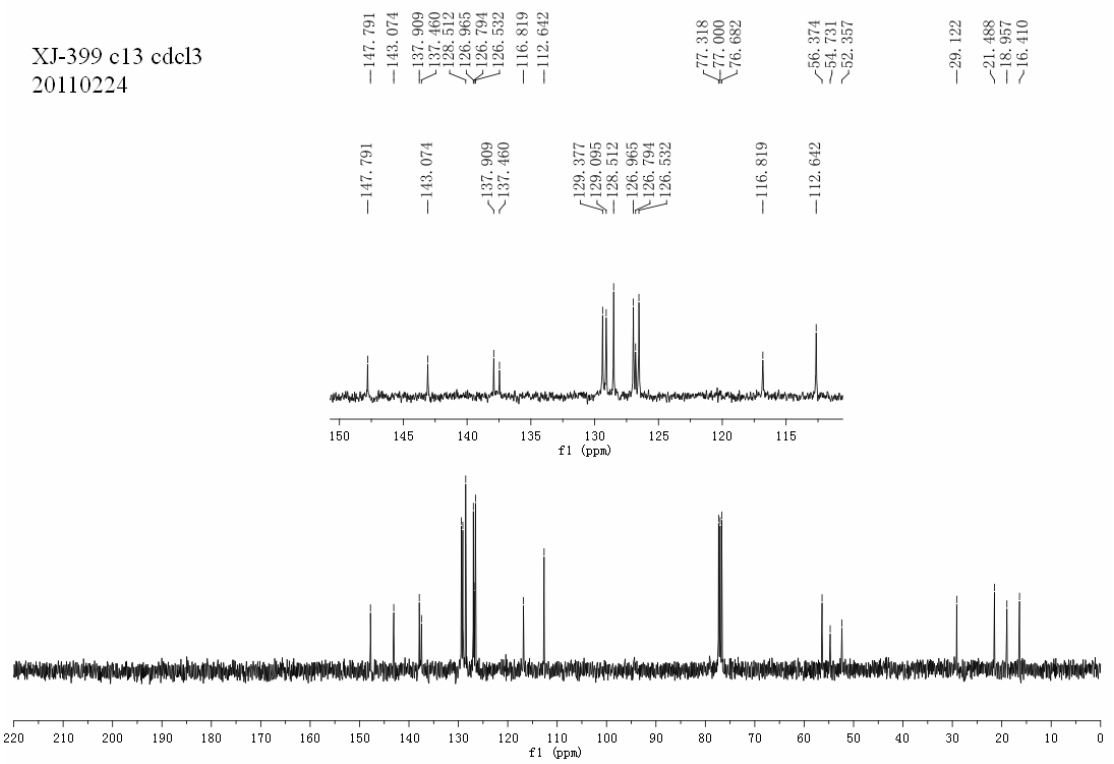
Analysis Name	D:\Data\MS\wj\0607\ysq000005.d	Acquisition Date	6/7/2011 10:10:39 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	cy-422	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





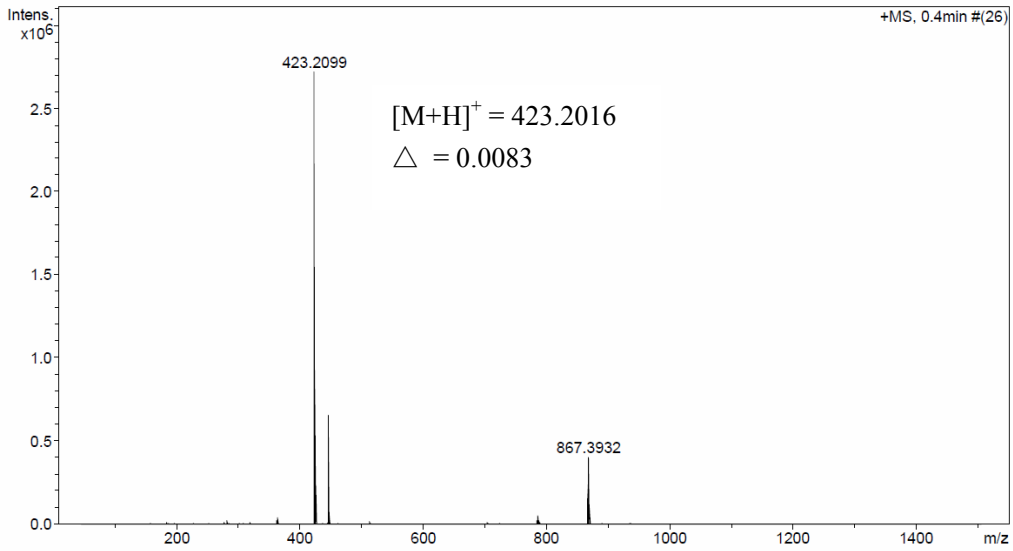


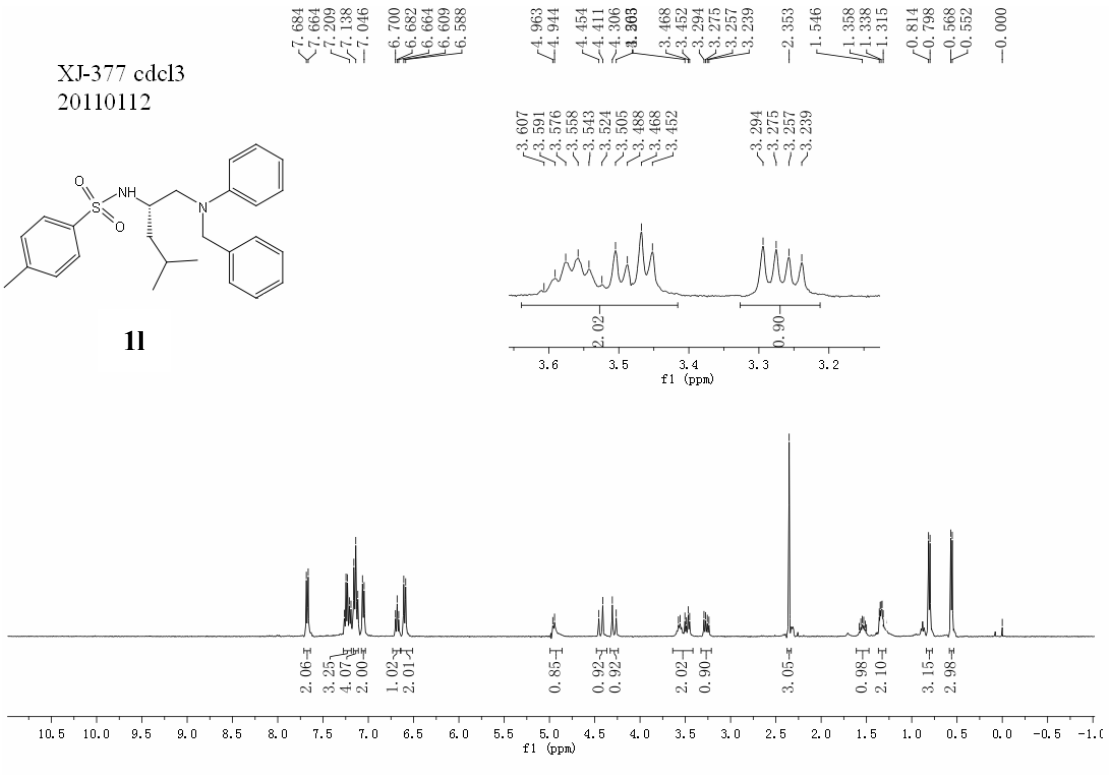
Analysis Info

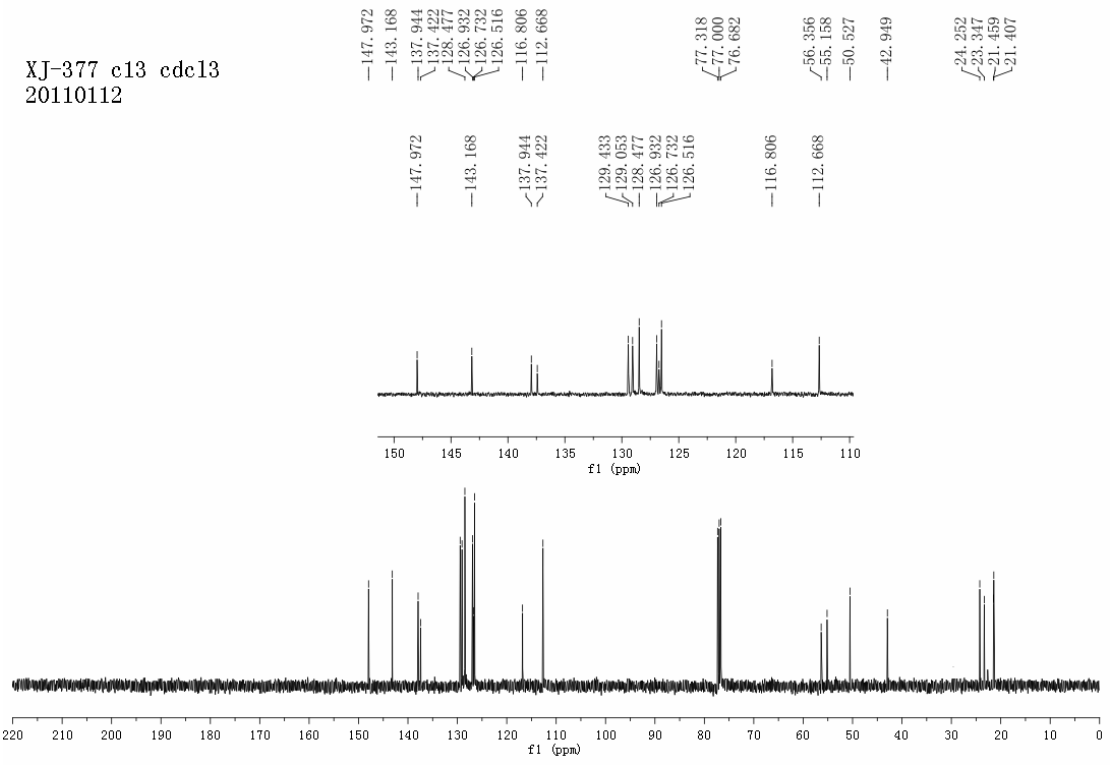
Analysis Name	D:\Data\MS\wj\0607\ysq000001.d	Acquisition Date	6/7/2011 9:45:40 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-399	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




XJ-377 cdcl3
20110112
11
f1 (ppm)

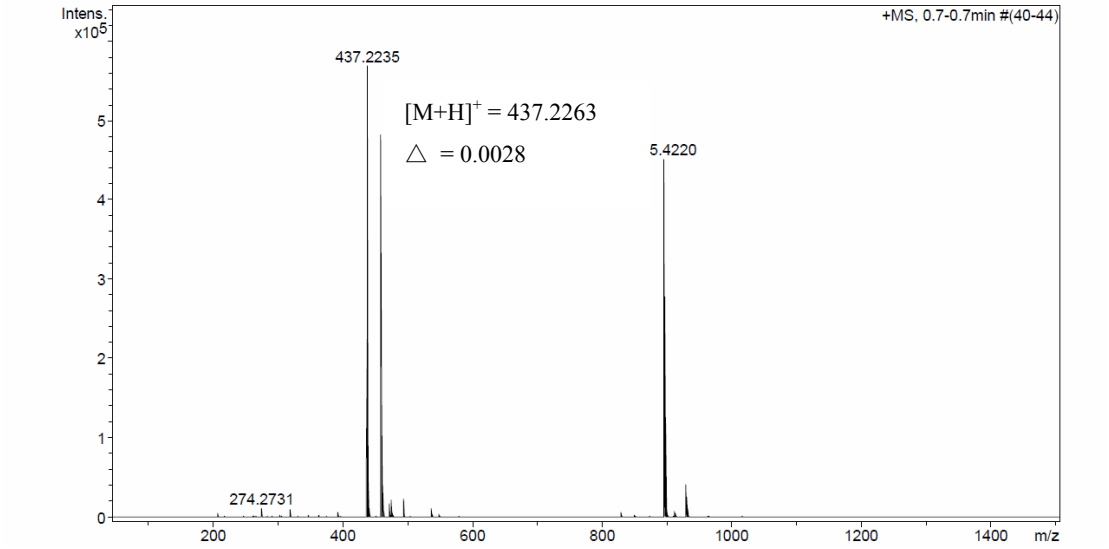

XJ-377 c13 cdcl3
20110112
f1 (ppm)

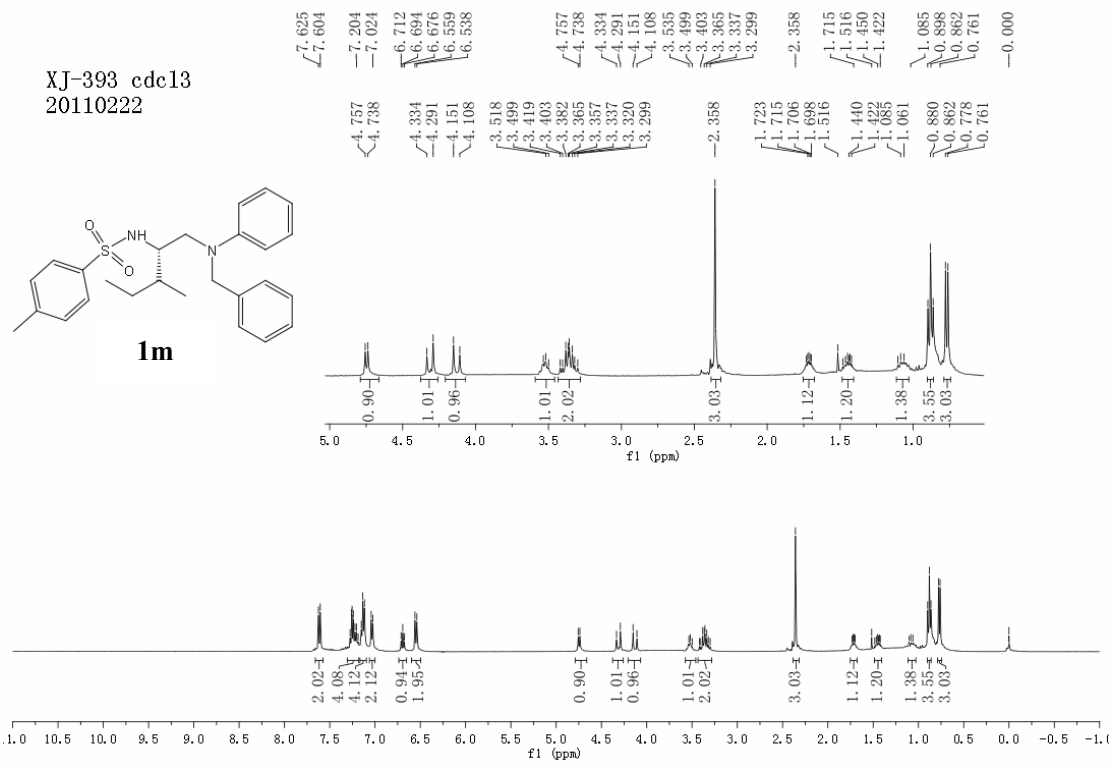
Analysis Info

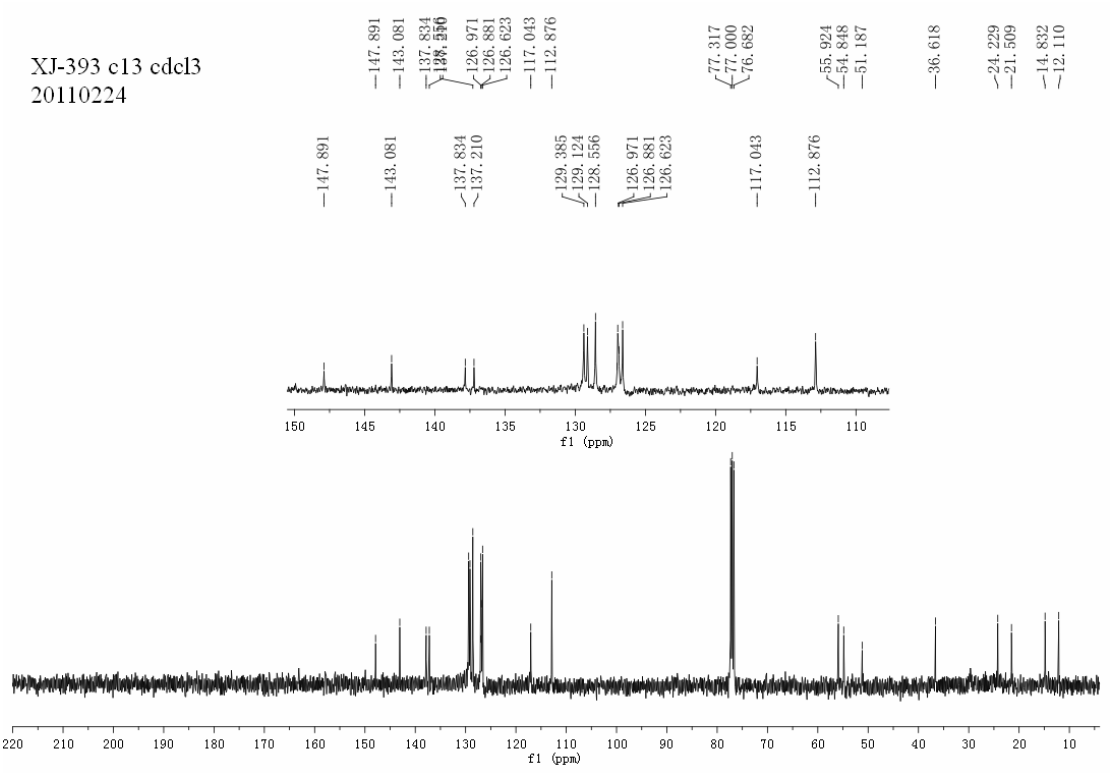
Analysis Name	D:\Data\MS\wj\0607\ysq000017.d	Acquisition Date	6/7/2011 11:07:39 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-377	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





