

Supporting Information
for
Enantio- and Diastereoselective Synthesis of
Spiro-Epoxyoxindoles

Amina Boucherif,[‡] Qing-Qing Yang,[‡] Qiang Wang,[‡] Jia-Rong Chen,[‡] Liang-Qiu

Lu,^{*,‡} 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;*

[§] *Collaborative Innovation Center of Chemical Science and
Engineering (Tianjin), China.*

E-mail: wxiao@mail.ccnu.edu.cn; luliangqiu@mail.ccnu.edu.cn

Table of Contents

1. General Information.....	1
2. Materials.....	1
3. Details for Condition Optimization.....	2
4. Absolute Configuration of Representative Product 3ka	3
5. Copies of HPLC for Products.....	4
6. Copies of ¹ H NMR and ¹³ C NMR Spectra.....	18
7. Copies of HRMS for Products.....	32

1. General Information

Proton and carbon nuclear magnetic resonance (^1H and ^{13}C NMR) spectra were recorded on 400/600 MHz spectrometers. Chemical shifts (δ) are reported in parts per million (ppm) relative to residual solvent signals (CHCl_3 , 7.26 ppm for ^1H NMR, CDCl_3 , 77.0 ppm for ^{13}C NMR). Data are reported as follows: chemical shift (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet, br = broad signal), coupling constants (Hz). Mass spectra were measured on MS spectrometer (EI) or LC/MS/MS (ESI-MS). HRMS analysis were taken on an analysis instrument. Chromatographic purification of products was accomplished using airforced- flow chromatography. The enantiomeric excess (ee) of the products was determined by chiral stationary phase HPLC. Optical rotations were measured with a polarimeter.

2. Materials

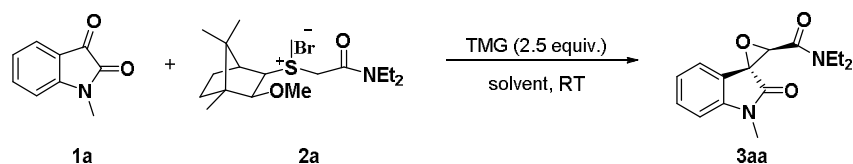
Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvents were treated according to general methods.¹ Flash column chromatography was performed using 200-300 mesh silica gel. *N*-methyl isatins **1a-l** were prepared according to literature procedures from commercially available isatins using a methyl protection reaction.² Sulfonium salts **2a-c** were prepared as described by Aggarwal et al.³ from optically active Camphor, which was commercially available and used as received.

References

- 1 Perrin, D. D. Armarego, W. L. F. Purification of Laboratory Chemicals, 4th ed.; Pergamon Press, Oxford, 1997.
- 2 Barry M. Trost; Y. Zhang; *J. Am. Chem. Soc.* **2007**, *129*, 14548.
- 3 (a) Aggarwal, V. K.; Hynd, G.; Picoul, W.; Vasse, J. *J. Am. Chem. Soc.* **2002**, *124*, 9964. (b) Aggarwal, V. K.; Charmant, J. P. H.; Fuentes, D.; Harvey, J. N.; Hynd, G.; Ohara, D.; Picoul, W.; Robiette, R.; Smith, C.; Vasse, J.; Winn, C. *J. Am. Chem. Soc.* **2006**, *128*, 2105, and references therein.

3. Details for Condition Optimization

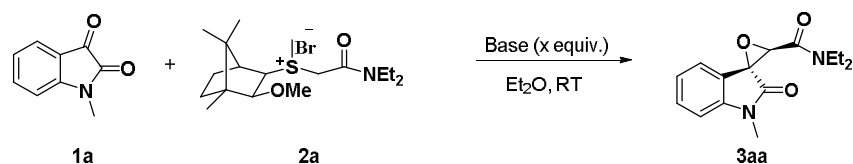
Table S1. Study of solvent and concentration effect^a



entry	solvent	conc. [M]	t (h)	yield (%) ^b	dr ^c	ee(%) ^d
1	MeCN	0.05	24	92%	> 95:5	74
2	CH ₂ Cl ₂	0.05	24	92%	> 95:5	85
3	CHCl ₃	0.05	24	64%	> 95:5	88
4	THF	0.05	24	95%	> 95:5	90
5	MeOH	0.05	48	43%	> 95:5	78
6	Toluene	0.05	24	99%	> 95:5	89
7	Xylene	0.05	24	99%	> 95:5	89
8	Et₂O	0.05	24	99%	> 95:5	91
9	Et ₂ O	0.1	24	99%	> 95:5	90
10	Et ₂ O	0.025	24	99%	> 95:5	91

^a Reaction conditions: **1a** (0.15 mmol), **2a** (0.18 mmol), TMG (0.375 mmol), solvent, rt. ^b Yield of isolated product. ^c Determined by ¹H NMR. ^d Determined by chiral HPLC analysis.

Table S2. Study of base effect^a



entry	base	x	yield (%) ^b	dr ^c	ee(%) ^d
1	TMG	2.5	99%	> 95:5	90
2	TMG	1.3	80%	> 95:5	90

3	TMG	1.5	89%	> 95:5	90
4	KOH	2.5	78%	> 95:5	90
5	CS ₂ CO ₃	2.5	98%	> 95:5	90
6	DBU	2.5	99%	> 95:5	90

^a Reaction conditions: **1a** (0.15 mmol), **2a** (0.18 mmol), Base (X equiv.), Et₂O (3 mL), RT. ^b Yield of isolated product. ^c Determined by ¹H NMR. ^d Determined by chiral HPLC analysis.

Table 3. Study of temperature effect^a

entry	T [°C]	t (h)	yield (%) ^b	dr ^c	ee(%) ^d
1	25 °C	24	99%	> 95:5	90
2	0 °C	48	99%	> 95:5	93
3	-10 °C	96	93%	> 95:5	93

^a Reaction conditions: **1a** (0.15 mmol), **2a** (0.18 mmol), DBU (0.375 mmol), Et₂O (3 mL). ^b Yield of isolated product. ^c Determined by ¹H NMR. ^d Determined by chiral HPLC analysis.