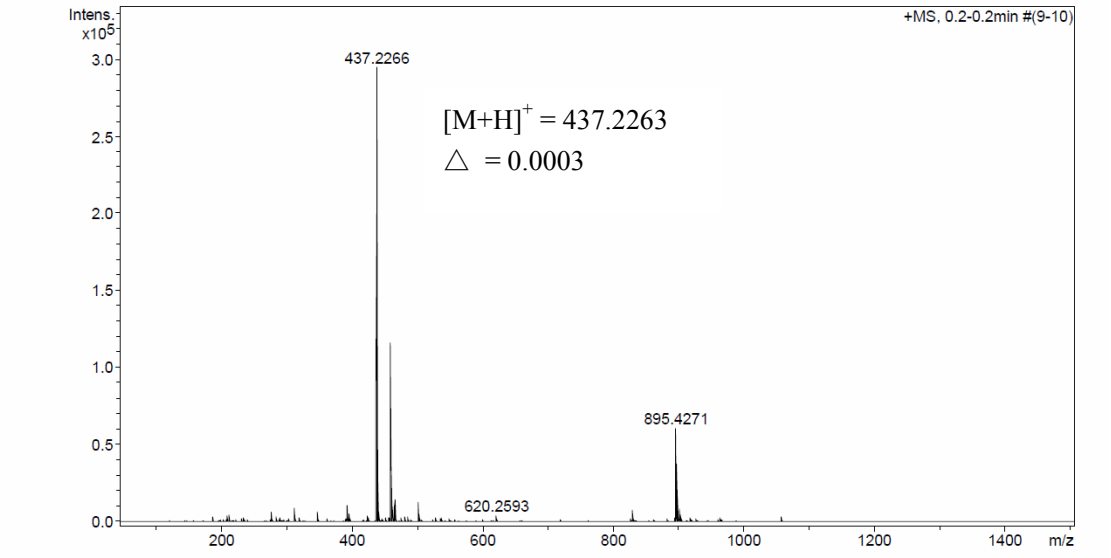


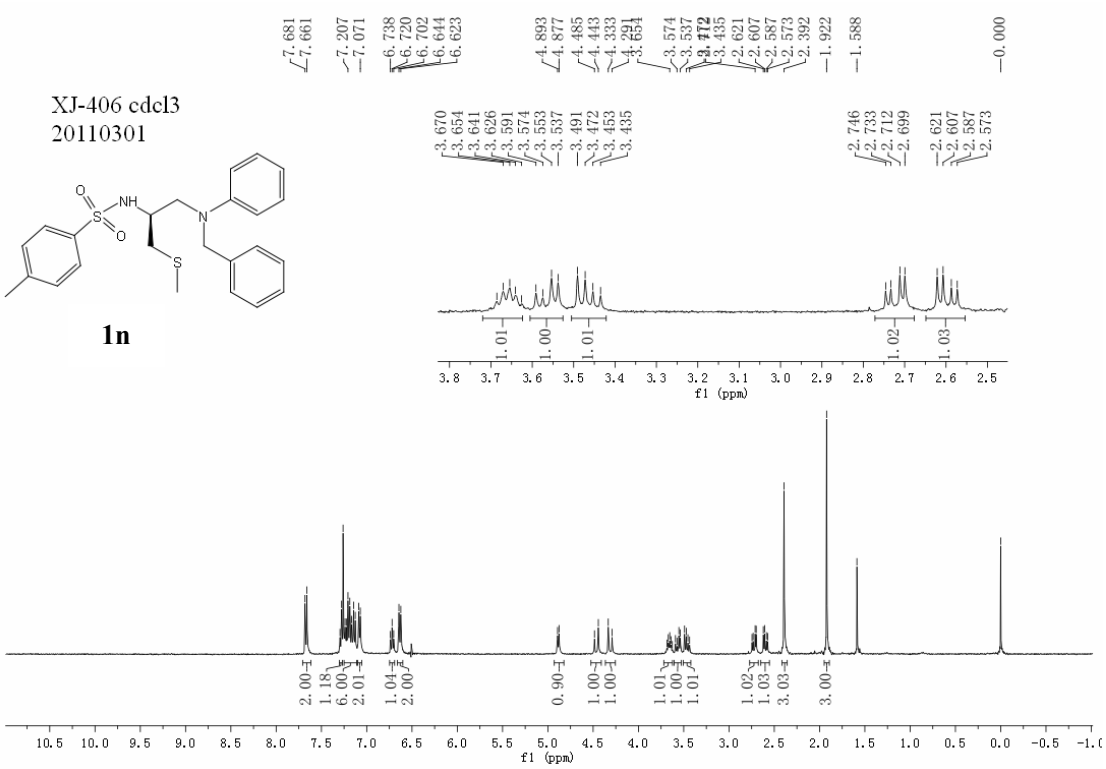
Analysis Info

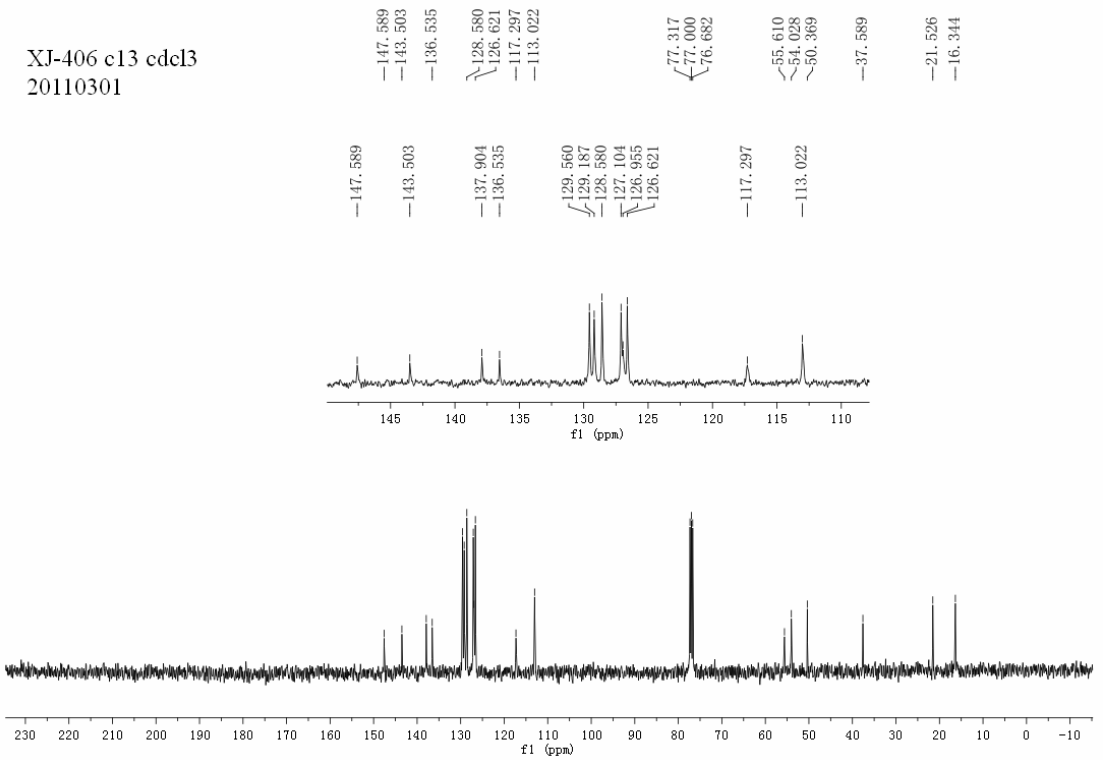
Analysis Name	D:\Data\MS\wj\0607\ysq000013.d	Acquisition Date	6/7/2011 10:46:08 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-393	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste




XJ-406 cdcl3
20110301
1n
f1 (ppm)

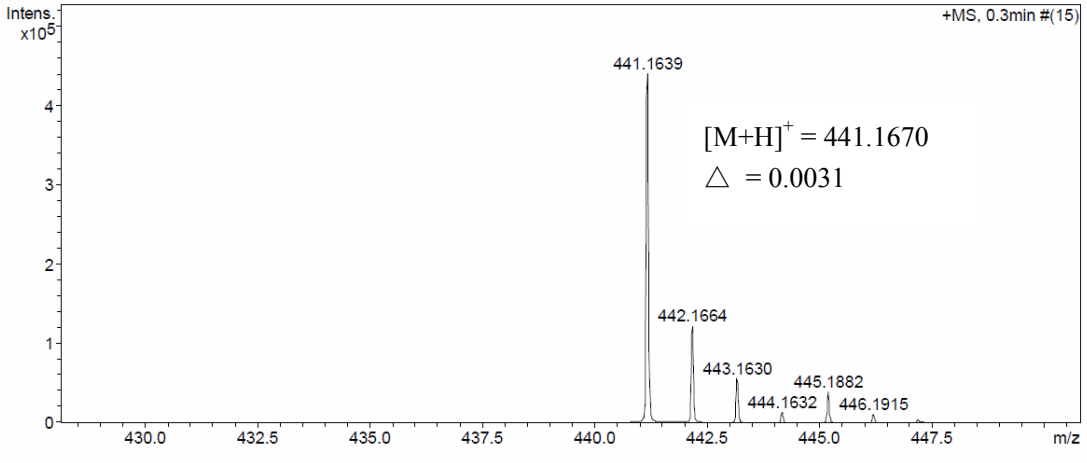

XJ-406 c13 cdcl3
20110301
f1 (ppm)

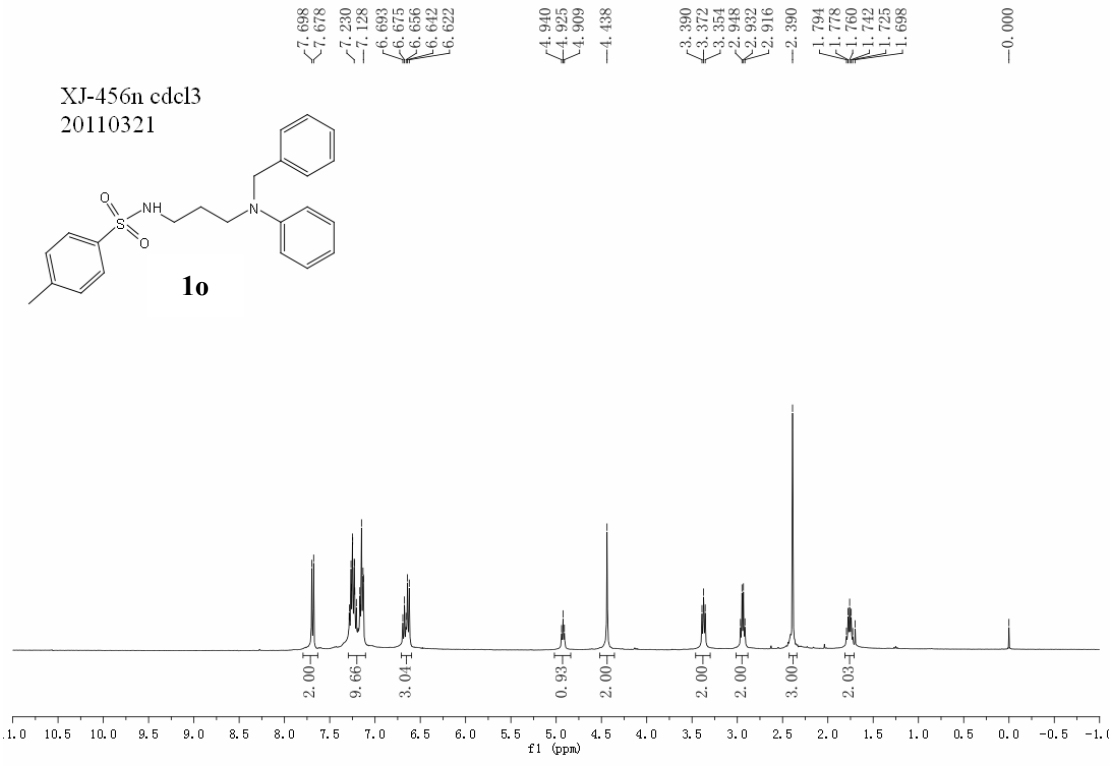
Analysis Info

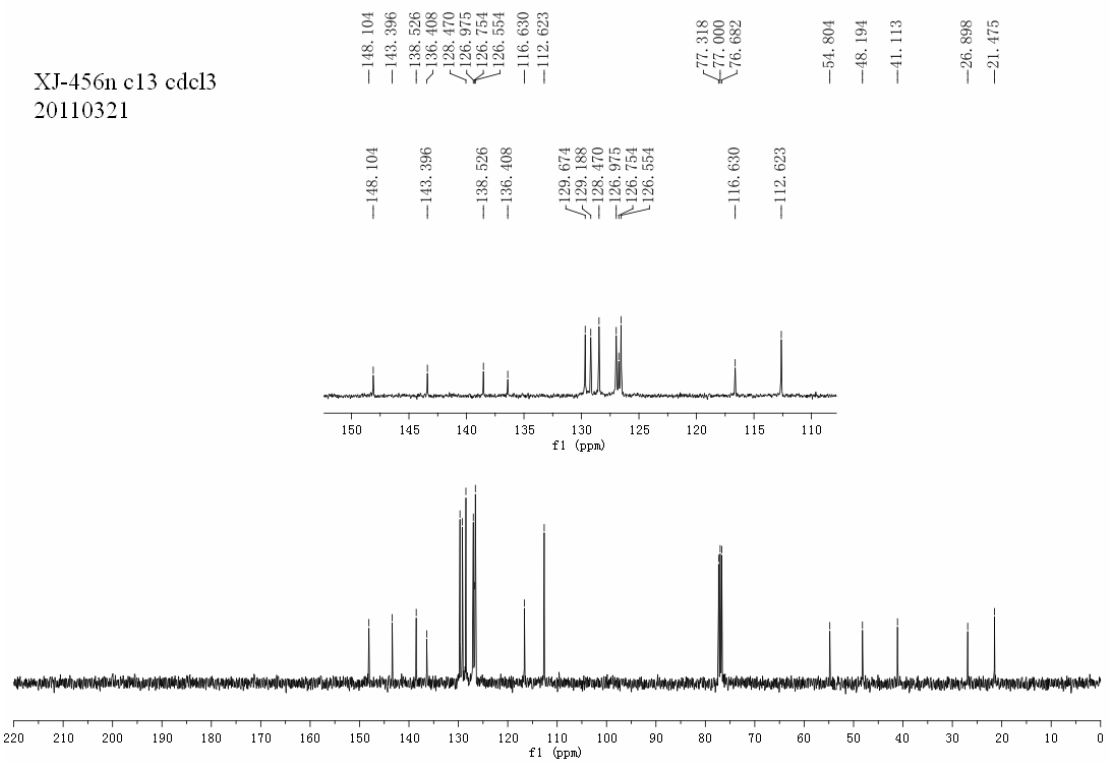
Analysis Name	D:\Data\MS\wj\0607\ysq000003.d	Acquisition Date	6/7/2011 10:00:00 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-406	Instrument / Ser#	micrOTOF II 10257
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste





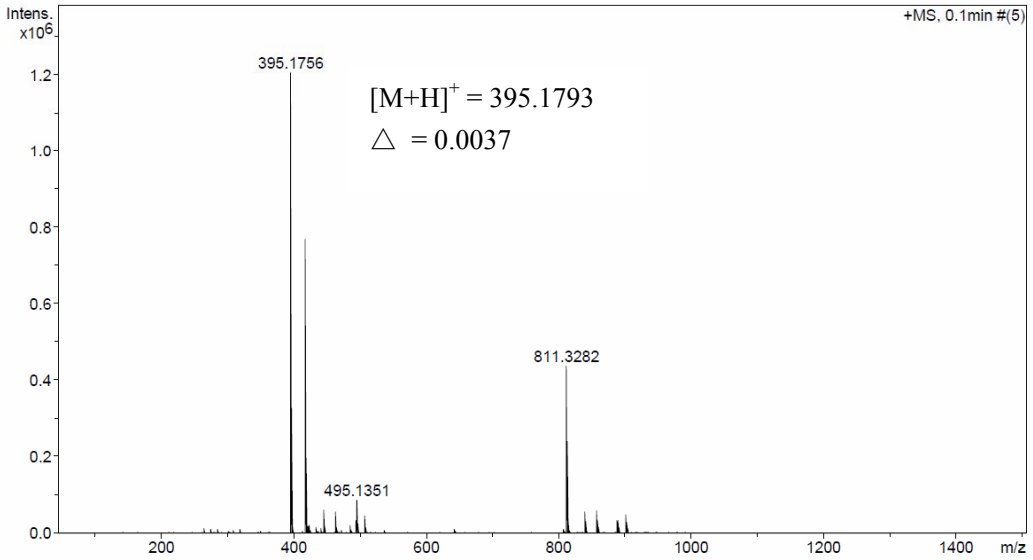


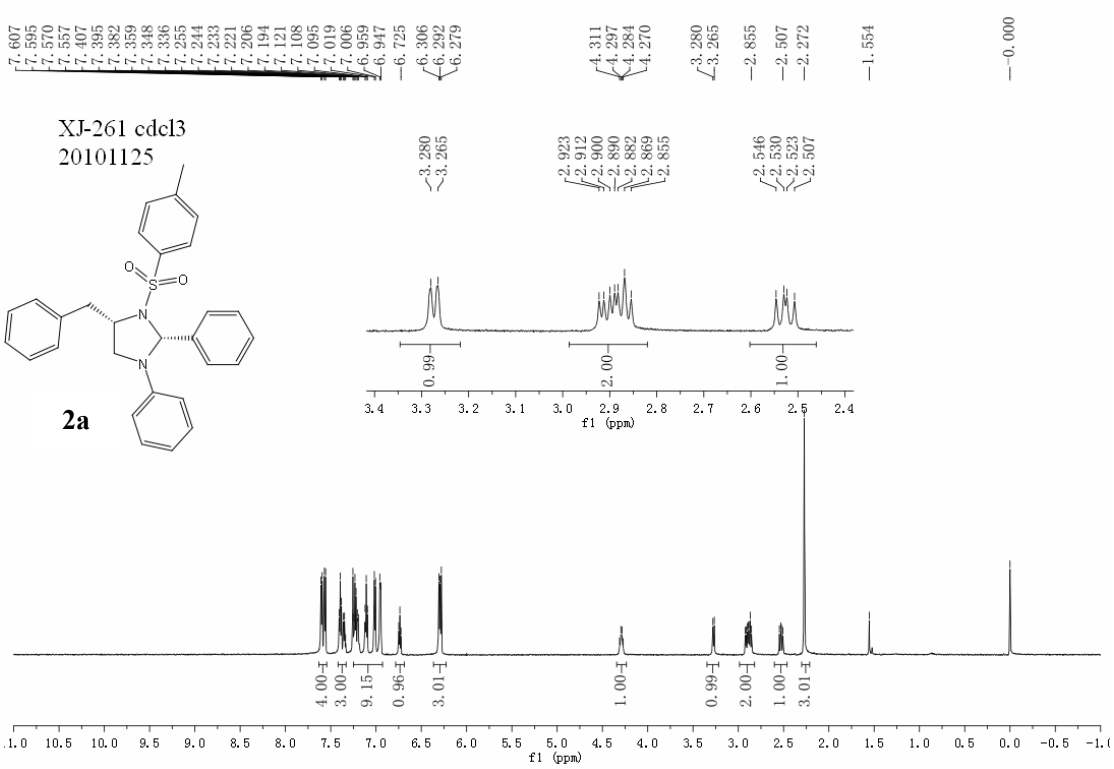
Analysis Info

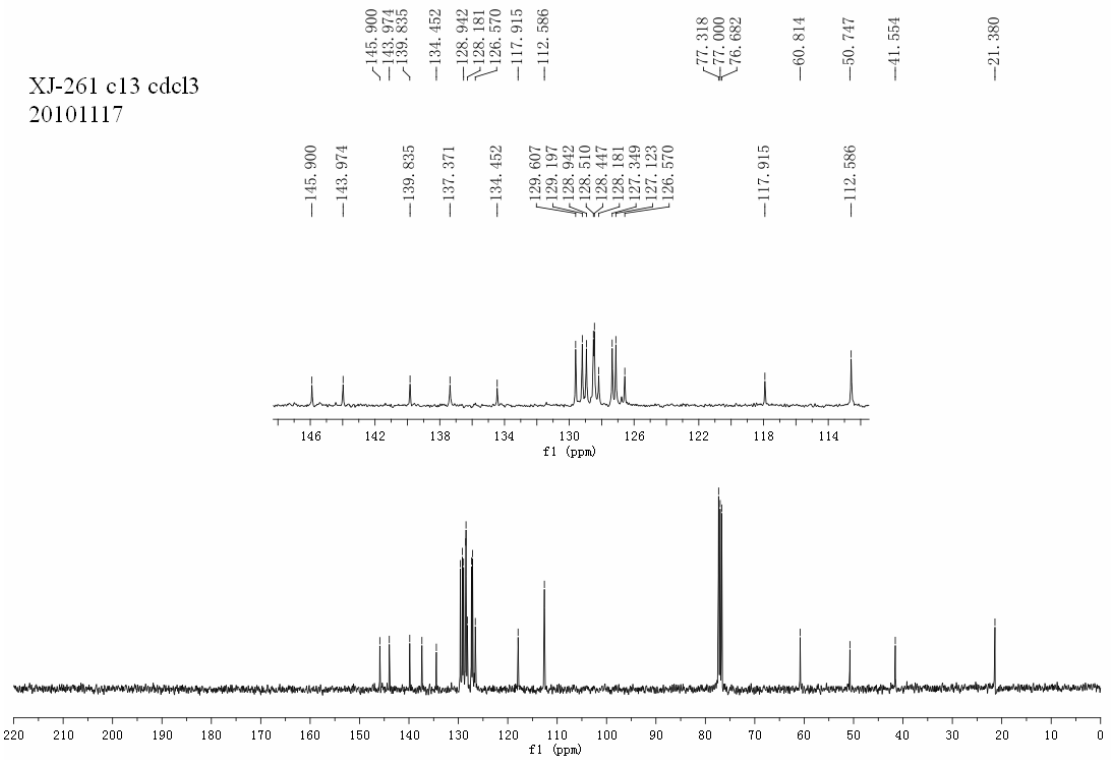
Analysis Name	D:\Data\MS\wj\0607\ysq000009.d	Acquisition Date	6/7/2011 10:19:59 AM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj-456	Instrument / Ser#	micrOTOF II 10257
Comment			