4. Absolute Configuration of Representative Product **3ka**

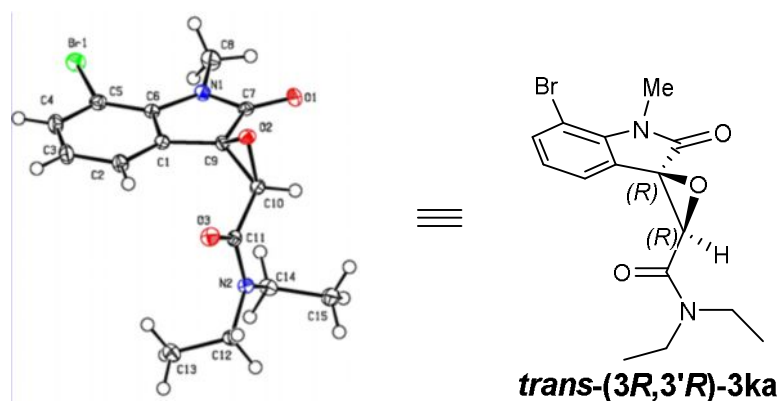
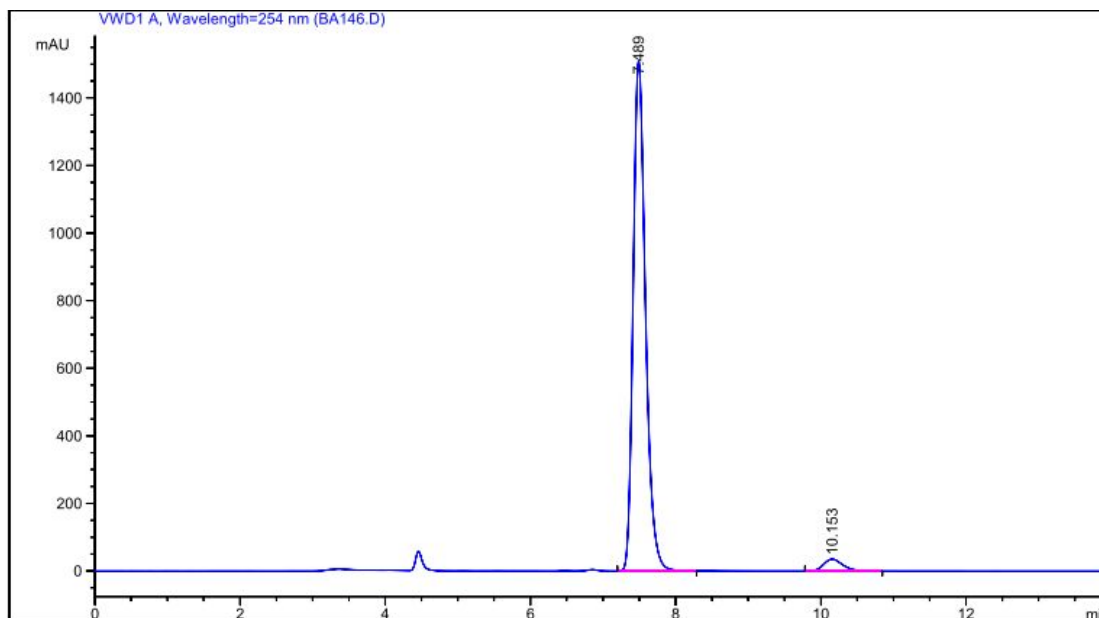
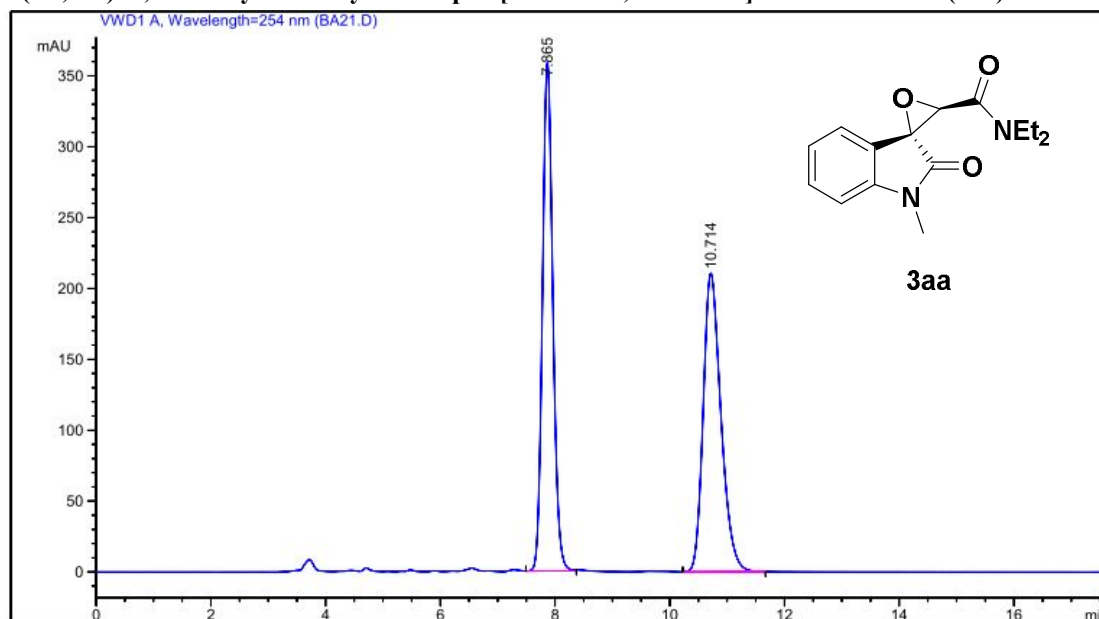