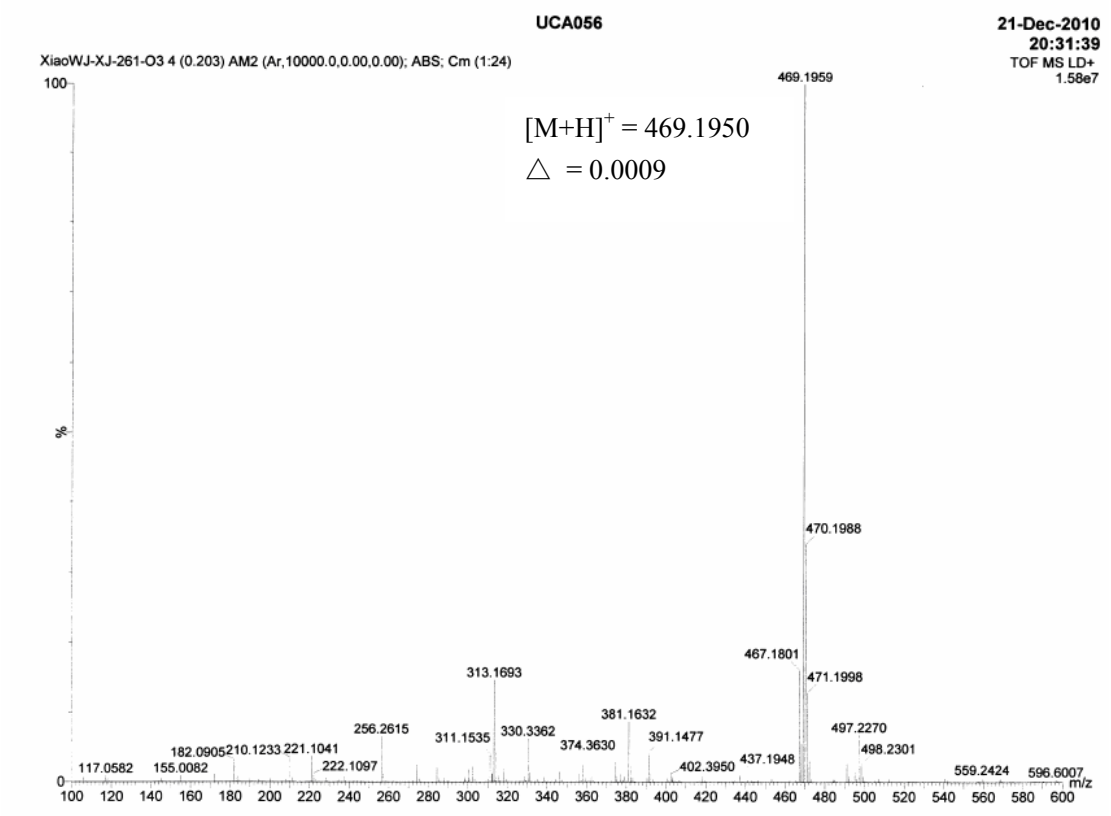
Acquisition Parameter

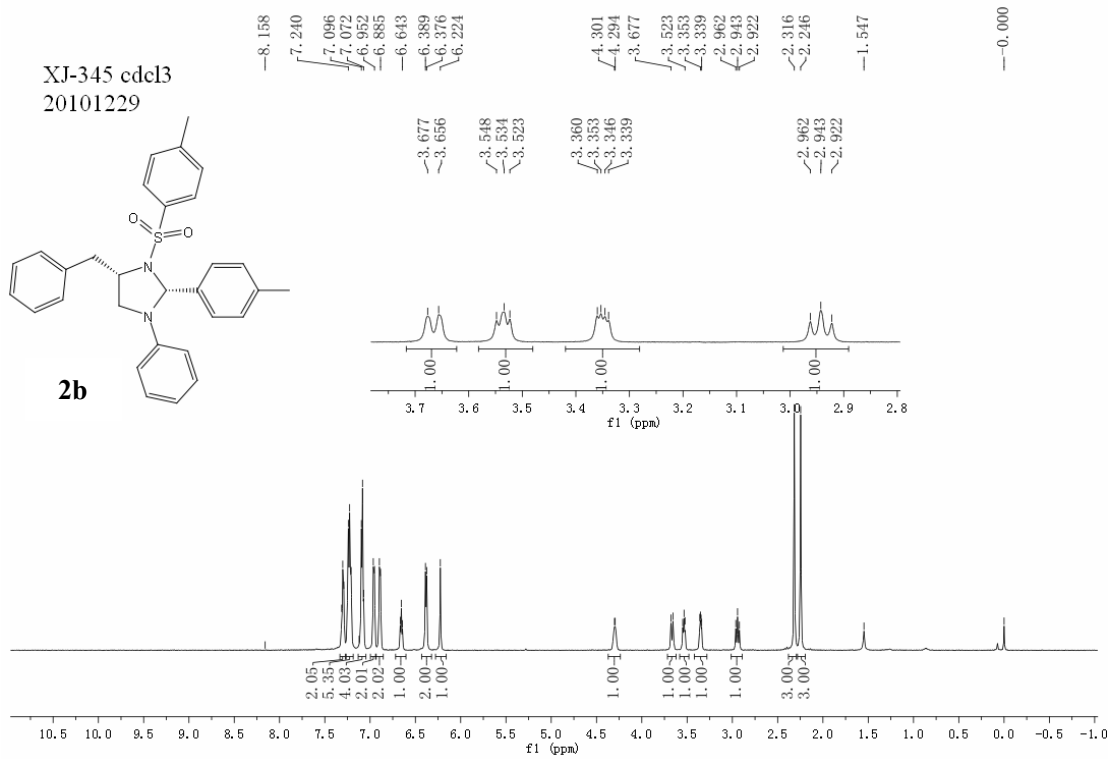
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active			Set Dry Heater	200 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

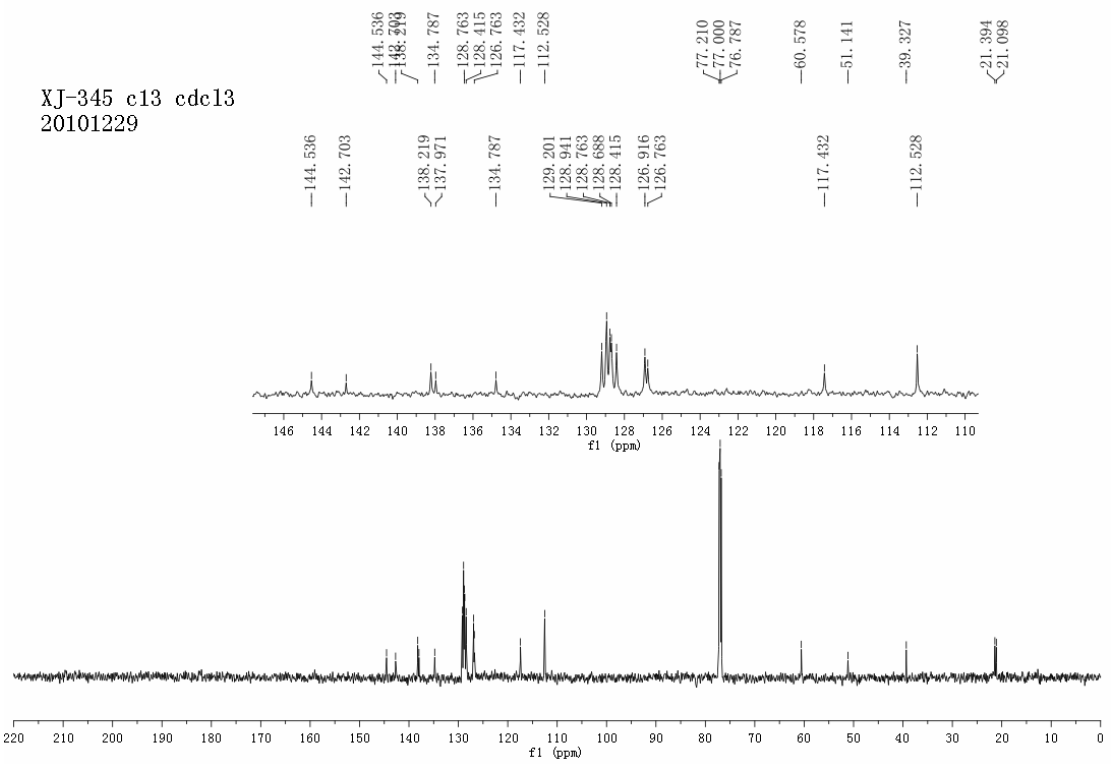


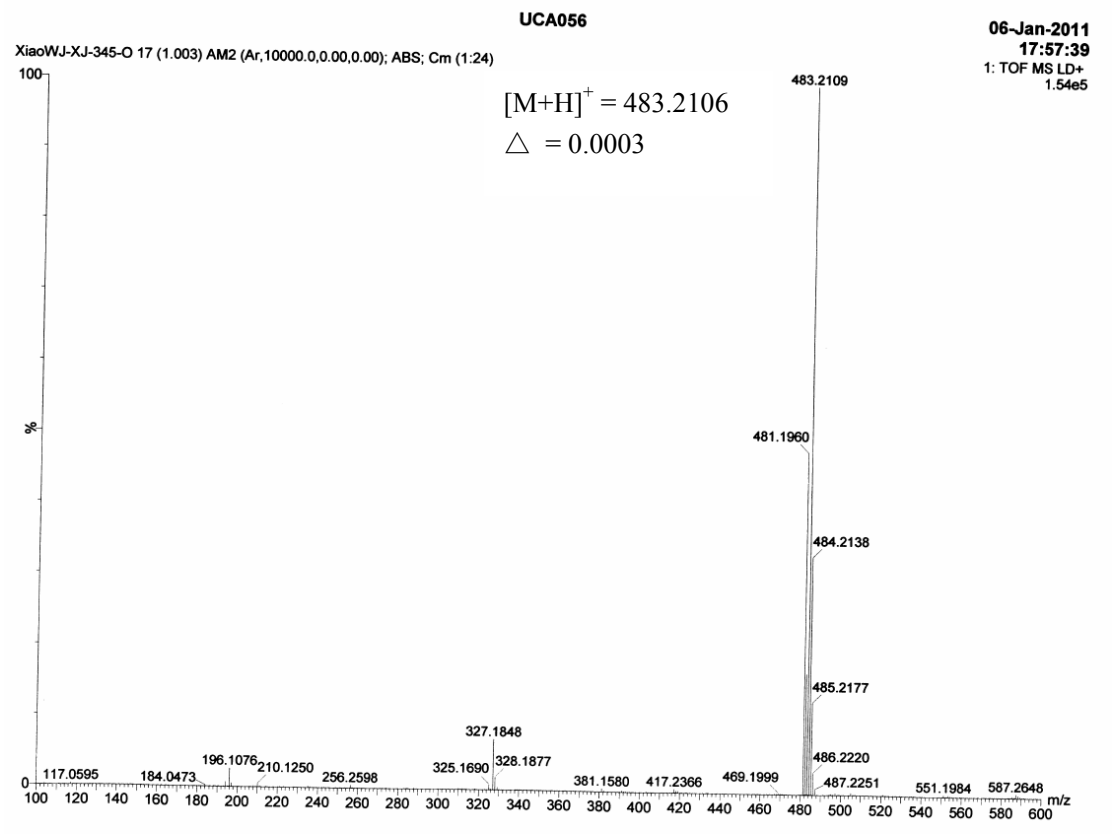

XJ-261 cdcl3
20101125
2a
f1 (ppm)

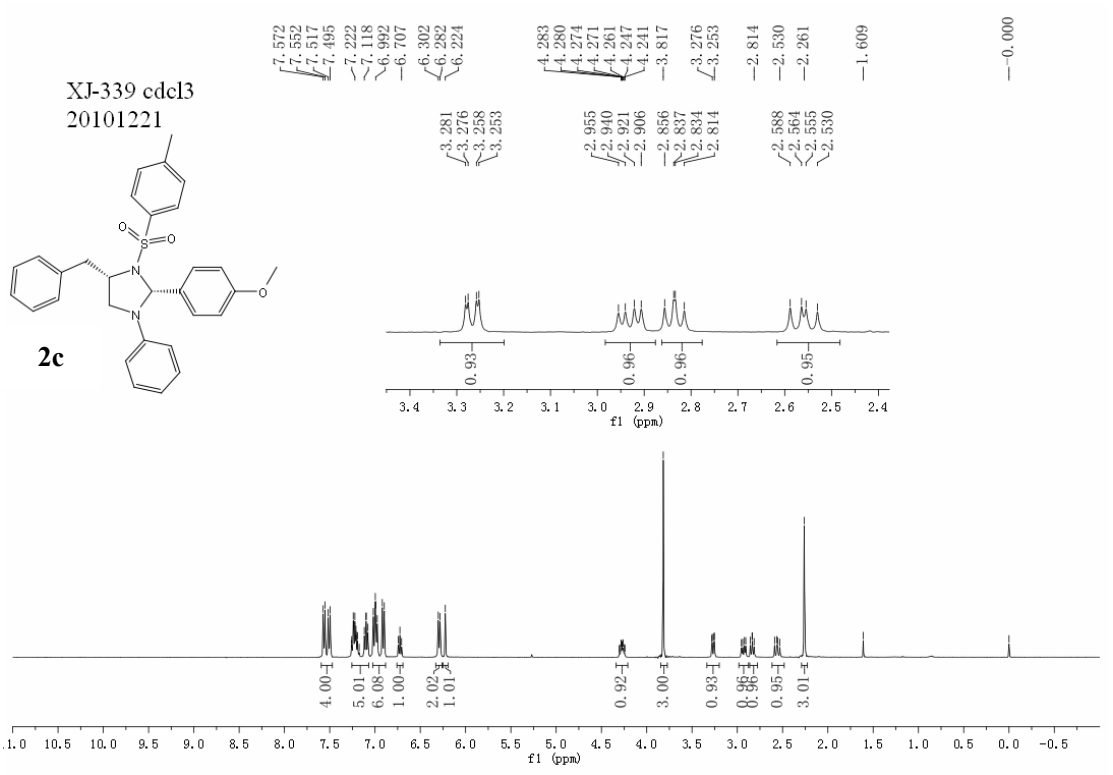

XJ-261 c13 cdcl3
20101117
f1 (ppm)

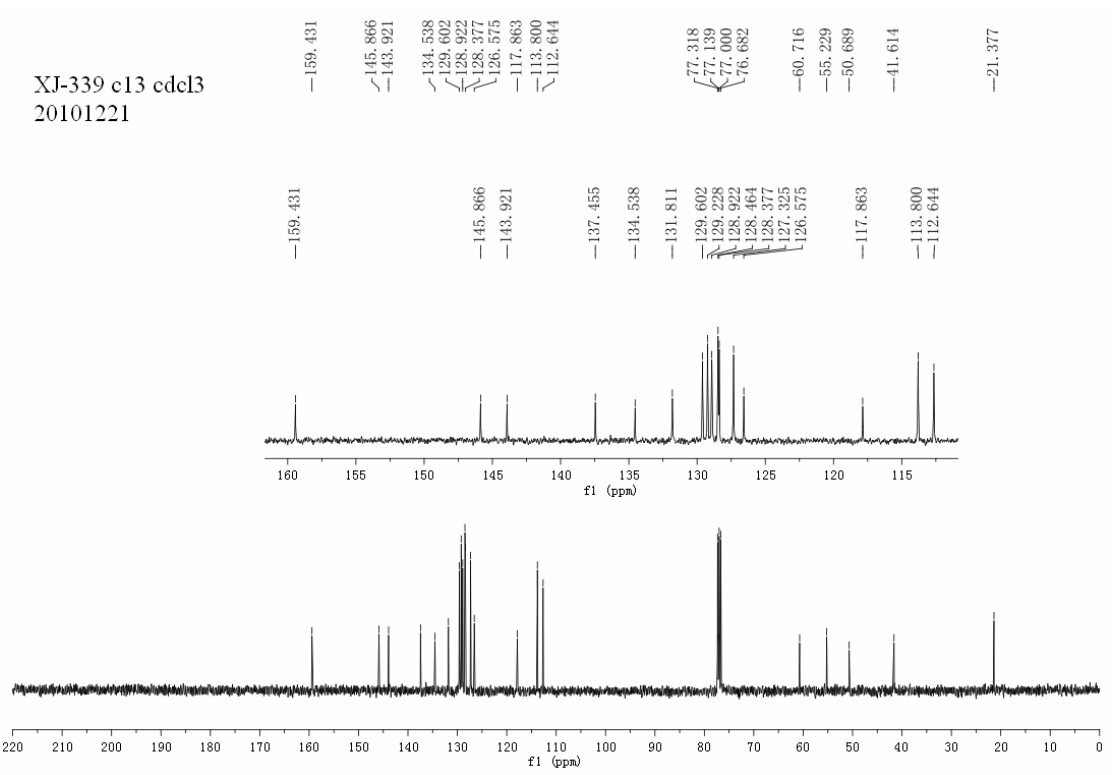

UCA056
21-Dec-2010
20:31:39
TOF MS LD+
1.58e7
XiaoWJ-XJ-261-O3 4 (0.203) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (1:24)
[M+H]+ = 469.1950
△ = 0.0009
469.1959
470.1988
467.1801
471.1998
313.1693
381.1632
256.2615
311.1535
330.3362
391.1477
374.3630
497.2270
498.2301
182.0905
210.1233
221.1041
222.1097
155.0082
117.0582
402.3950
437.1948
559.2424
596.6007
m/z

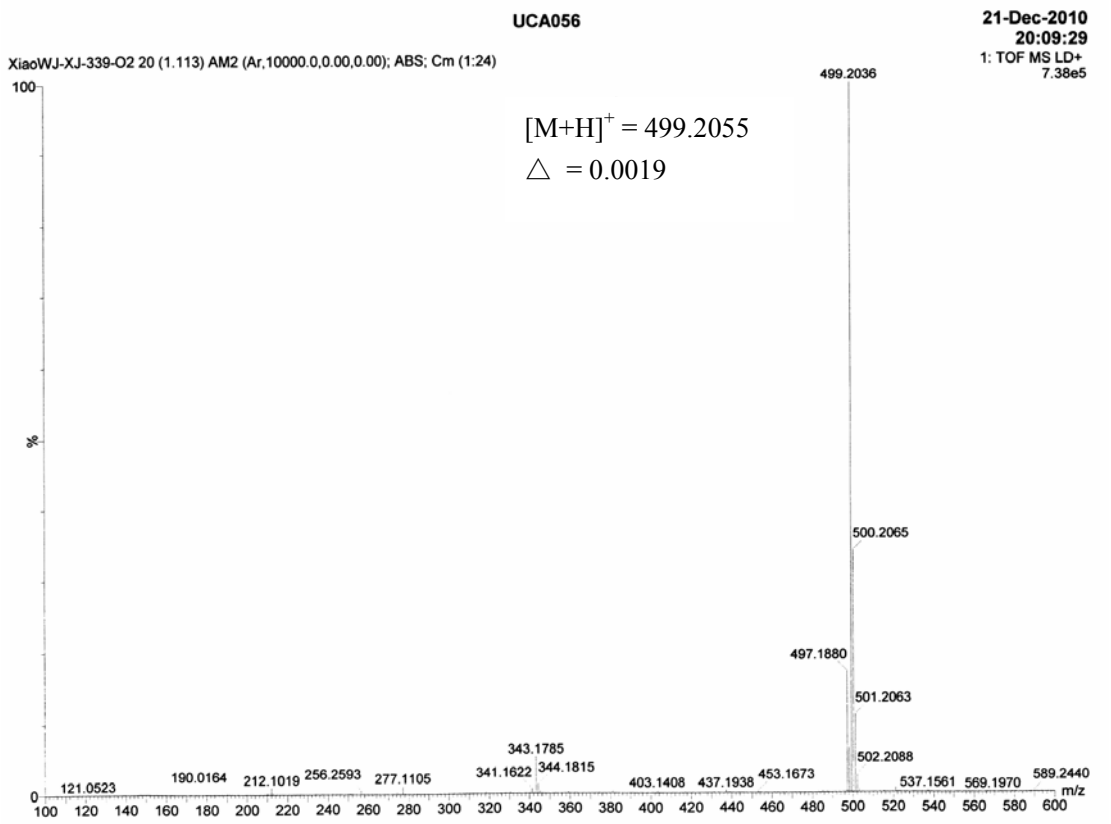

XJ-345 cdcl3
20101229
2b
f1 (ppm)

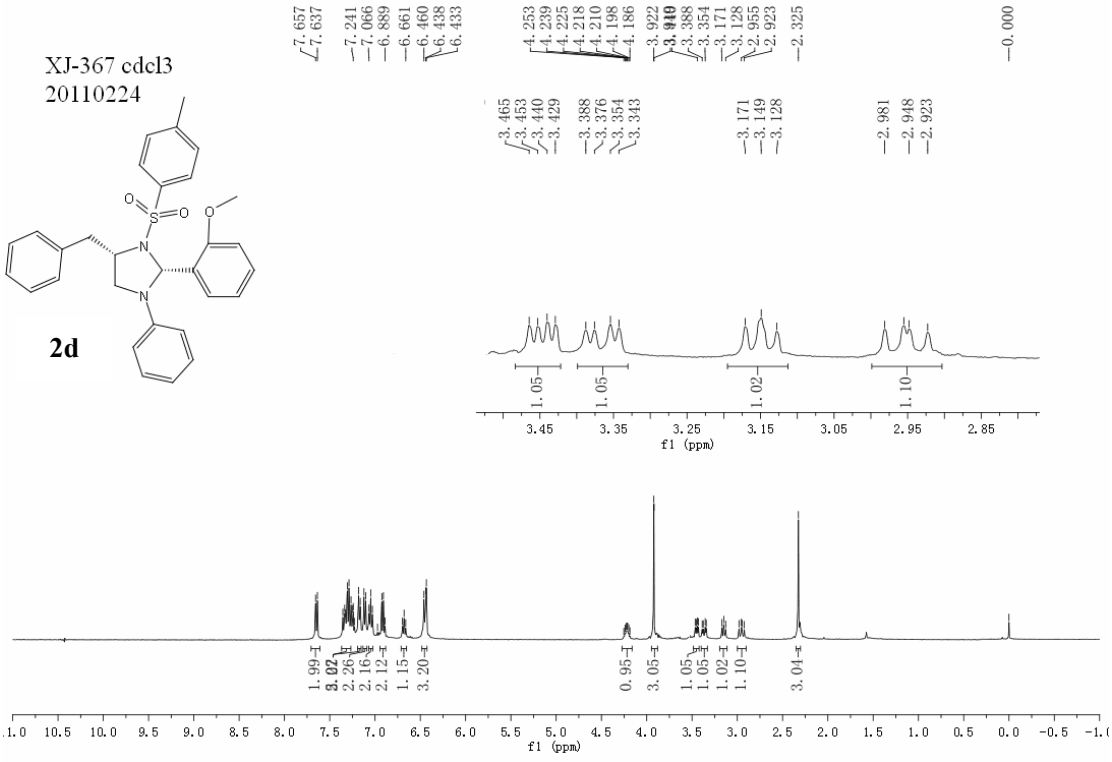

XJ-345 c13 cdcl3
20101229
144.536
142.703
138.219
137.971
134.787
129.201
128.941
128.763
128.688
128.415
126.916
126.763
117.432
112.528
77.210
77.000
76.787
60.578
51.141
39.327
21.394
21.098
f1 (ppm)

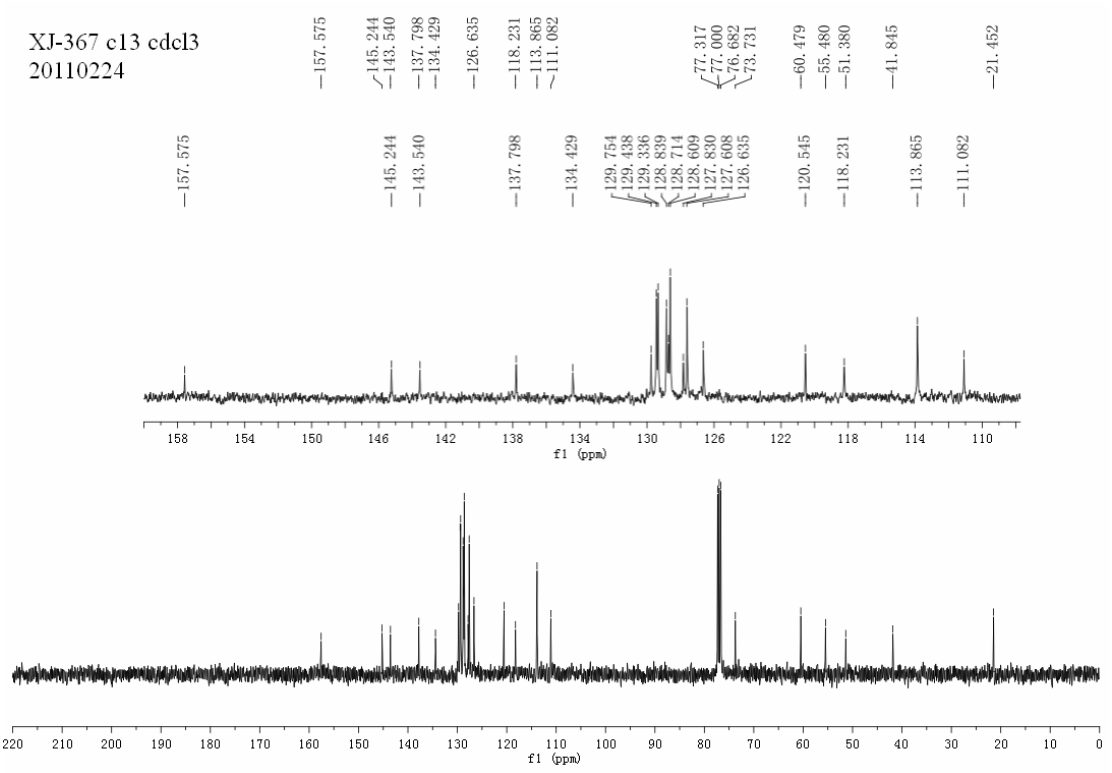

UCA056
06-Jan-2011
17:57:39
1: TOF MS LD+
1.54e5
XiaoWJ-XJ-345-O 17 (1.003) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (1:24)
[M+H]+ = 483.2106
△ = 0.0003
483.2109
481.1960
484.2138
485.2177
486.2220
487.2251
327.1848
328.1877
325.1690
196.1076
210.1250
256.2598
184.0473
117.0595
381.1580
417.2366
469.1999
551.1984
587.2648
%
m/z

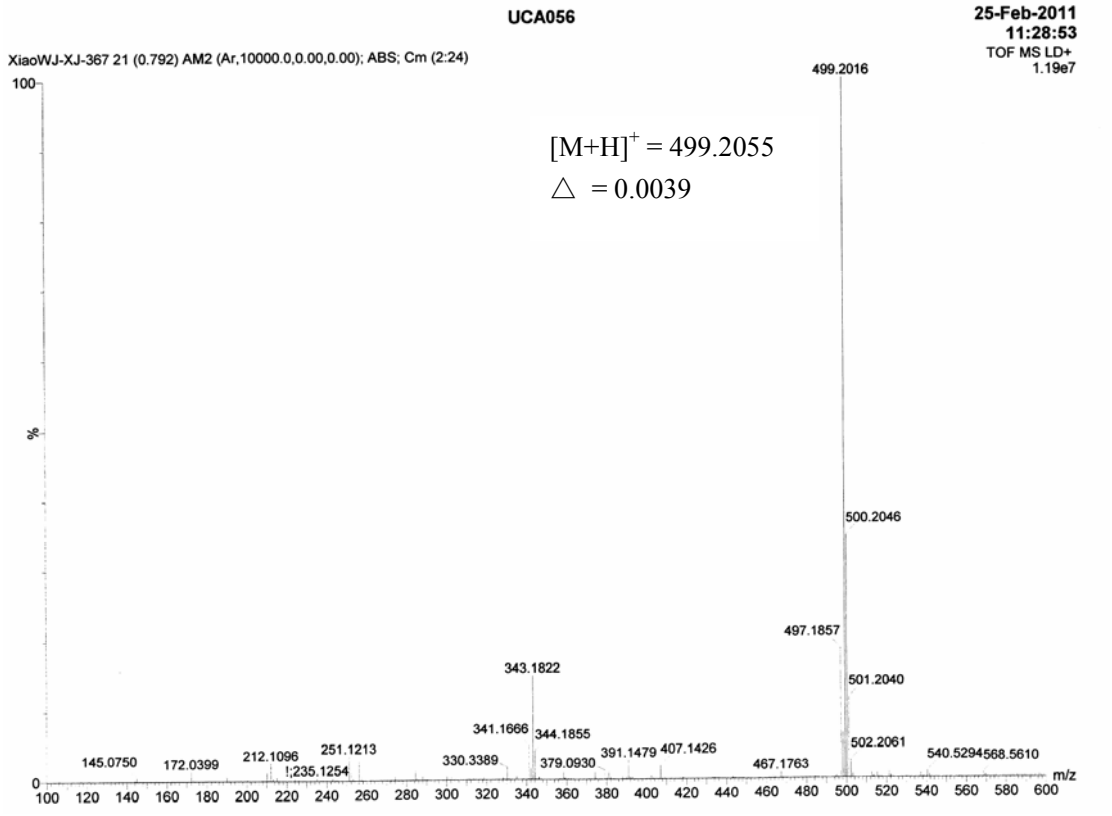

XJ-339 cdcl3
20101221
2c
f1 (ppm)

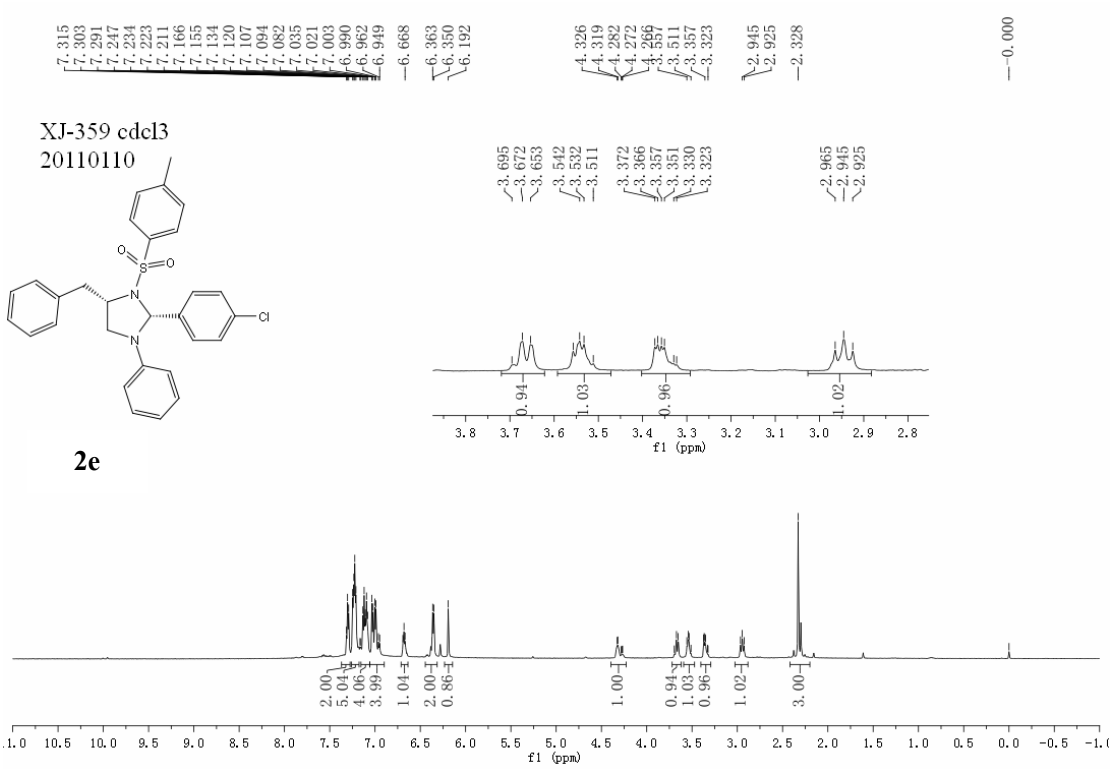

XJ-339 c13 cdcl3
20101221
f1 (ppm)

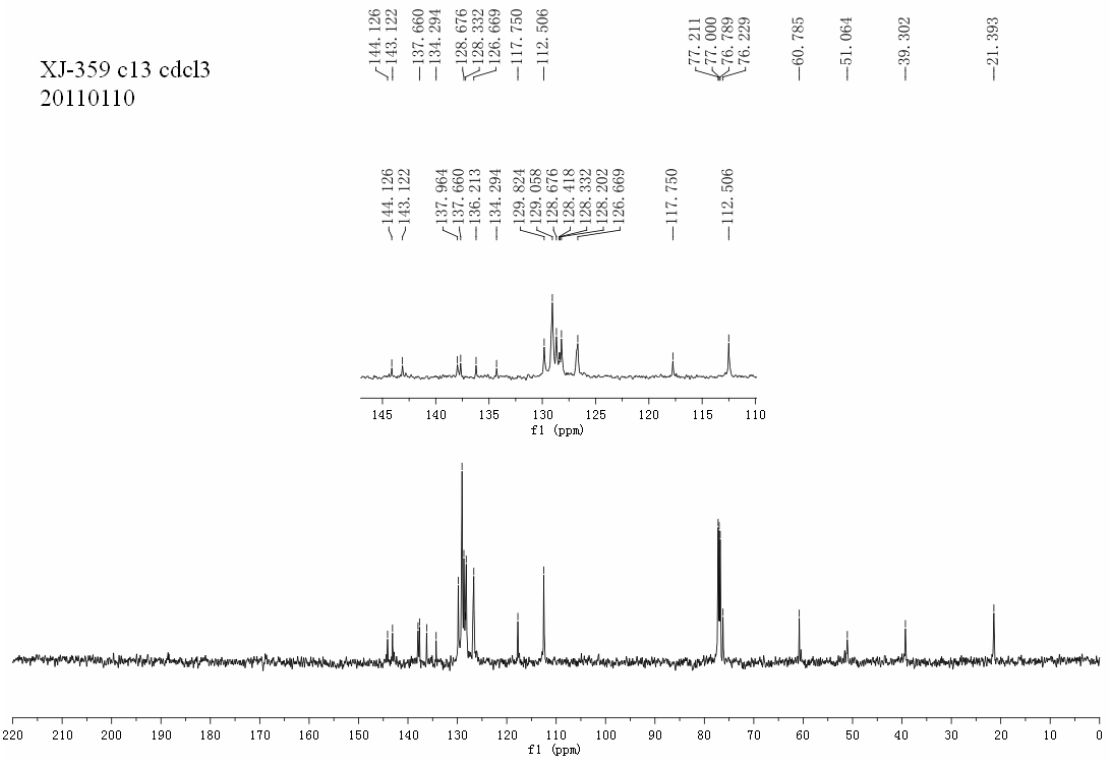

UCA056
21-Dec-2010
20:09:29
1: TOF MS LD+
7.38e5
XiaoWJ-XJ-339-O2 20 (1.113) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (1:24)
[M+H]+ = 499.2055
△ = 0.0019
499.2036
500.2065
497.1880
501.2063
502.2088
343.1785
344.1815
341.1622
121.0523
190.0164
212.1019
256.2593
277.1105
403.1408
437.1938
453.1673
537.1561
569.1970
589.2440
%
m/z

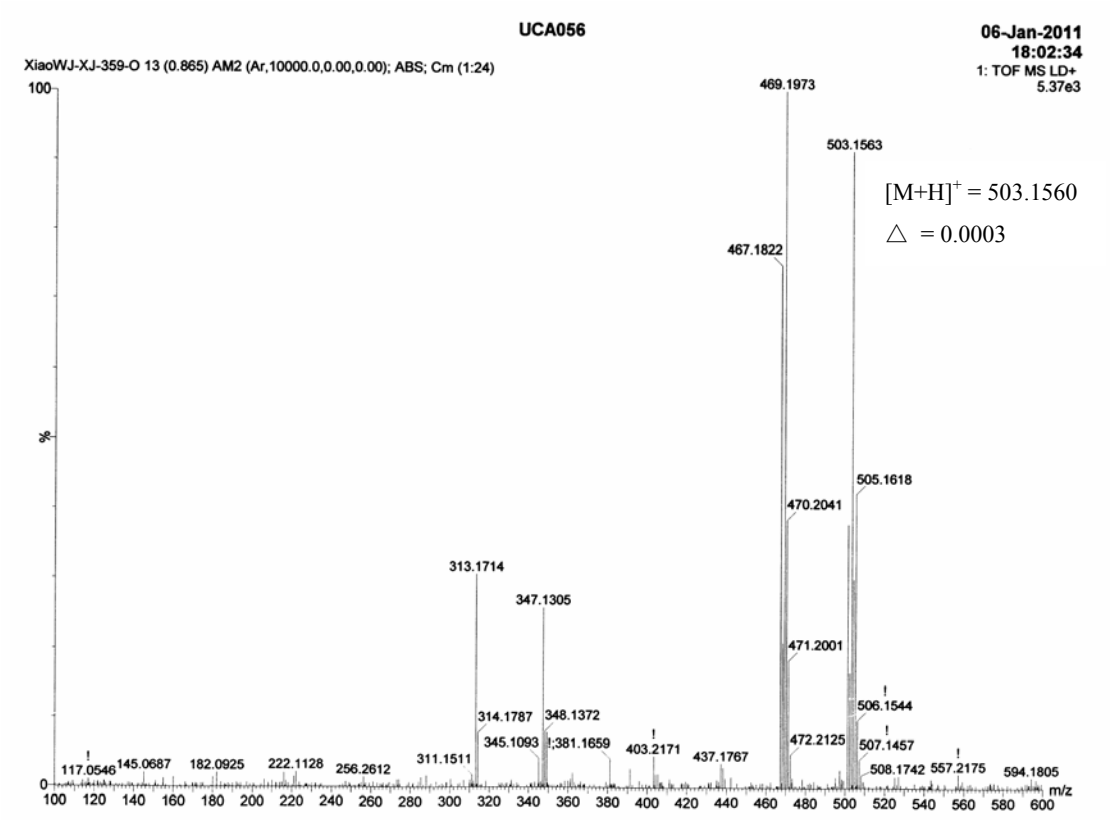

XJ-367 cdcl3
20110224
2d
f1 (ppm)

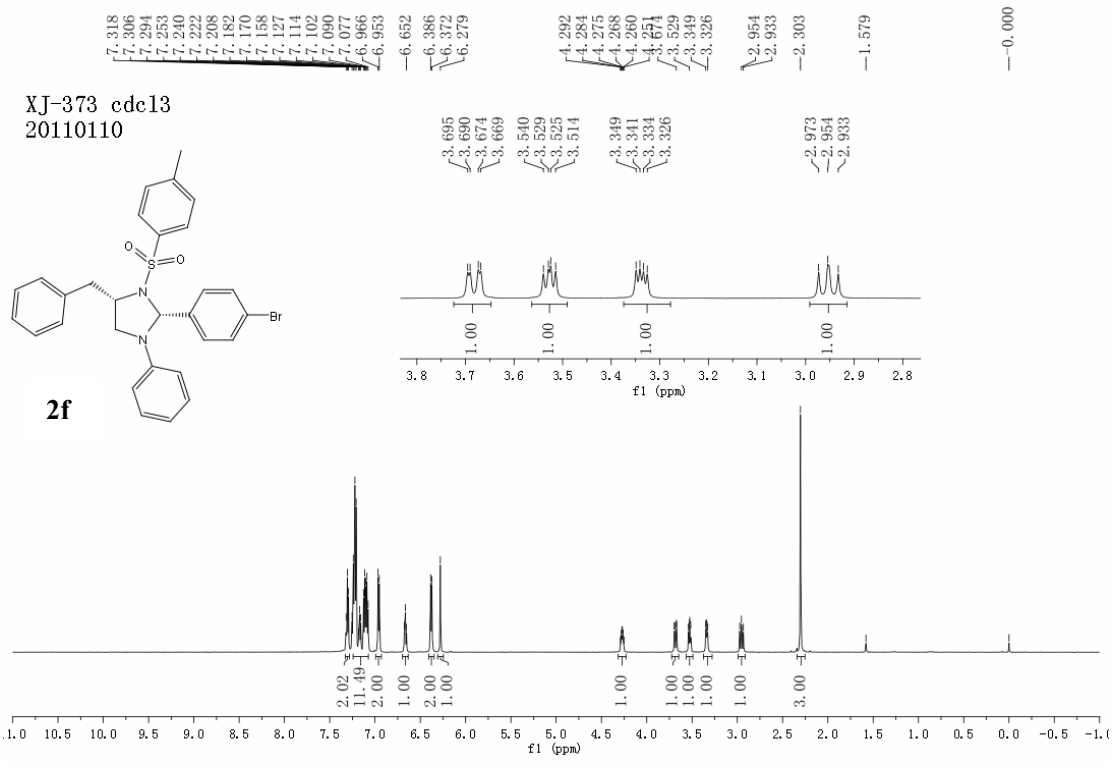

XJ-367 c13 cdcl3
20110224
157.575
145.244
143.540
137.798
134.429
126.635
118.231
113.865
111.082
77.317
77.000
76.682
73.731
60.479
55.480
51.380
41.845
21.452
f1 (ppm)

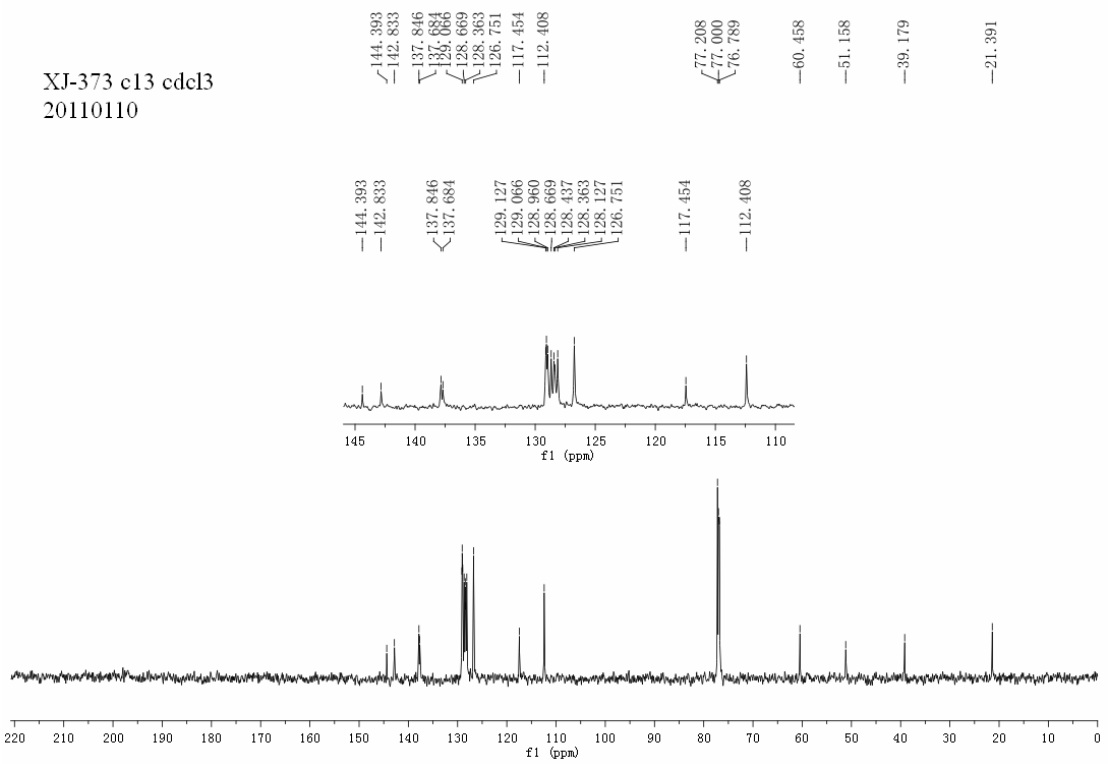

UCA056
25-Feb-2011
11:28:53
TOF MS LD+
1.19e7
XiaoWJ-XJ-367 21 (0.792) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (2:24)
499.2016
[M+H]+ = 499.2055
△ = 0.0039
500.2046
497.1857
501.2040
343.1822
341.1666
344.1855
502.2061
145.0750
172.0399
212.1096
251.1213
235.1254
330.3389
379.0930
391.1479
407.1426
467.1763
540.5294
568.5610
m/z