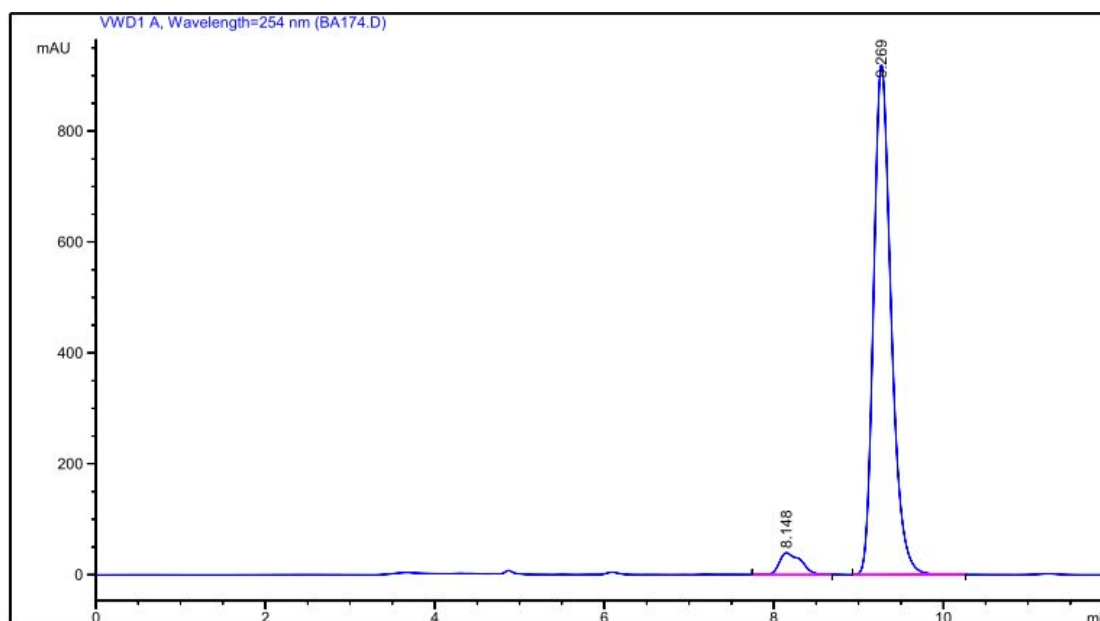
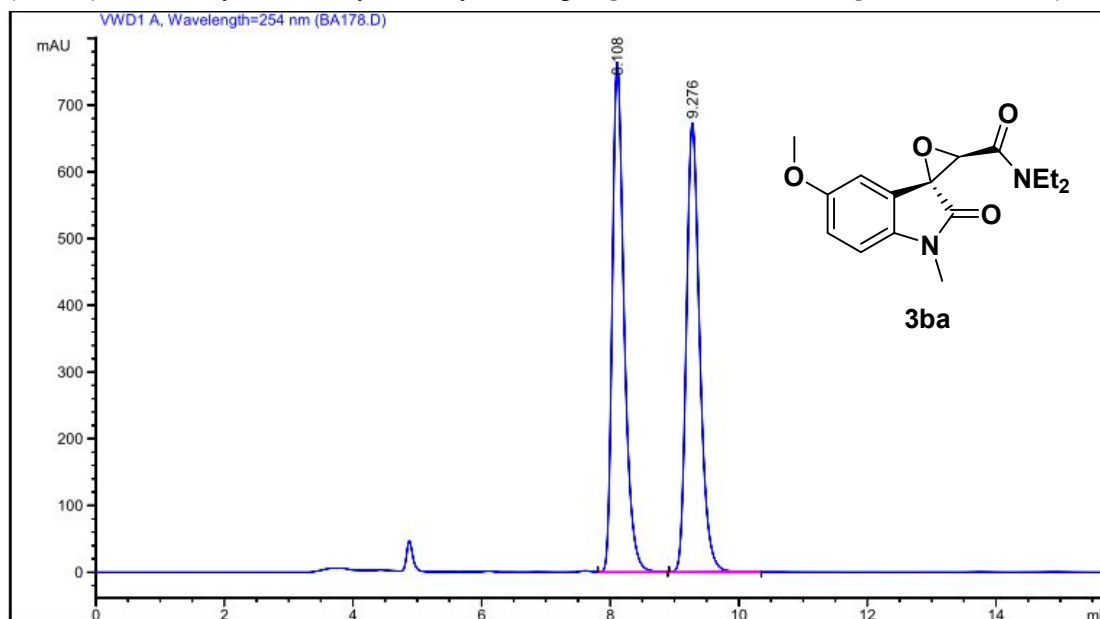
Figure 1. Absolute configuration of product **3ka** established by X-ray analysis.