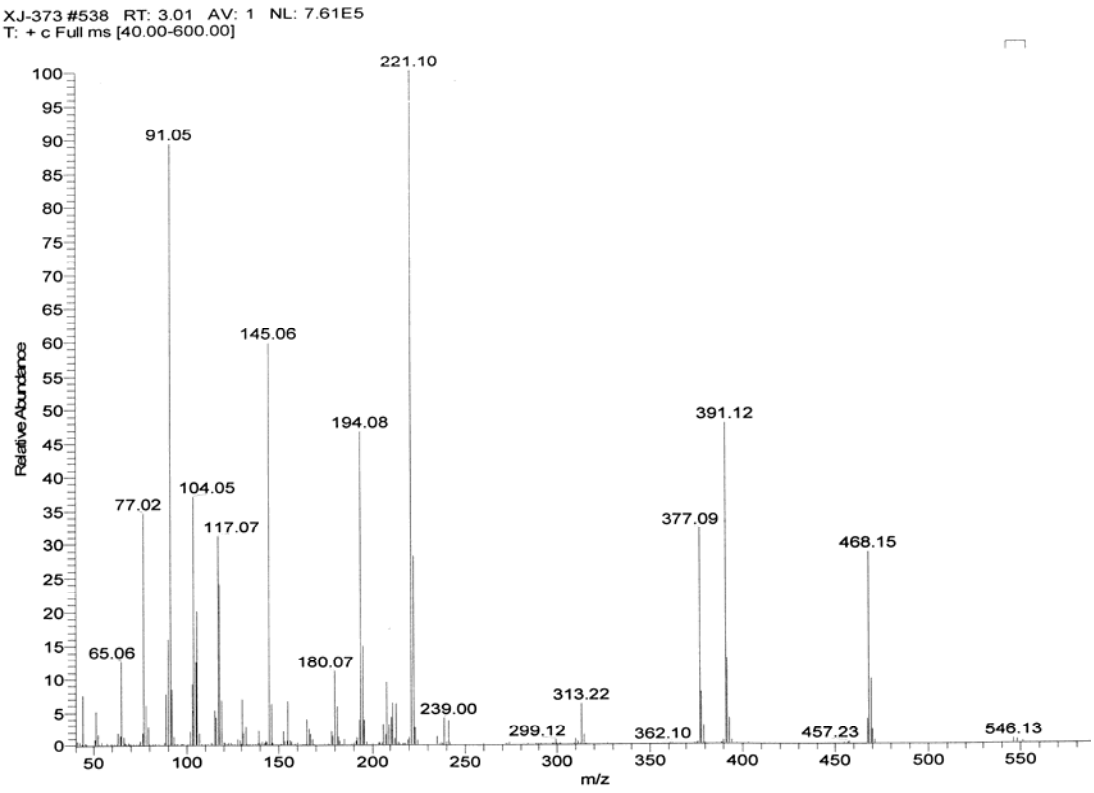

XJ-359 cdcl3
20110110
2e
f1 (ppm)

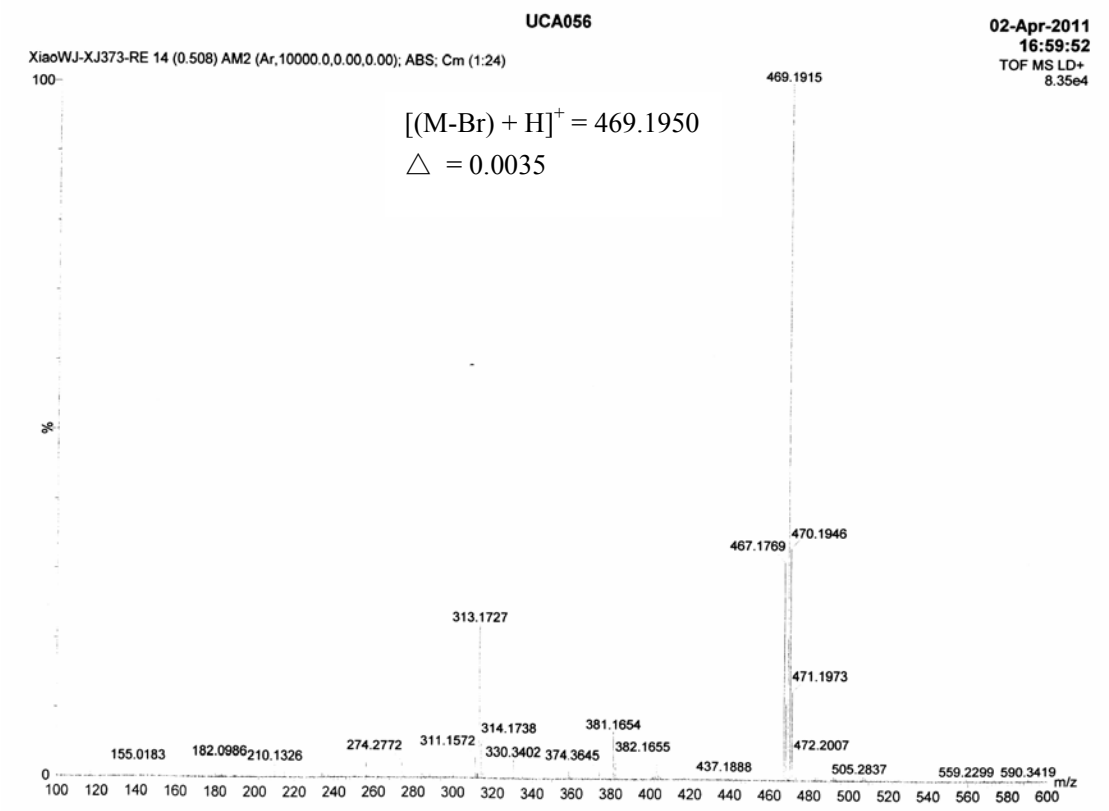

XJ-359 c13 cdcl3
20110110
f1 (ppm)

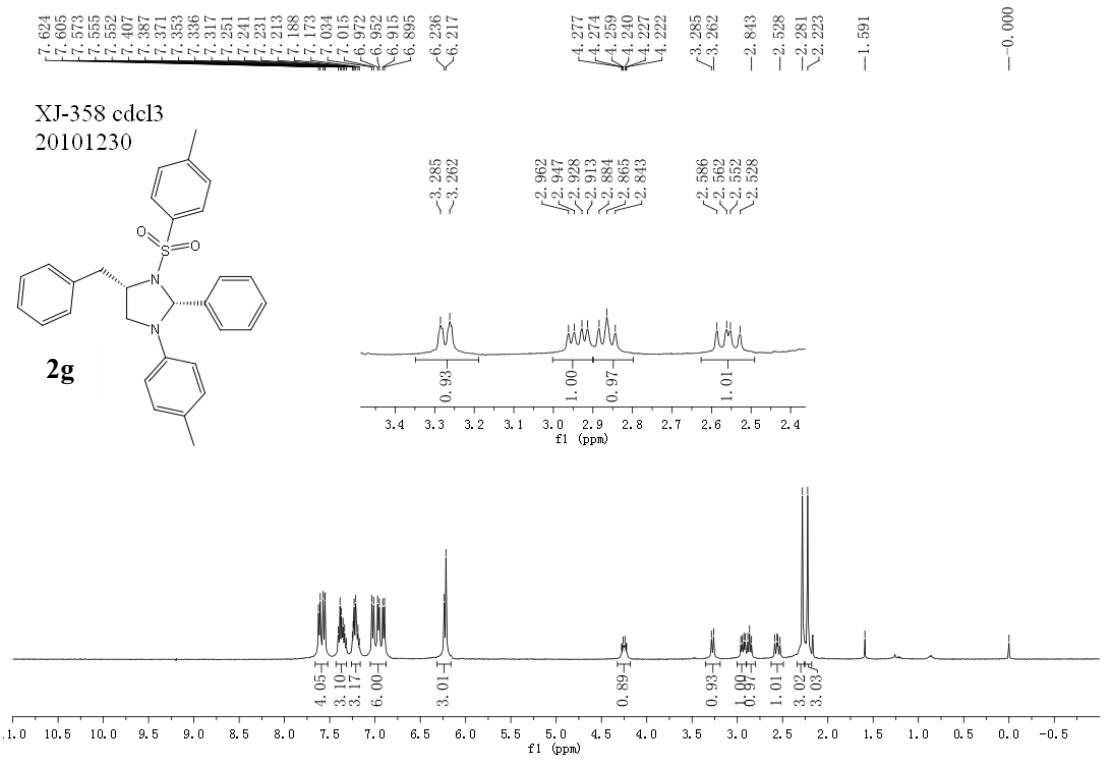

UCA056
06-Jan-2011
18:02:34
1: TOF MS LD+
5.37e3
XiaoWJ-XJ-359-O 13 (0.865) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (1:24)
[M+H]+ = 503.1560
△ = 0.0003
469.1973
503.1563
467.1822
505.1618
470.2041
313.1714
347.1305
471.2001
506.1544
314.1787
348.1372
345.1093
381.1659
403.2171
437.1767
472.2125
507.1457
117.0546
145.0687
182.0925
222.1128
256.2612
311.1511
508.1742
557.2175
594.1805
m/z

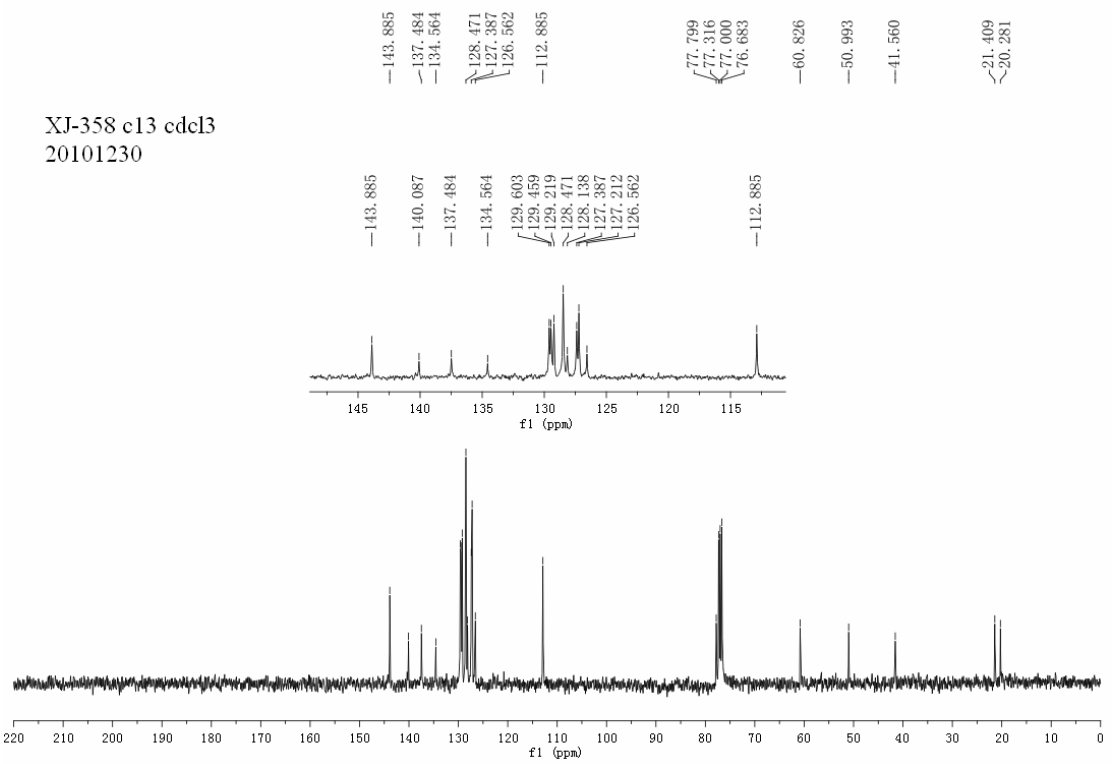

XJ-373 cdcl3
20110110
2f
Br
f1 (ppm)

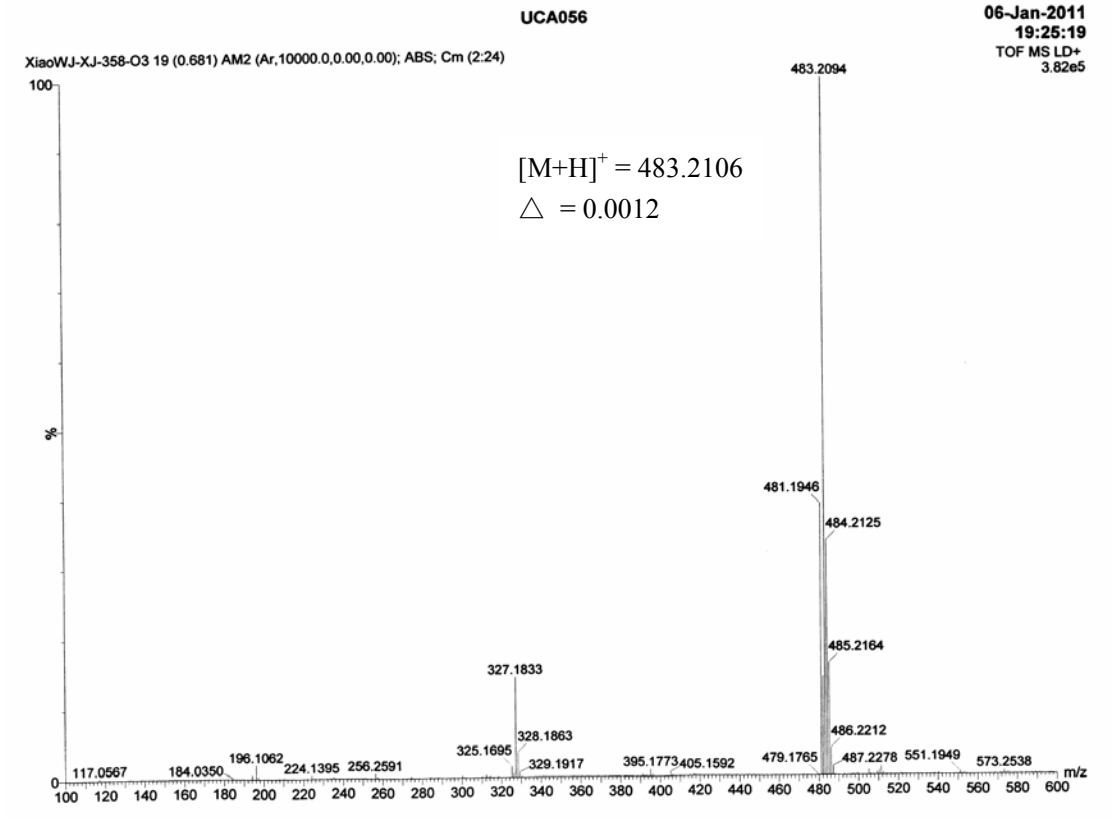

XJ-373 c13 cdcl3
20110110
144.393
142.833
137.846
137.684
129.066
128.960
128.669
128.437
128.363
128.127
126.751
117.454
112.408
77.208
77.000
76.789
60.458
51.158
39.179
21.391
f1 (ppm)

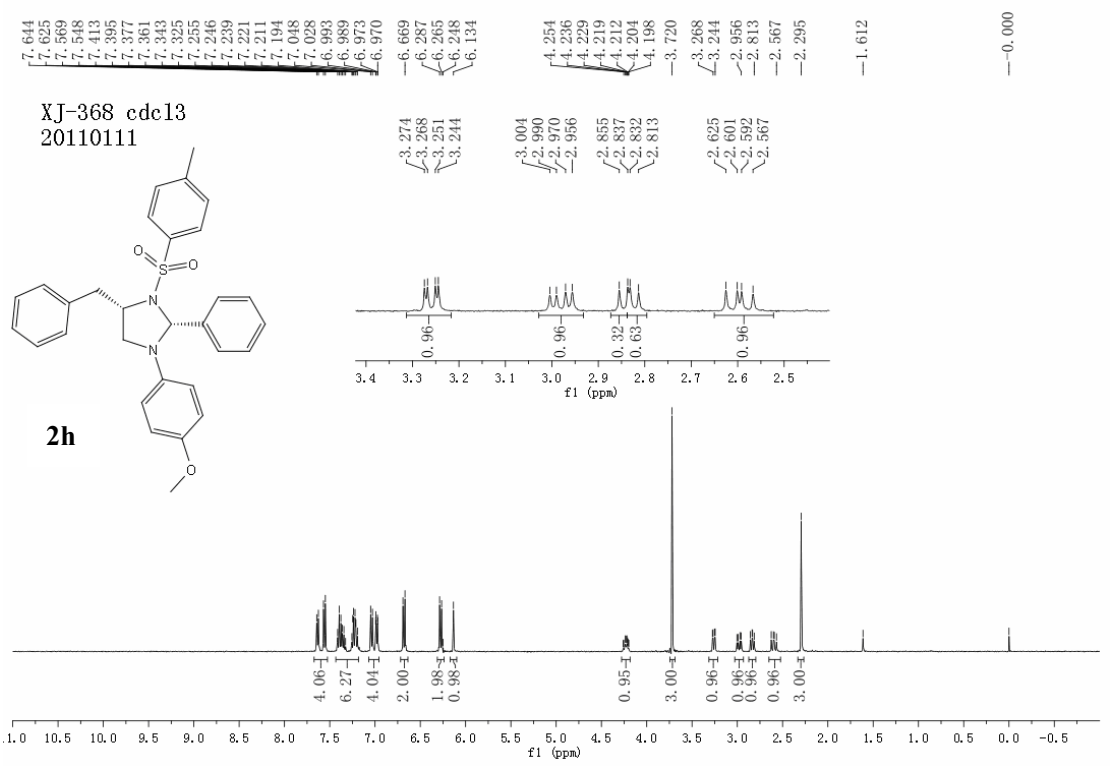

XJ-373 #538 RT: 3.01 AV: 1 NL: 7.61E5
T: + c Full ms [40.00-600.00]
Relative Abundance
m/z
221.10
91.05
145.06
194.08
391.12
104.05
77.02
117.07
377.09
468.15
65.06
180.07
239.00
313.22
299.12
362.10
457.23
546.13

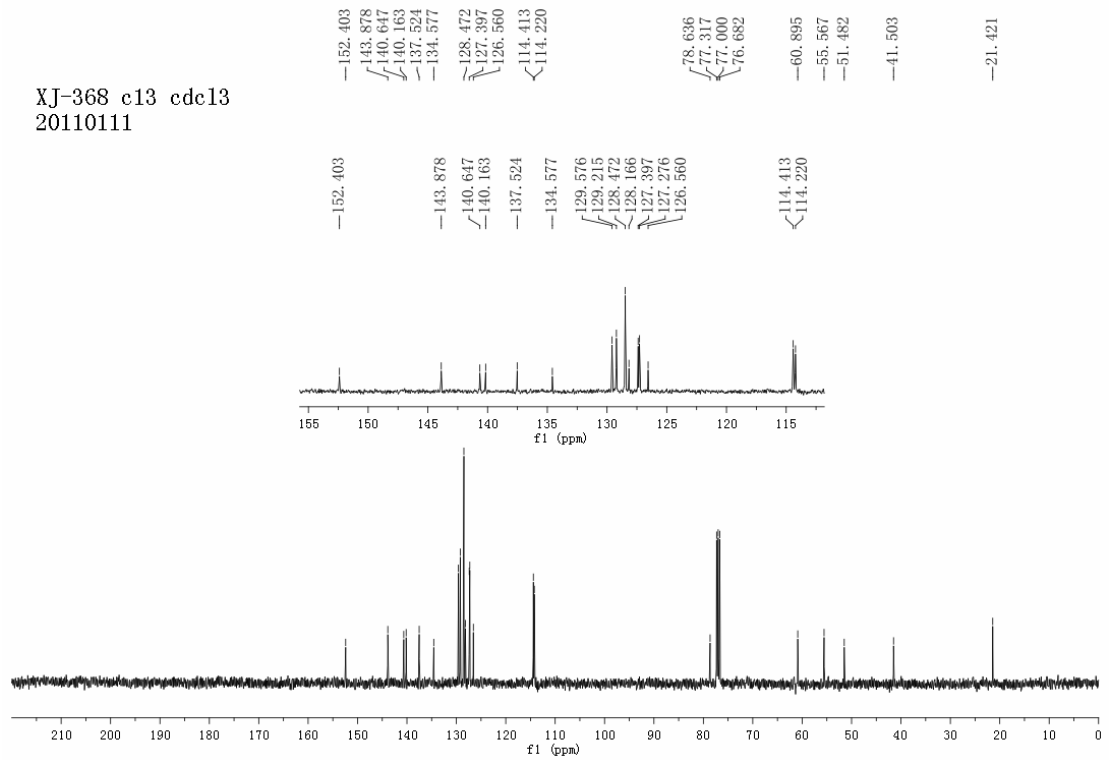

UCA056
02-Apr-2011
16:59:52
TOF MS LD+
8.35e4
XiaoWJ-XJ373-RE 14 (0.508) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (1:24)
100
%
0
[(M-Br) + H]+ = 469.1950
△ = 0.0035
469.1915
470.1946
467.1769
313.1727
471.1973
314.1738
381.1654
382.1655
330.3402
374.3645
311.1572
274.2772
155.0183
182.0986
210.1326
472.2007
437.1888
505.2837
559.2299
590.3419
m/z

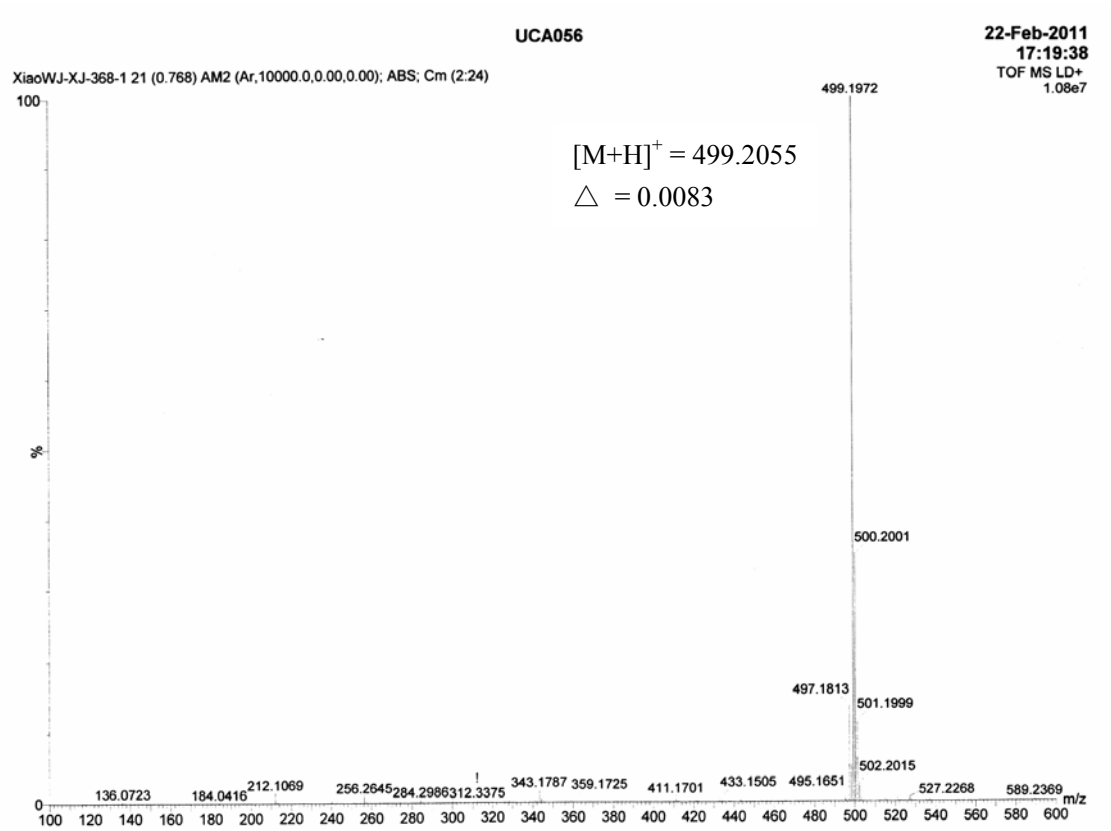

XJ-358 cdcl3
20101230
2g
f1 (ppm)

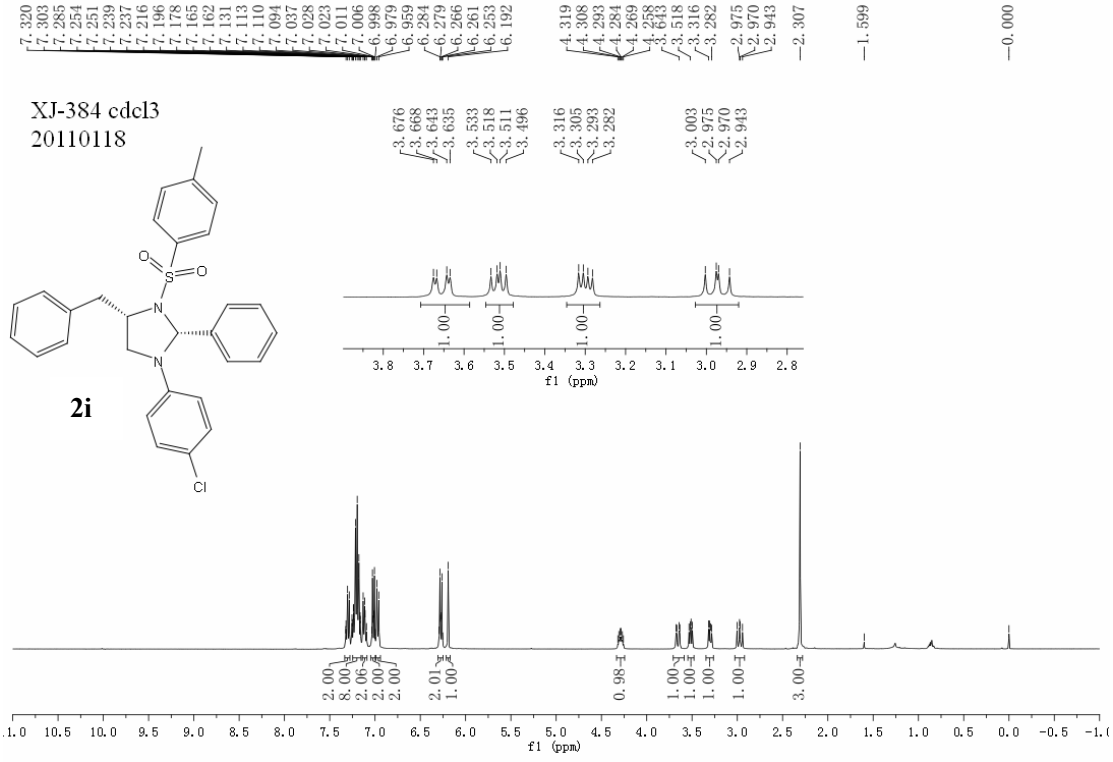

143.885
137.484
134.564
128.471
127.387
126.562
112.885
77.799
77.316
77.000
76.683
60.826
50.993
41.560
21.409
20.281
XJ-358 c13 cdcl3
20101230
143.885
140.087
137.484
134.564
129.603
129.459
129.219
128.471
128.138
127.387
127.212
126.562
112.885
145 140 135 130 125 120 115
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

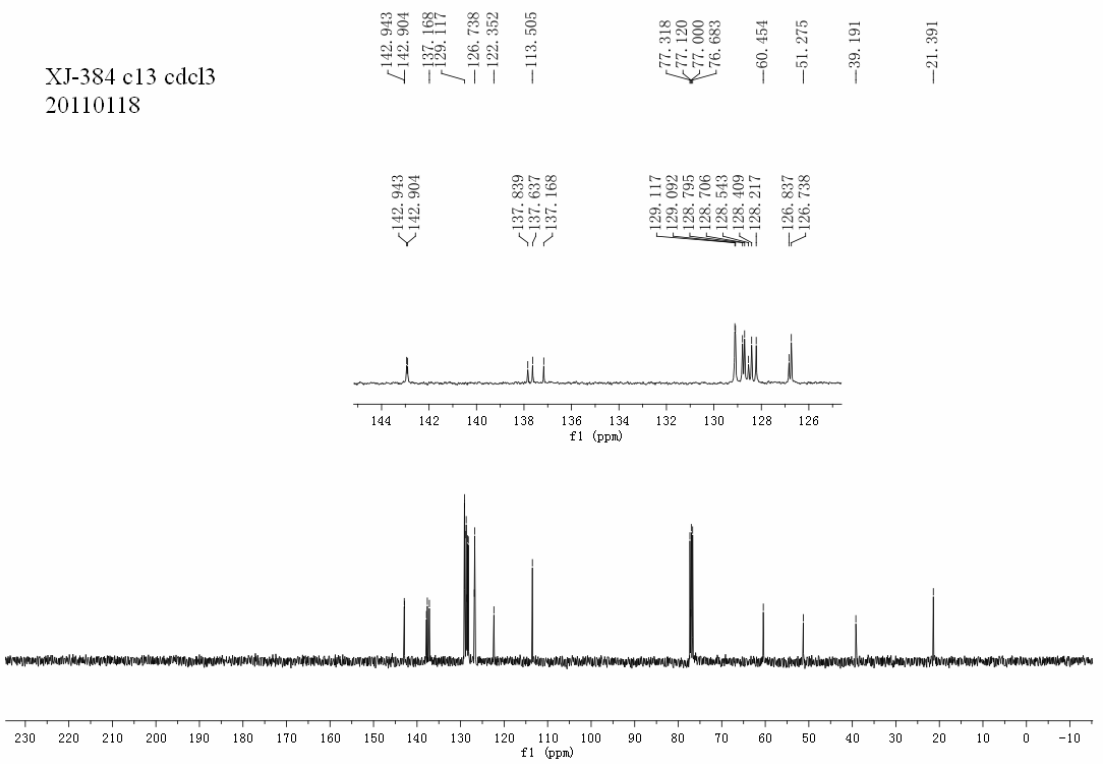

UCA056
06-Jan-2011
19:25:19
TOF MS LD+
3.82e5
XiaoWJ-XJ-358-O3 19 (0.681) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (2:24)
100
%
0
483.2094
481.1946
484.2125
485.2164
327.1833
328.1863
486.2212
325.1695
329.1917
196.1062
224.1395
256.2591
117.0567
184.0350
395.1773
405.1592
479.1765
487.2278
551.1949
573.2538
m/z
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
[M+H]+ = 483.2106
△ = 0.0012

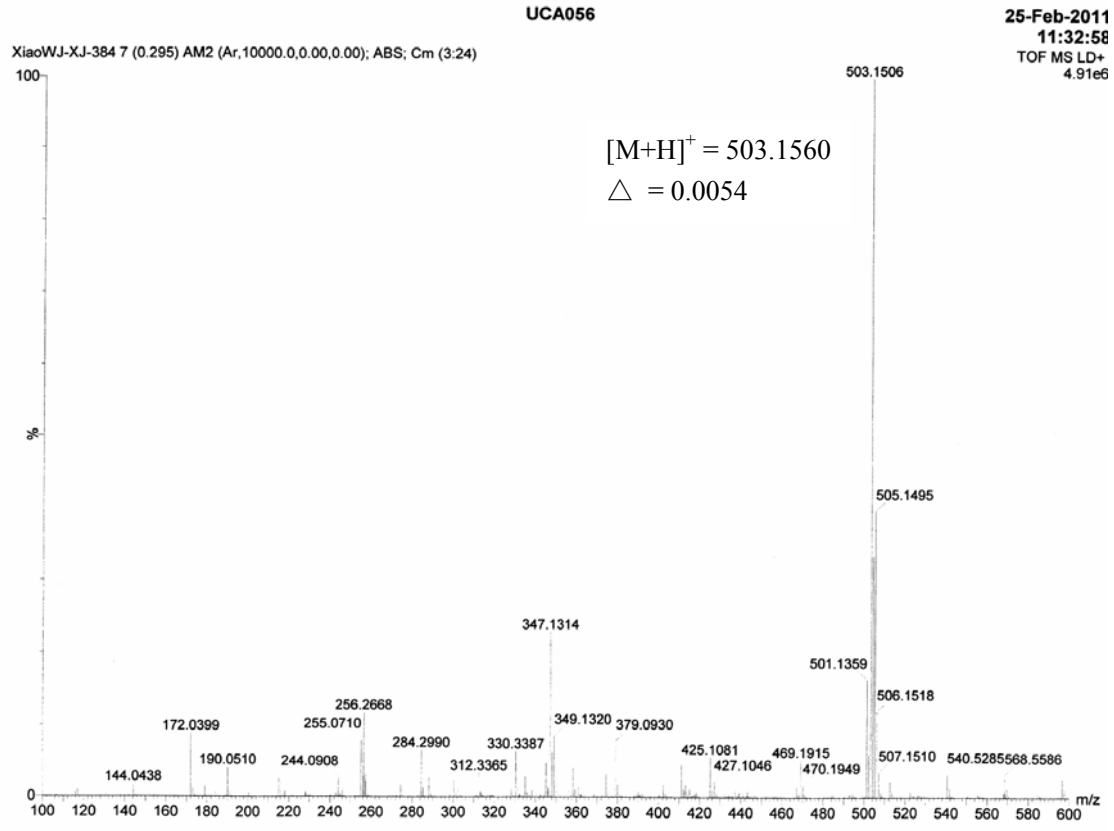

XJ-368 cdcl3
20110111
2h
f1 (ppm)


XJ-368 c13 cdcl3
20110111
f1 (ppm)


UCA056
22-Feb-2011
17:19:38
TOF MS LD+
1.08e7
XiaoWJ-XJ-368-1 21 (0.768) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (2:24)
[M+H]+ = 499.2055
△ = 0.0083
499.1972
500.2001
497.1813
501.1999
502.2015
m/z

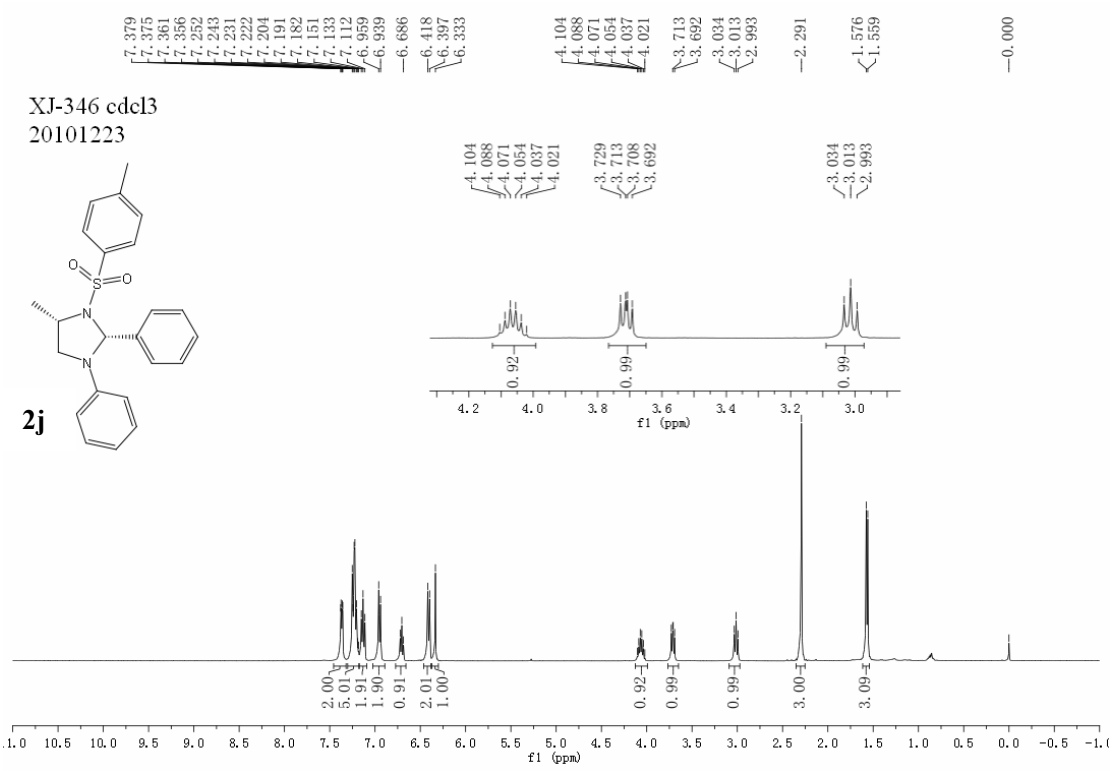

XJ-384 cdcl3
20110118
2i
f1 (ppm)