5. Copies of HPLC for Products

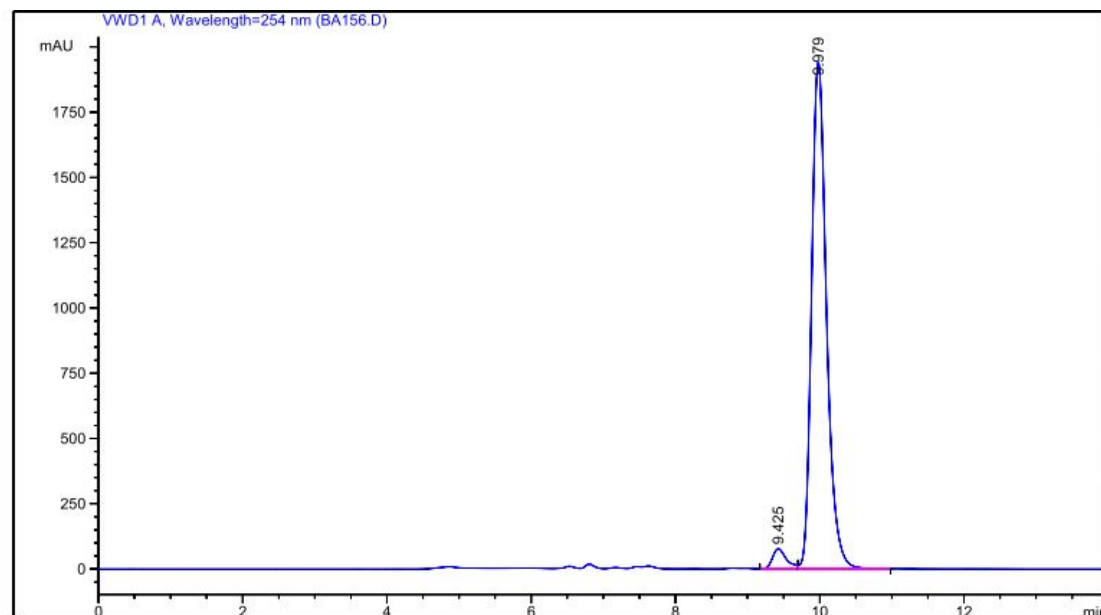
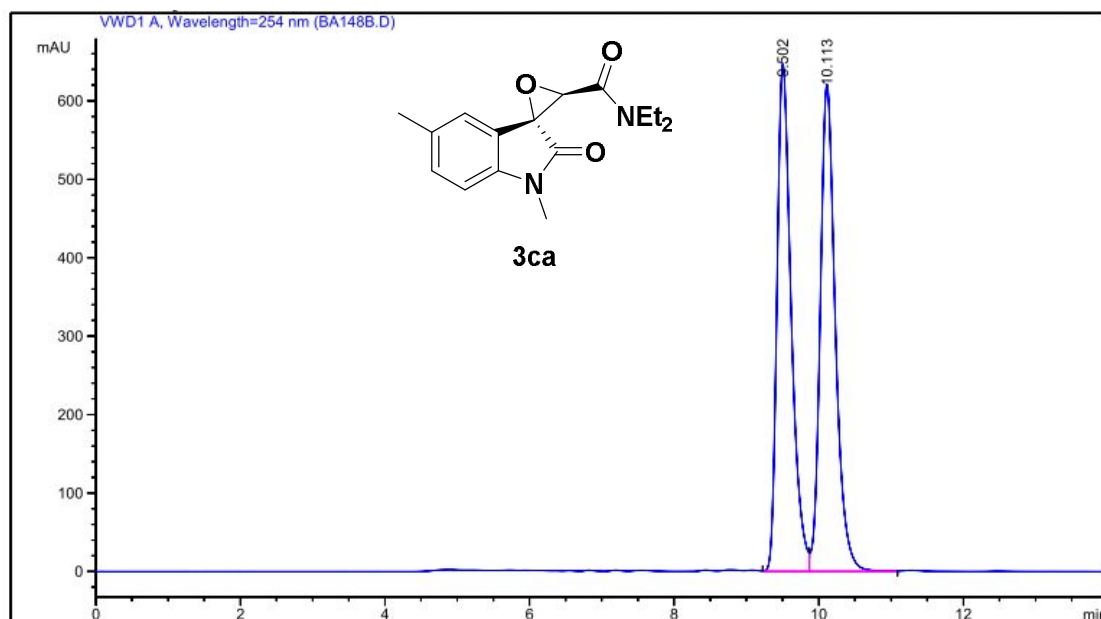
(3*R*,3'*R*)-*N,N*-Diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3aa):



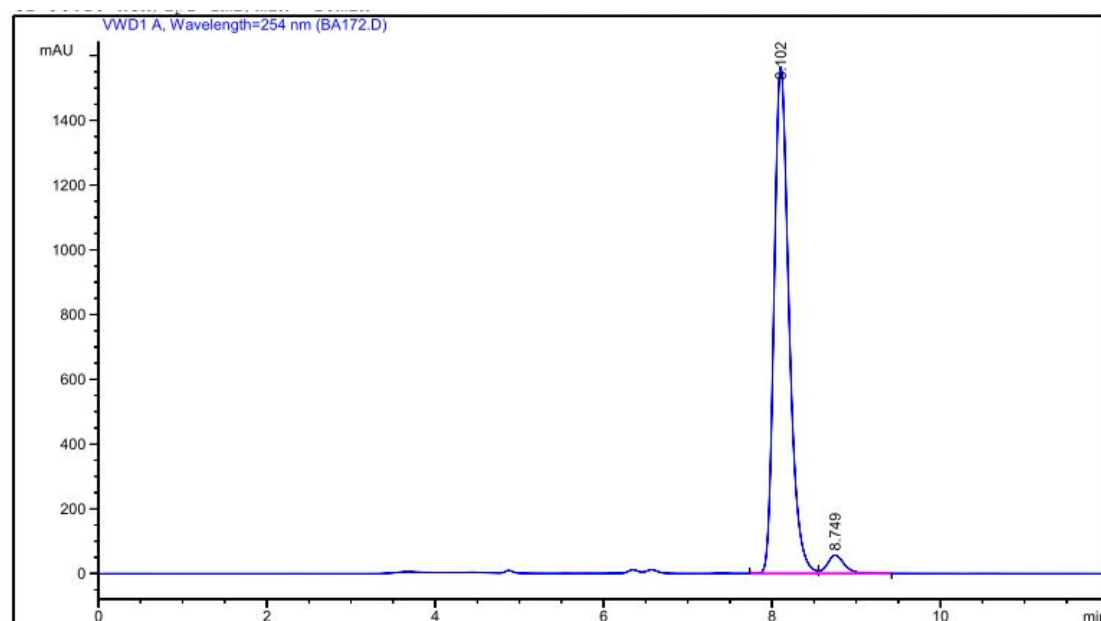
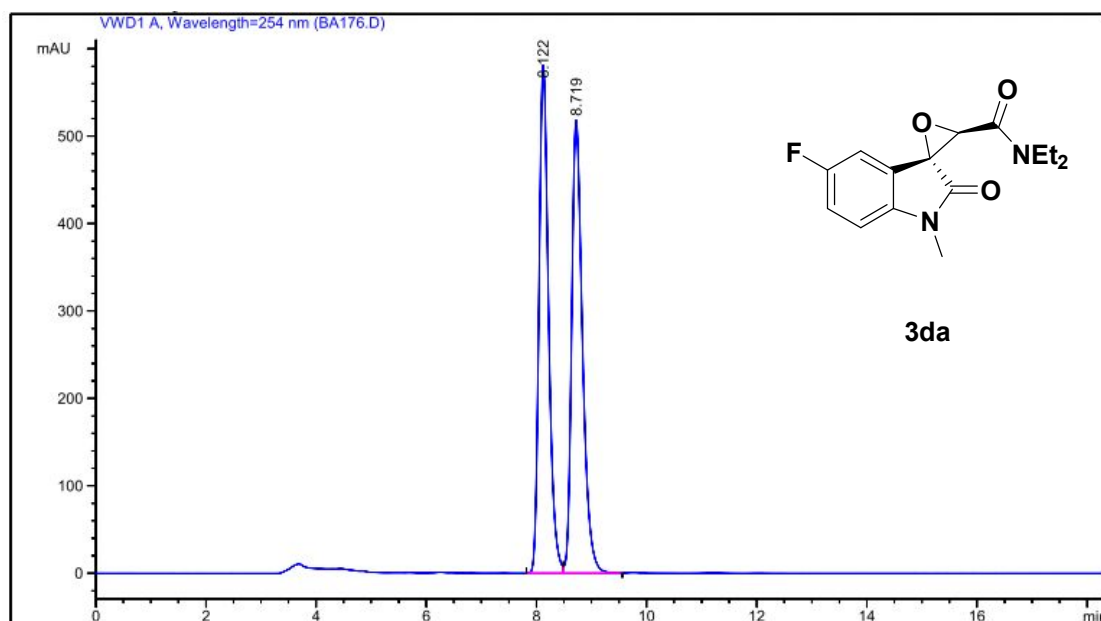
(3*R*,3'*R*)-*N,N*-diethyl-5-methoxy-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide(3ba):



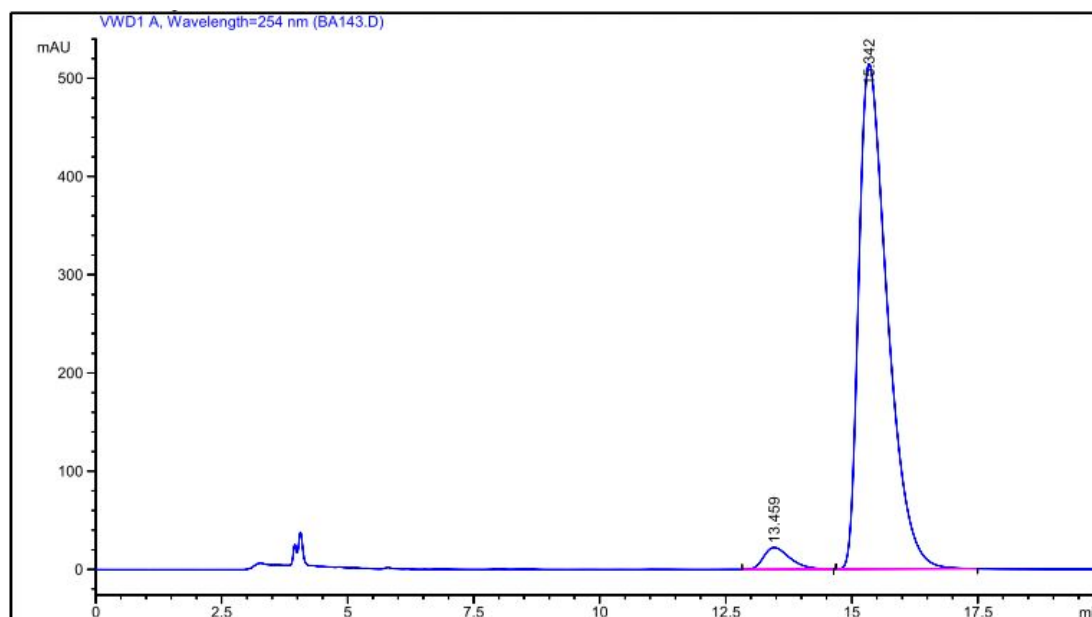
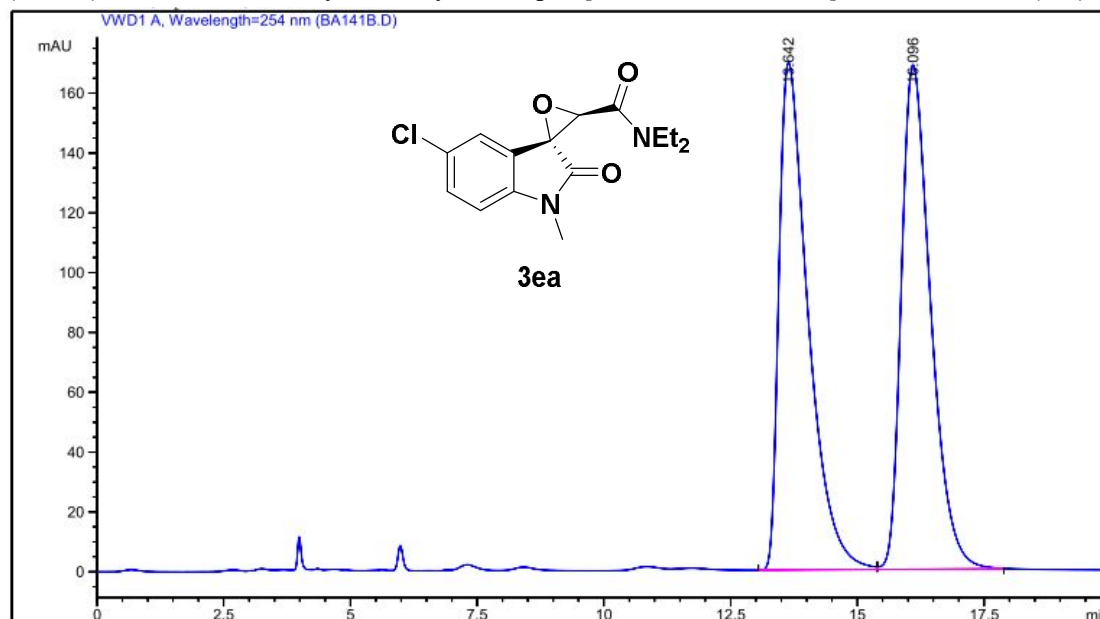
(3*R*,3'*R*)-*N,N*-diethyl-1,5-dimethyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3ca):