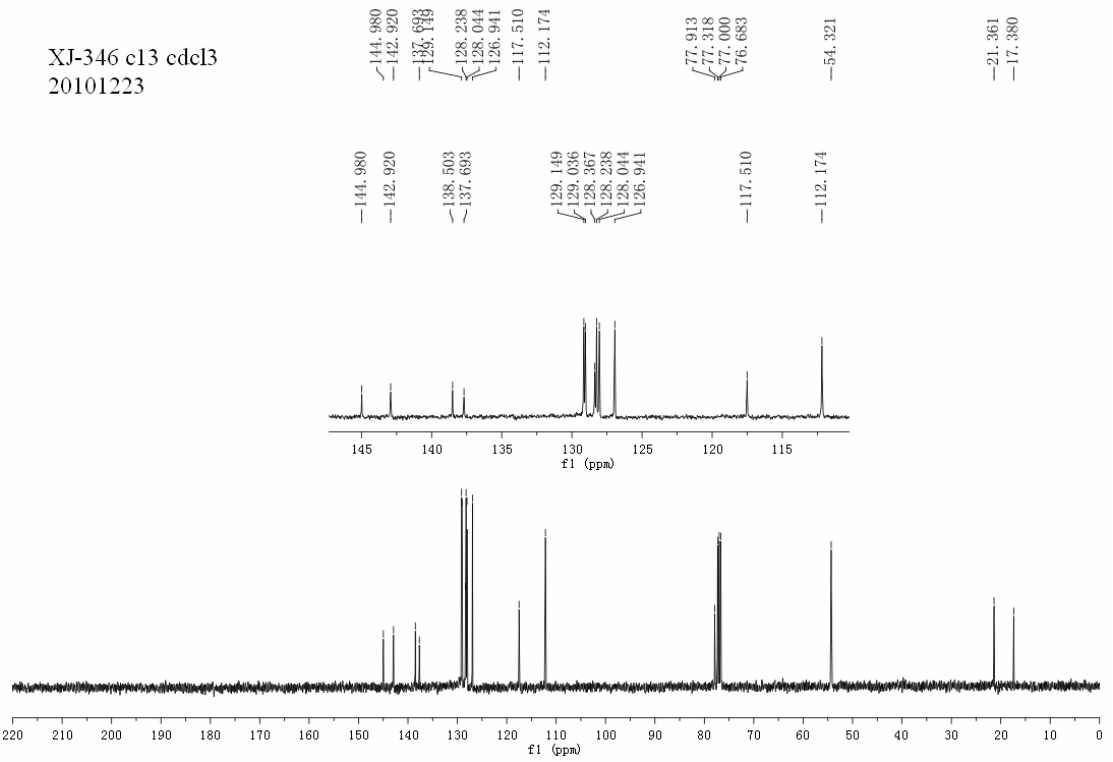


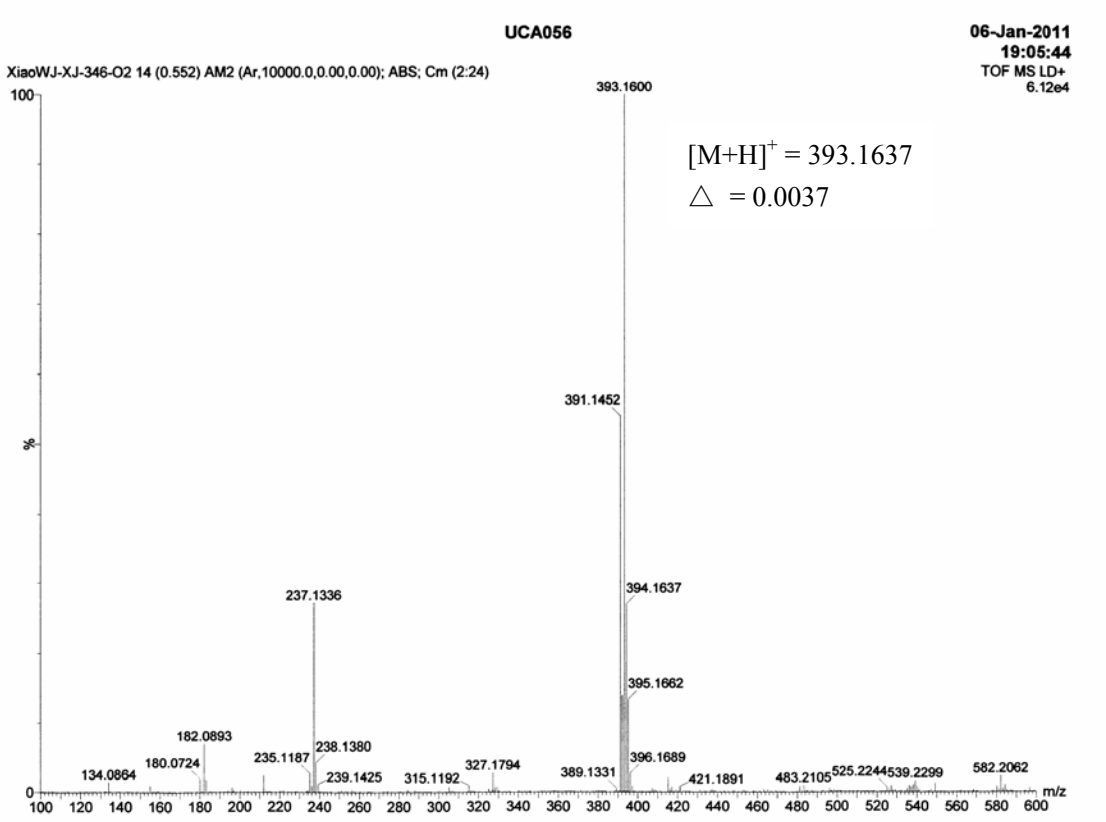


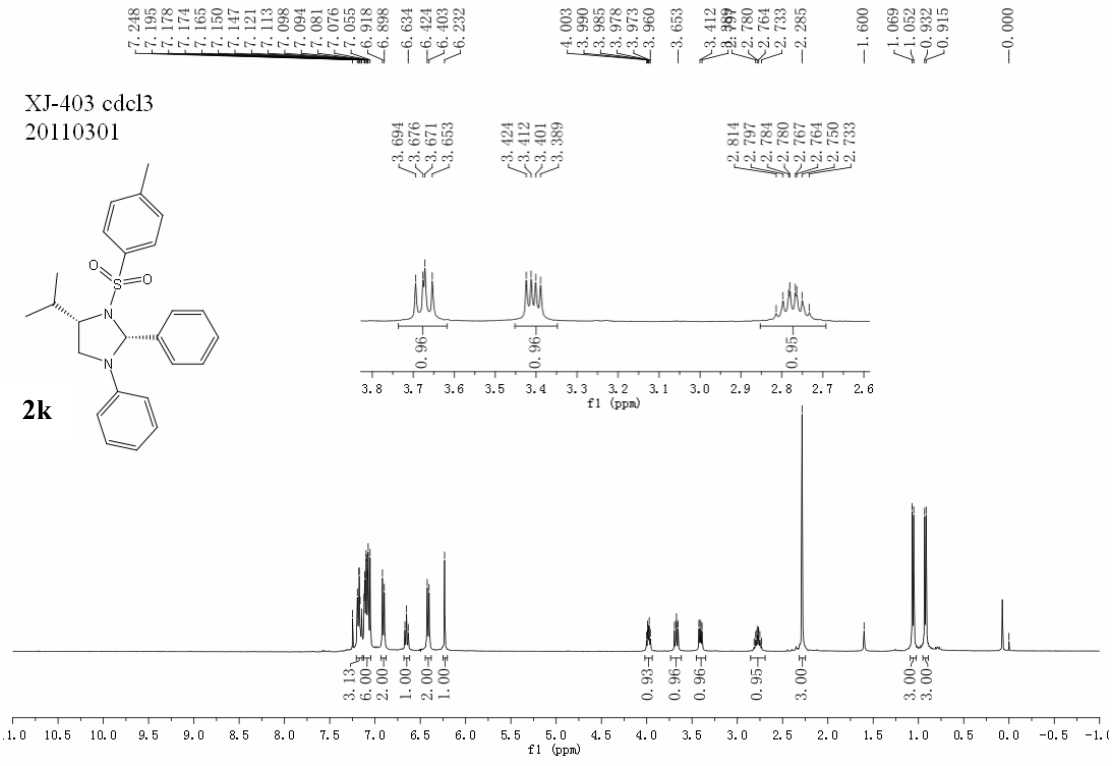
$[M+H]^+ = 503.1560$

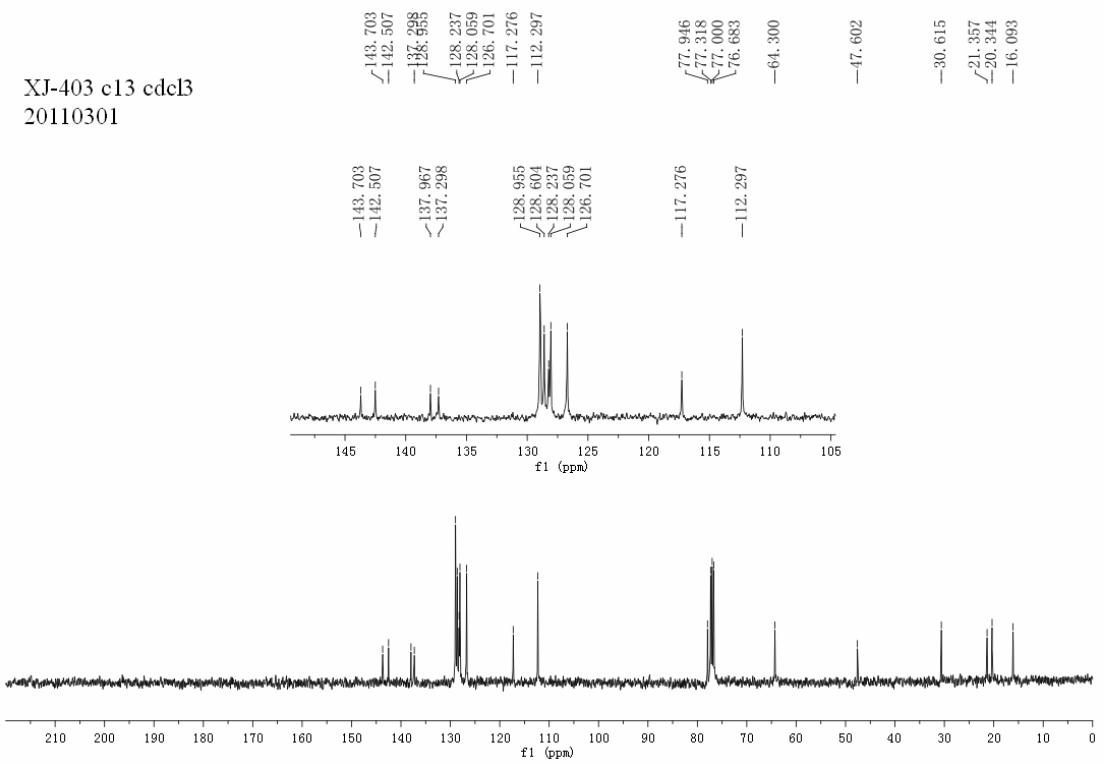
$\triangle = 0.0054$


XJ-346 cdcl3
20101223
2j


XJ-346 c13 cdcl3
20101223


UCA056
06-Jan-2011
19:05:44
TOF MS LD+
6.12e4
XiaoWJ-XJ-346-O2 14 (0.552) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (2:24)
[M+H]+ = 393.1637
△ = 0.0037
393.1600
391.1452
394.1637
237.1336
395.1662
182.0893
238.1380
235.1187
396.1689
180.0724
239.1425
315.1192
327.1794
389.1331
421.1891
483.2105
525.2244
539.2299
582.2062
134.0864
%
m/z


XJ-403 cdcl3
20110301
2k
f1 (ppm)

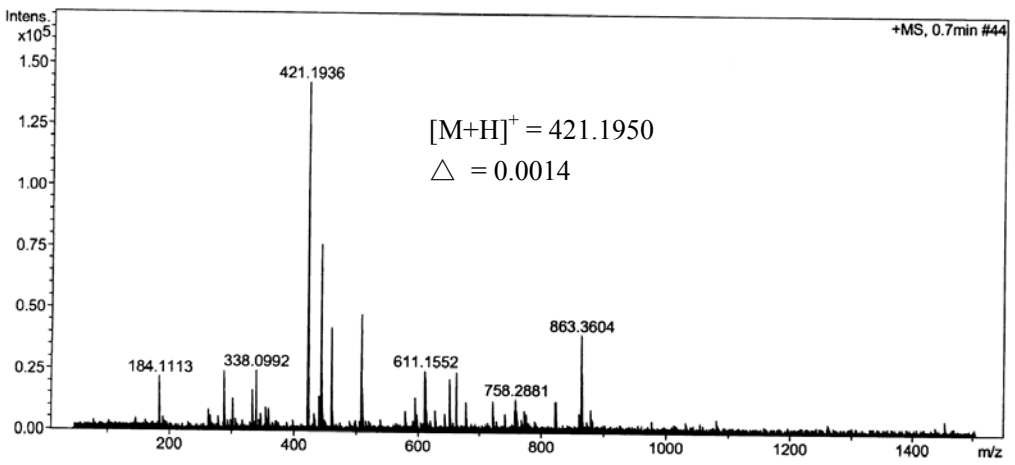


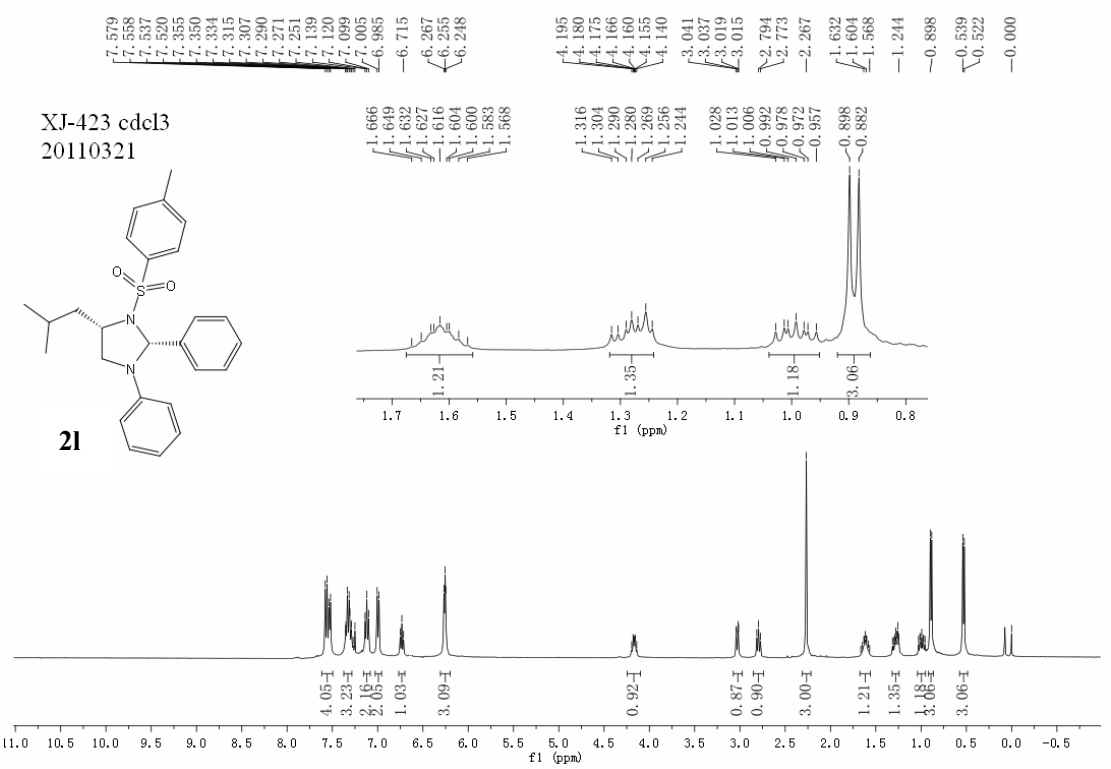
Analysis Info

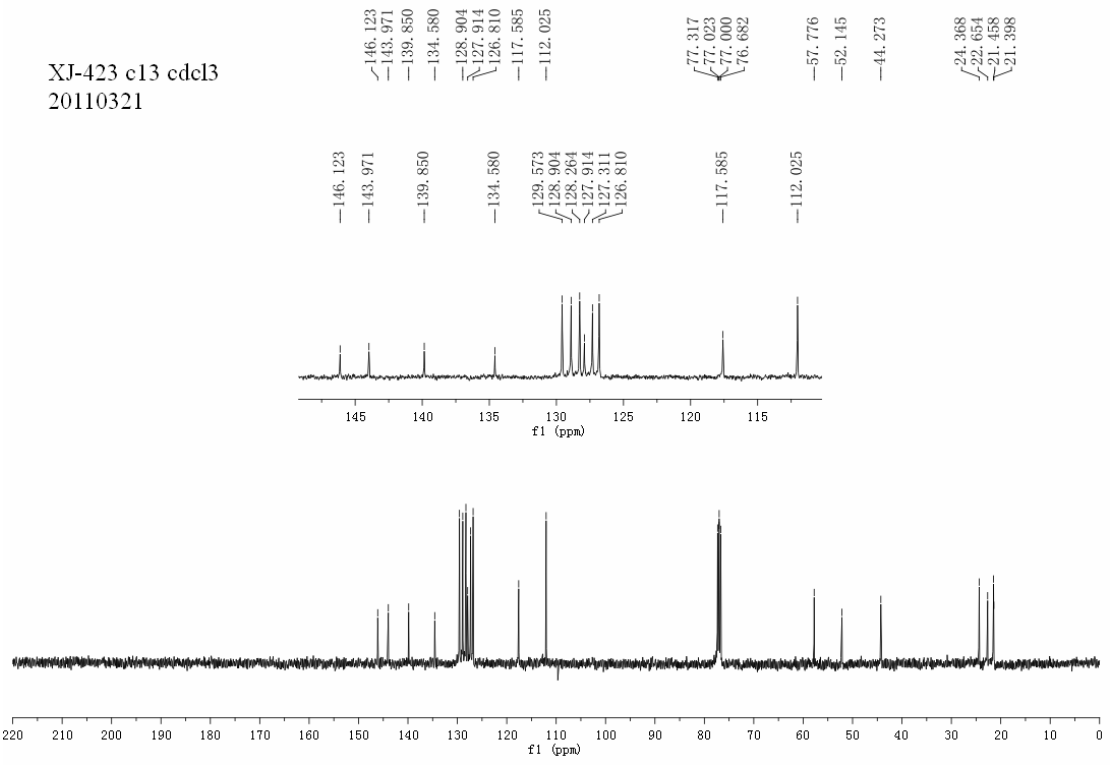
Analysis Name	D:\Data\MS\wj\0324\wc-ysq000015.d	Acquisition Date	3/24/2011 3:33:40 PM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	403	Instrument / Ser#	micrOTOF II 10257
Comment			

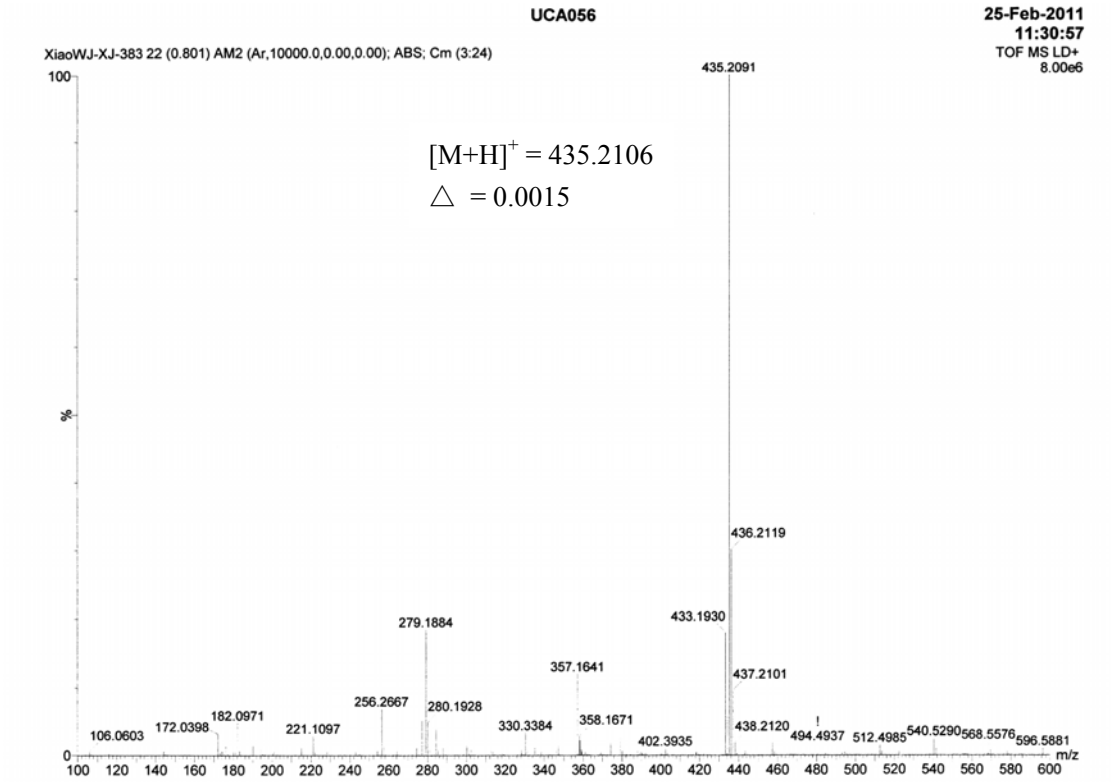
Acquisition Parameter

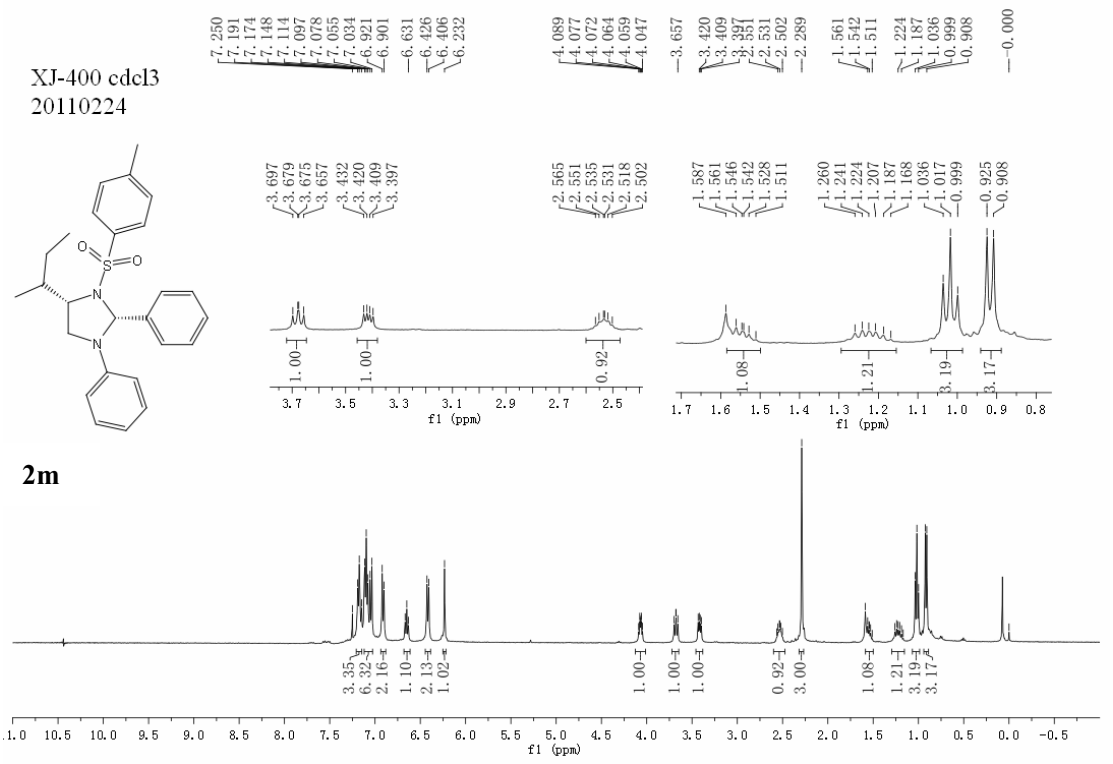
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