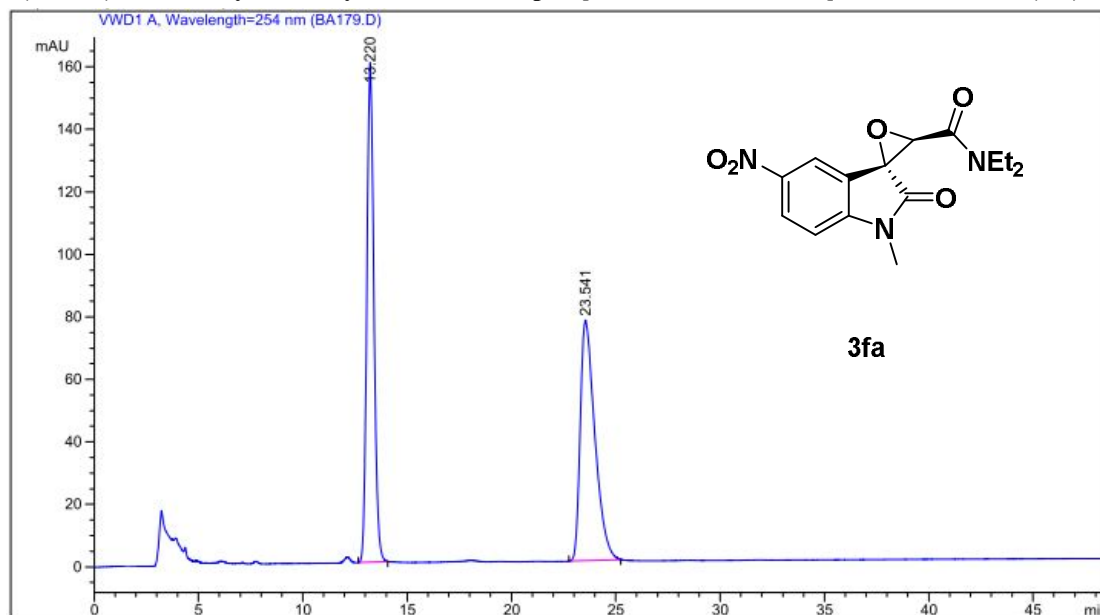
(3*R*,3'*R*)-*N,N*-diethyl-5-fluoro-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3da):



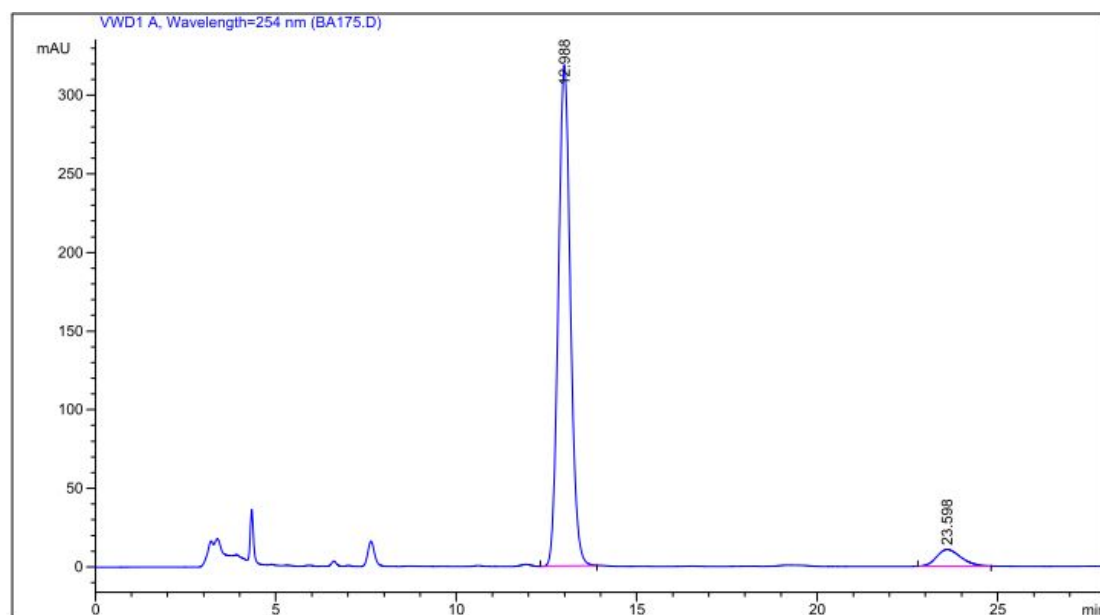
(3*R*,3'*R*)-5-chloro-*N,N*-diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3ea):



(3*R*,3'*R*)-*N,N*-diethyl-1-methyl-5-nitro-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3fa):