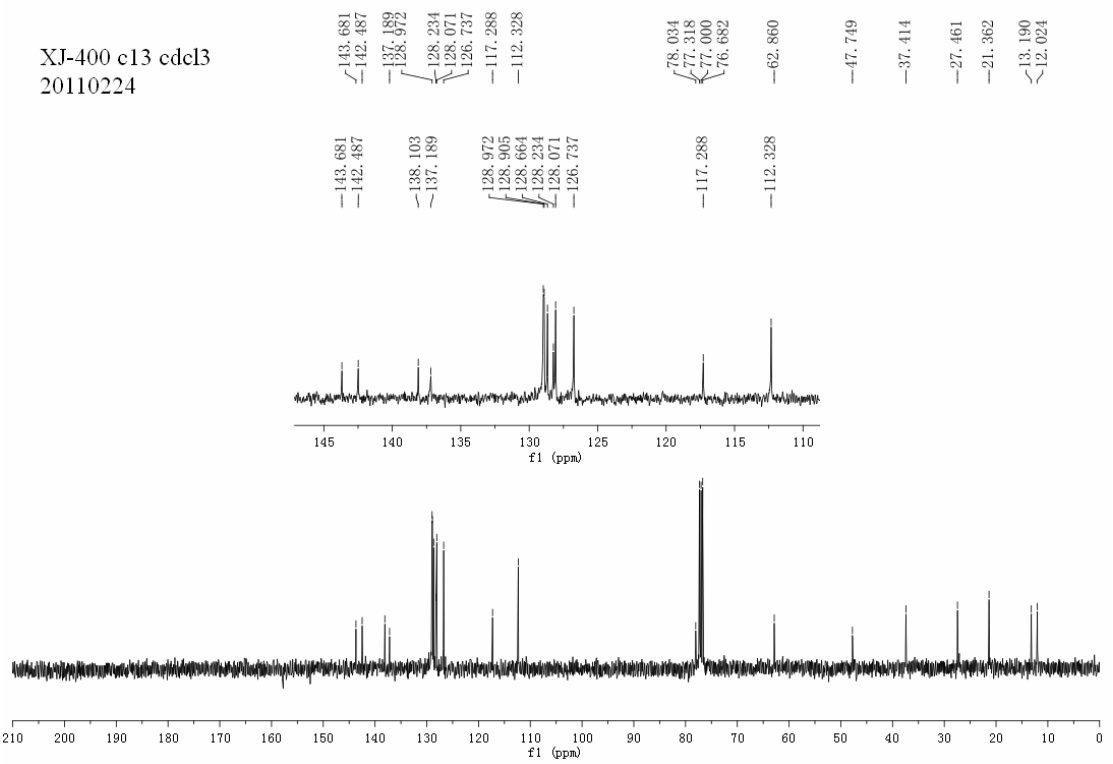


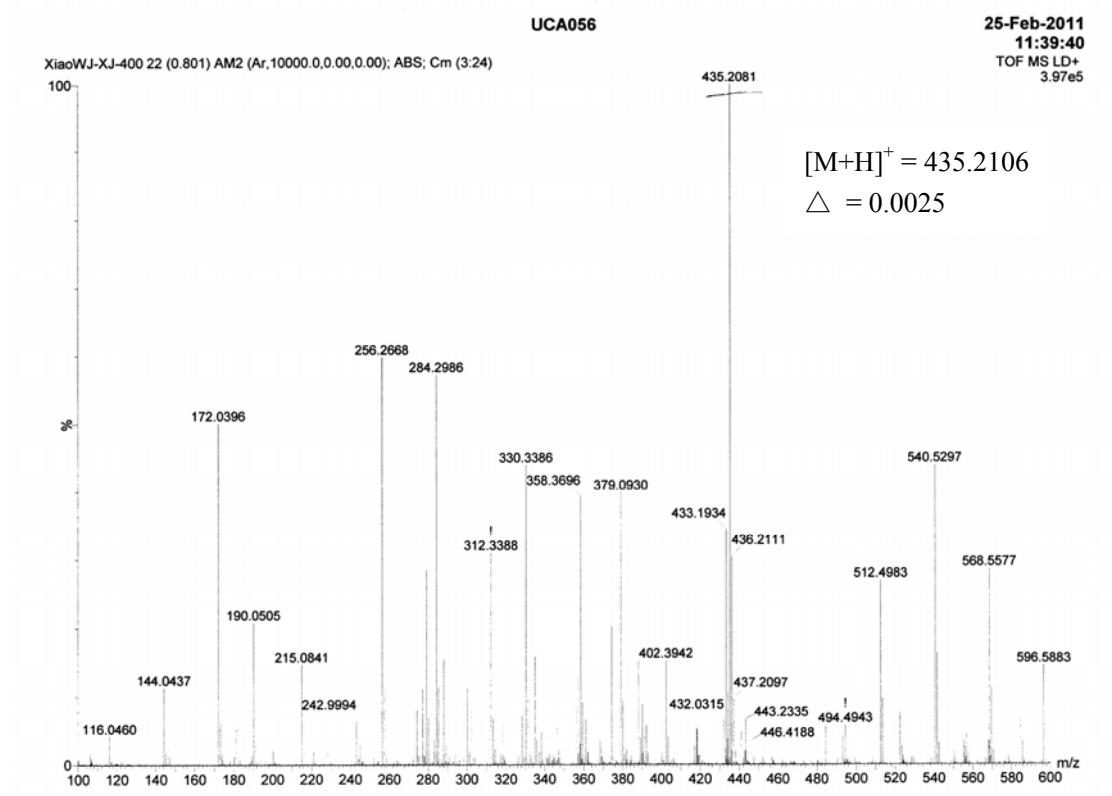

XJ-423 cdcl3
20110321
2l
f1 (ppm)

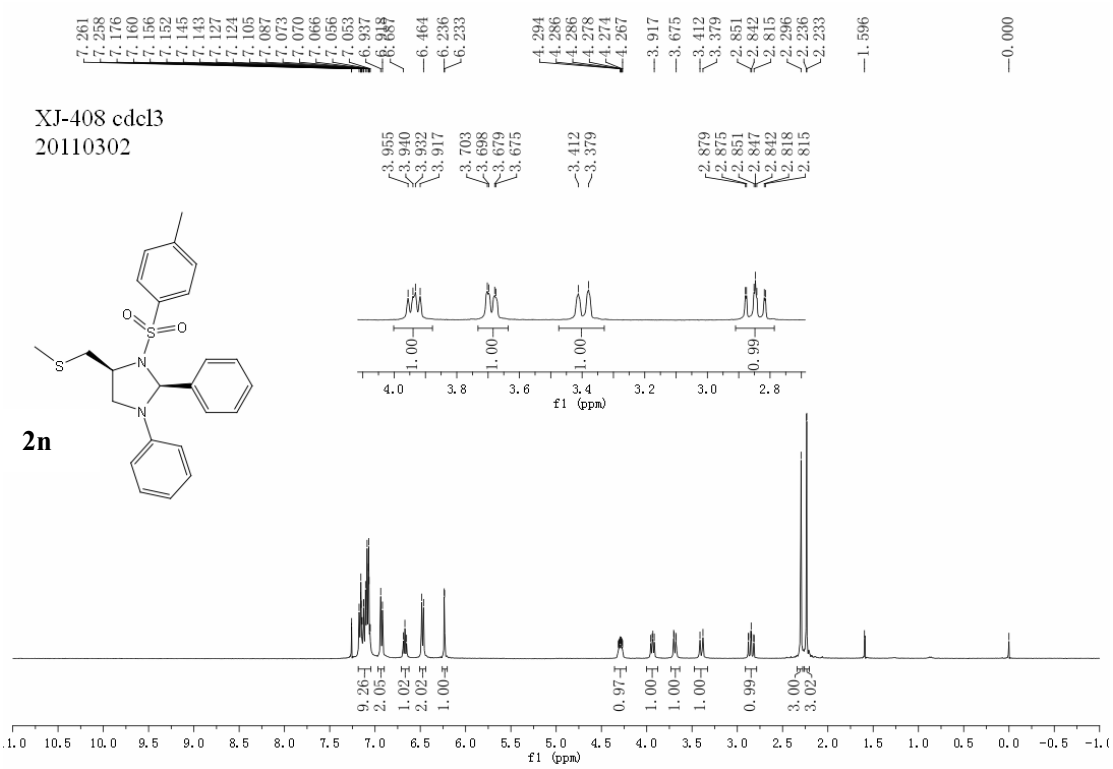

XJ-423 c13 cdcl3
20110321
f1 (ppm)

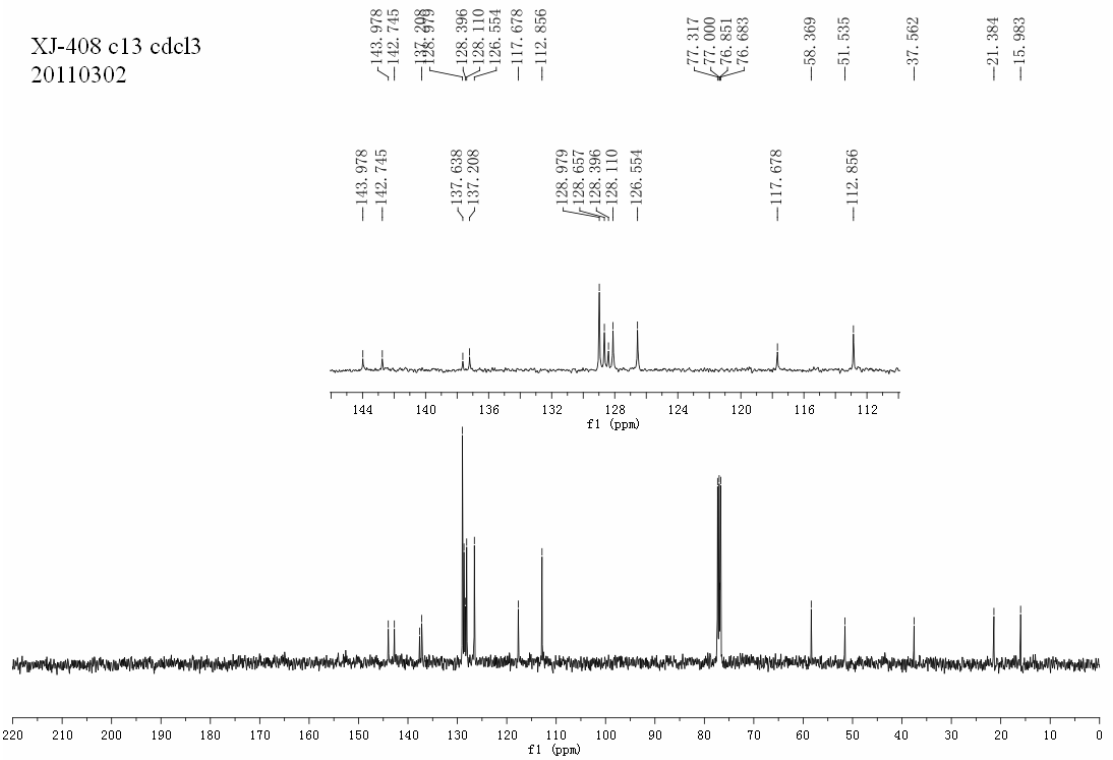

UCA056
25-Feb-2011
11:30:57
TOF MS LD+
8.00e6
XiaoWJ-XJ-383 22 (0.801) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (3:24)
[M+H]+ = 435.2106
△ = 0.0015
435.2091
436.2119
433.1930
437.2101
279.1884
357.1641
256.2667
280.1928
182.0971
172.0398
106.0603
221.1097
330.3384
358.1671
402.3935
438.2120
494.4937
512.4985
540.5290
568.5576
596.5881
%
m/z


XJ-400 cdcl3
20110224
2m
f1 (ppm)


XJ-400 c13 cdcl3
20110224
143.681
142.487
137.189
128.972
128.234
128.071
126.737
117.288
112.328
78.034
77.318
77.000
76.682
62.860
47.749
37.414
27.461
21.362
13.190
12.024
f1 (ppm)


UCA056
25-Feb-2011
11:39:40
TOF MS LD+
3.97e5
XiaoWJ-XJ-400 22 (0.801) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (3:24)
435.2081
[M+H]+ = 435.2106
△ = 0.0025
256.2668
284.2986
172.0396
330.3386
358.3696
379.0930
433.1934
436.2111
540.5297
312.3388
512.4983
568.5577
190.0505
215.0841
402.3942
596.5883
144.0437
437.2097
242.9994
432.0315
443.2335
494.4943
446.4188
116.0460
%
m/z


XJ-408 cdcl3
20110302
2n
f1 (ppm)

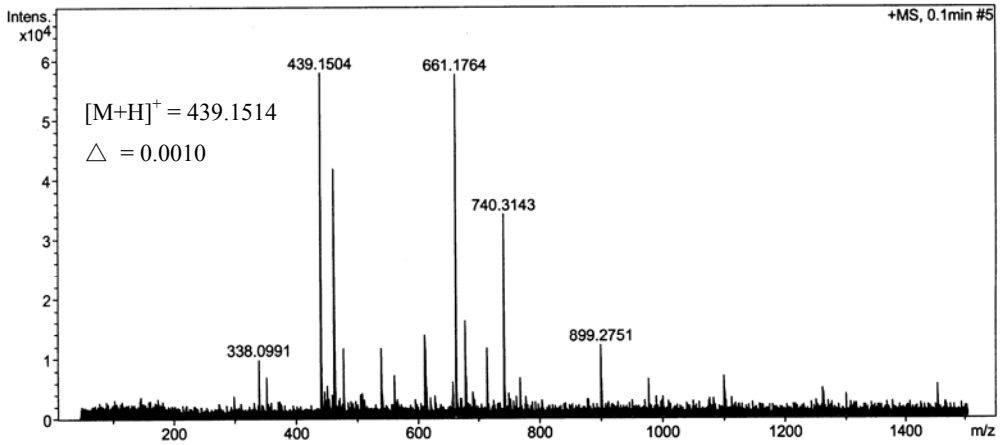

XJ-408 c13 cdcl3
20110302
f1 (ppm)

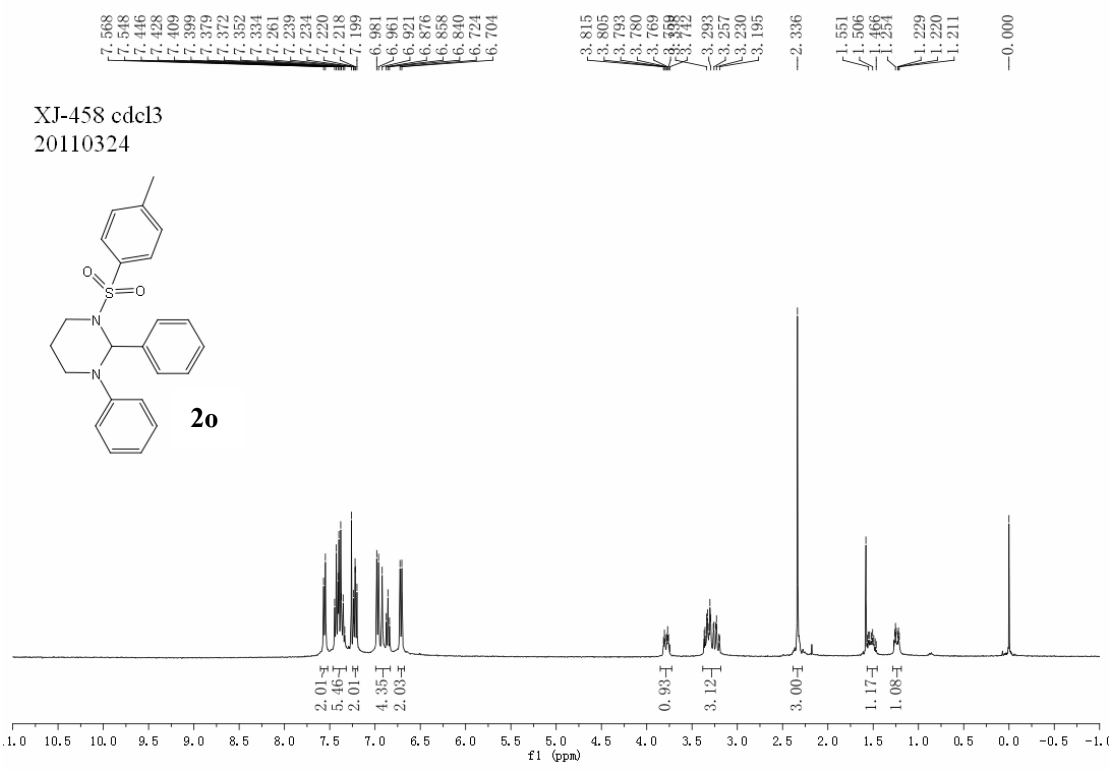
Analysis Info

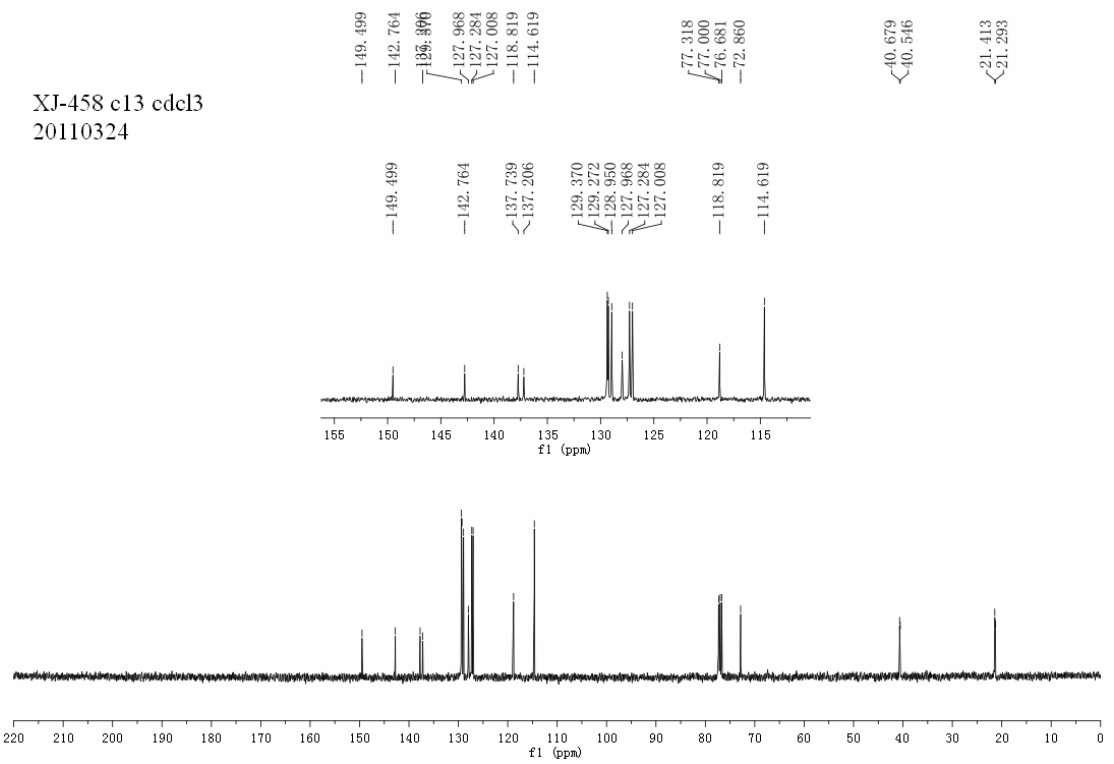
Analysis Name	D:\Data\MS\wj\0324\wc-ysq000014.d	Acquisition Date	3/24/2011 3:32:23 PM
Method	tune_200-800_hcoona-POS.m	Operator	gftang
Sample Name	xj408505	Instrument / Ser#	micrOTOF II 10257
Comment			

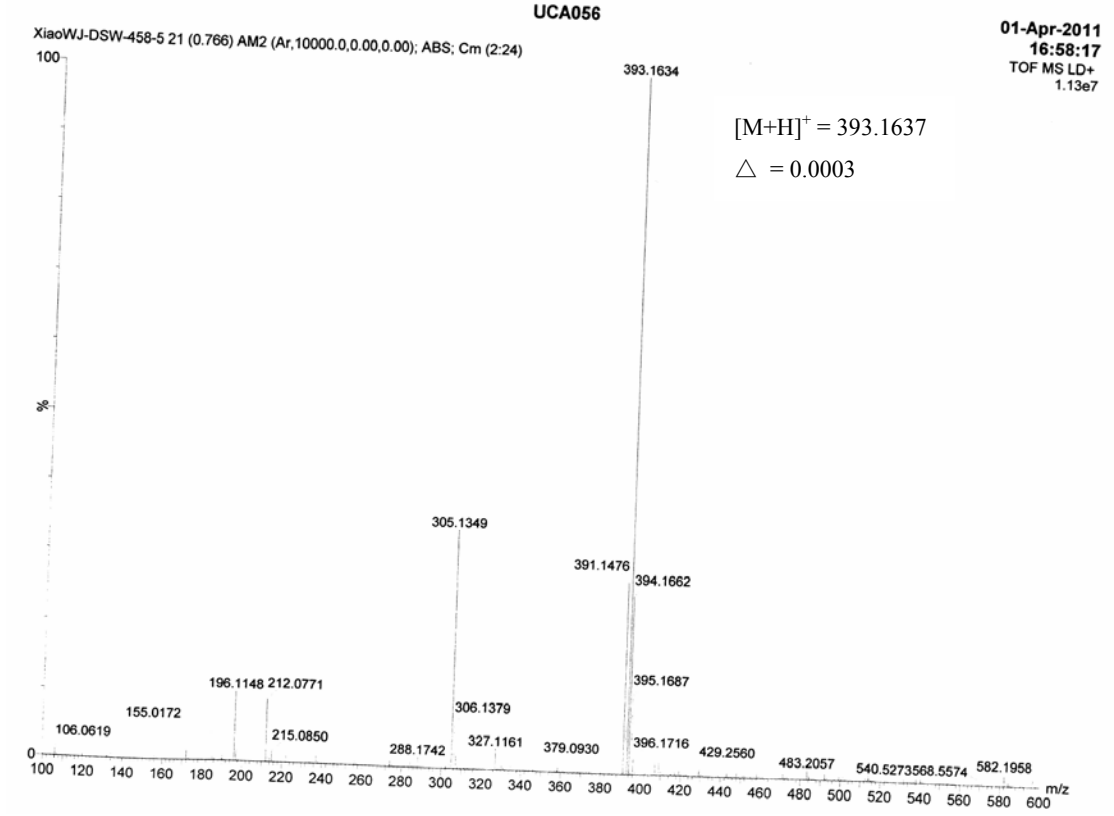
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.6 Bar
Focus	Not active			Set Dry Heater	180 ℃
Scan Begin	50 m/z	Set Capillary	4000 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste






XJ-458 c13 cdcl3
20110324
149.499
142.764
137.739
137.206
129.370
129.272
128.950
127.968
127.284
127.008
118.819
114.619
77.318
77.000
76.681
72.860
40.679
40.546
21.413
21.293
f1 (ppm)


UCA056
XiaoWJ-DSW-458-5 21 (0.766) AM2 (Ar,10000.0,0.00,0.00); ABS; Cm (2:24)
01-Apr-2011
16:58:17
TOF MS LD+
1.13e7
[M+H]+ = 393.1637
△ = 0.0003
393.1634
305.1349
391.1476
394.1662
395.1687
306.1379
196.1148
212.0771
155.0172
106.0619
215.0850
288.1742
327.1161
379.0930
396.1716
429.2560
483.2057
540.5273
568.5574
582.1958
%
m/z