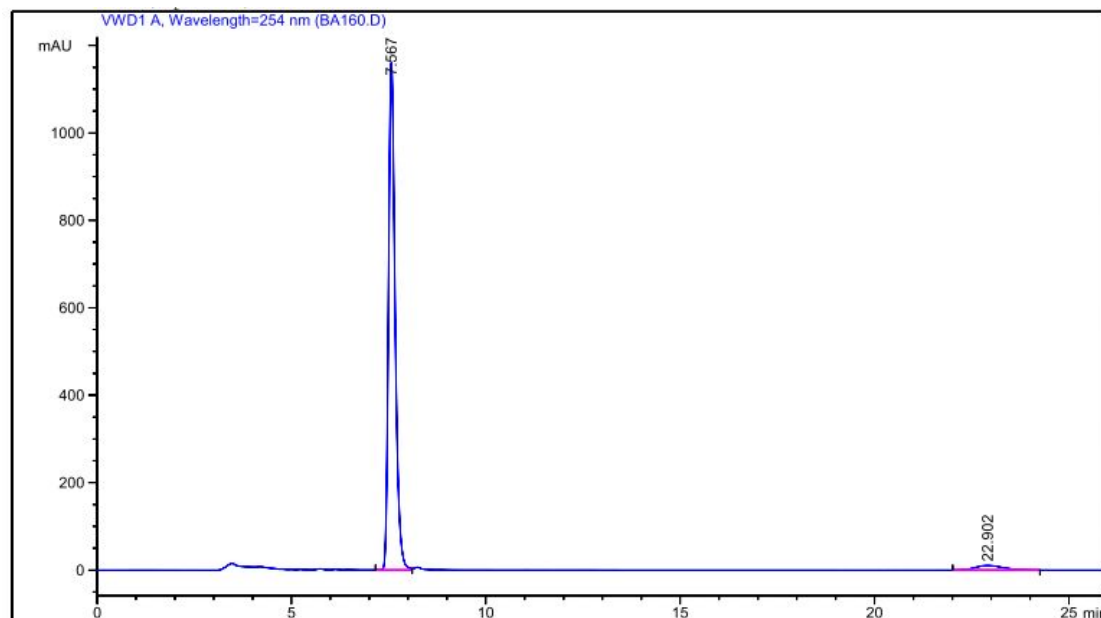
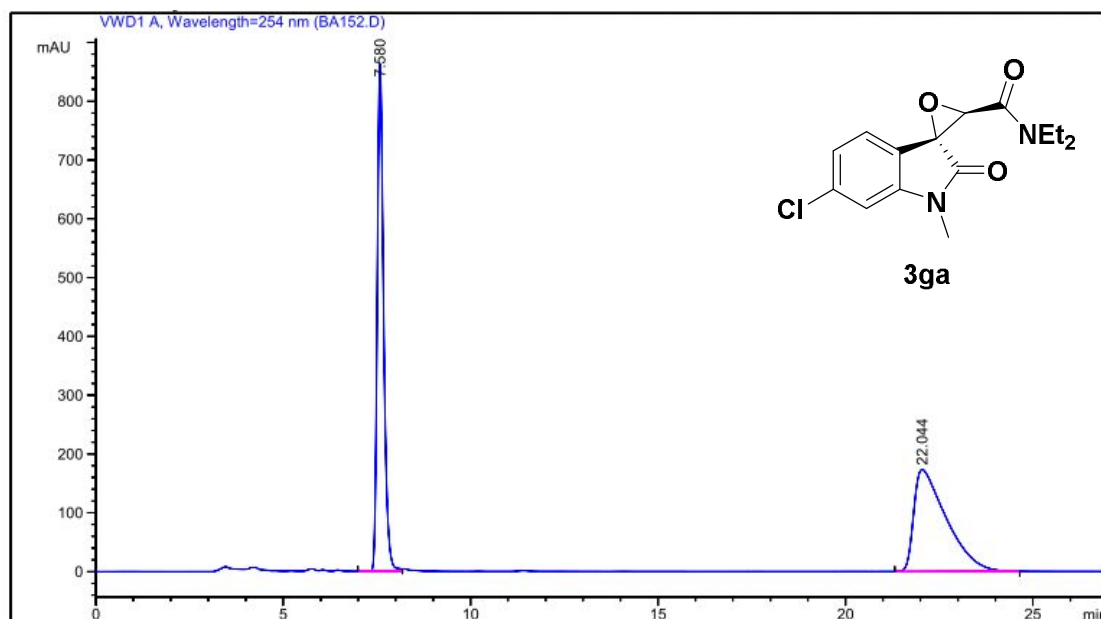


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	13.220	BB	0.3629	3754.49536		159.82578	50.0439
2	23.541	BB	0.7340	3747.90649		76.98526	49.9561

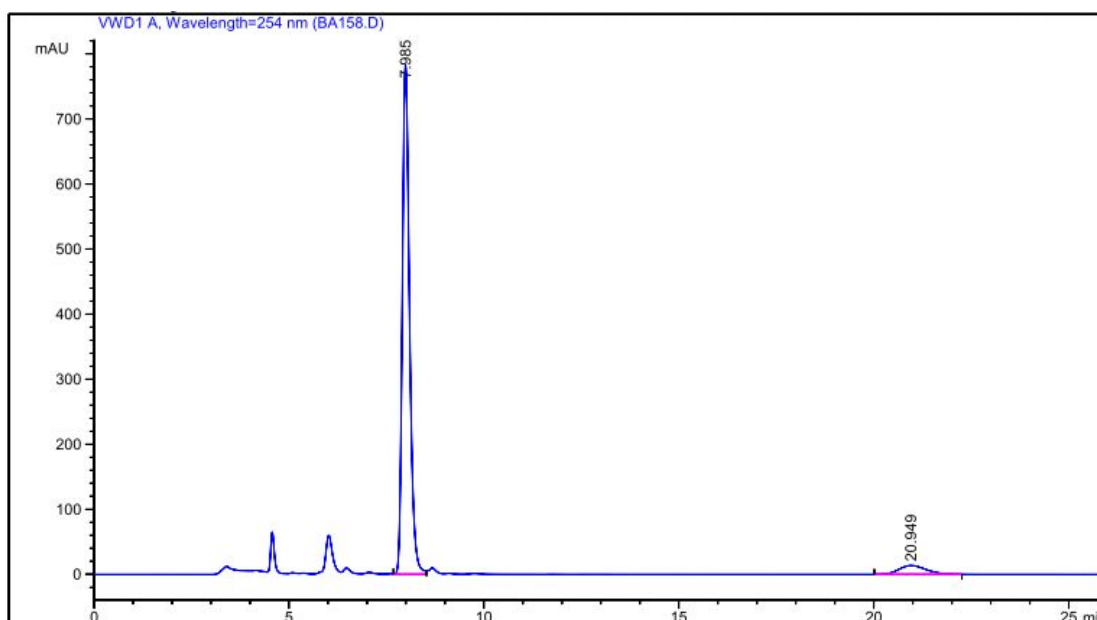
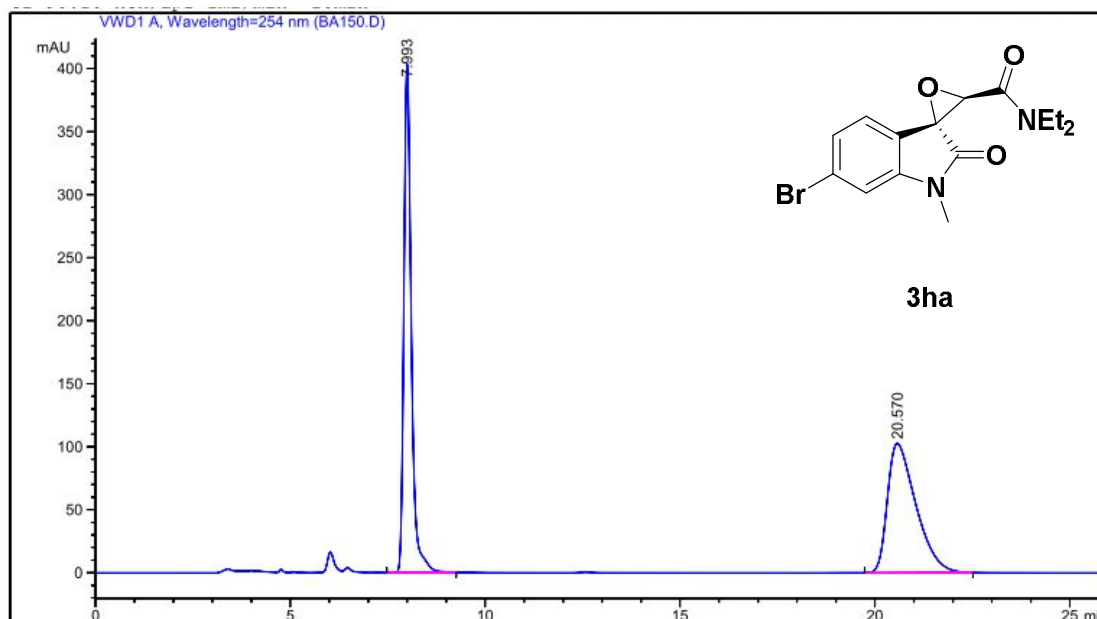


Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area *s	Height [mAU]	Area %
1	12.988	VB	0.3616	7413.45068		318.73776	93.6466
2	23.598	BB	0.7216	502.96320		10.67270	6.3534

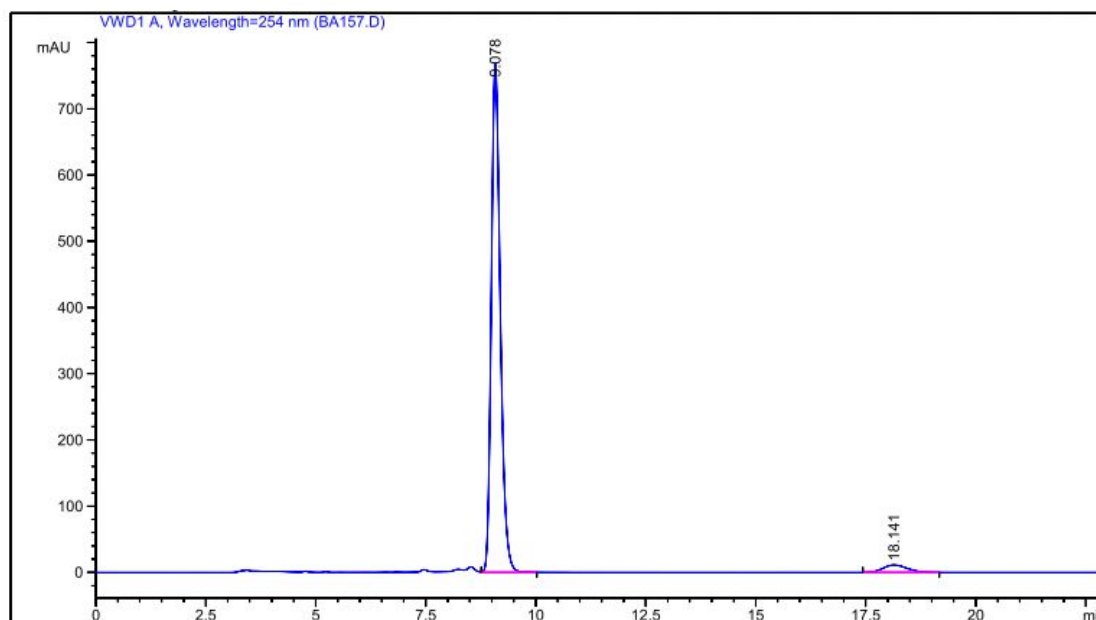
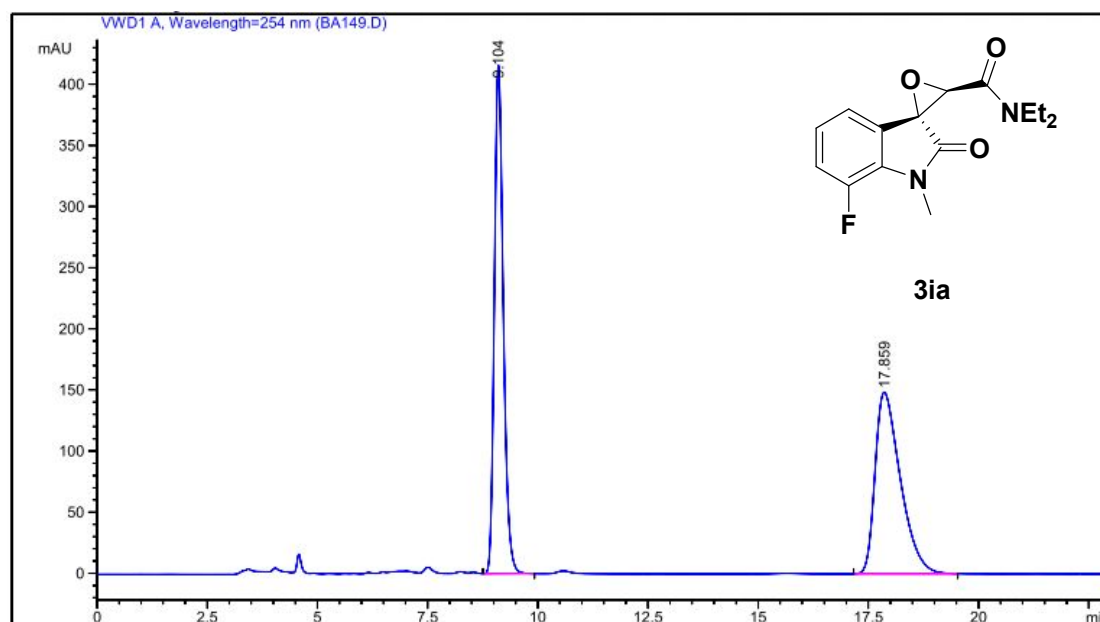
(3R,3'R)-6-chloro-N,N-diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3ga):



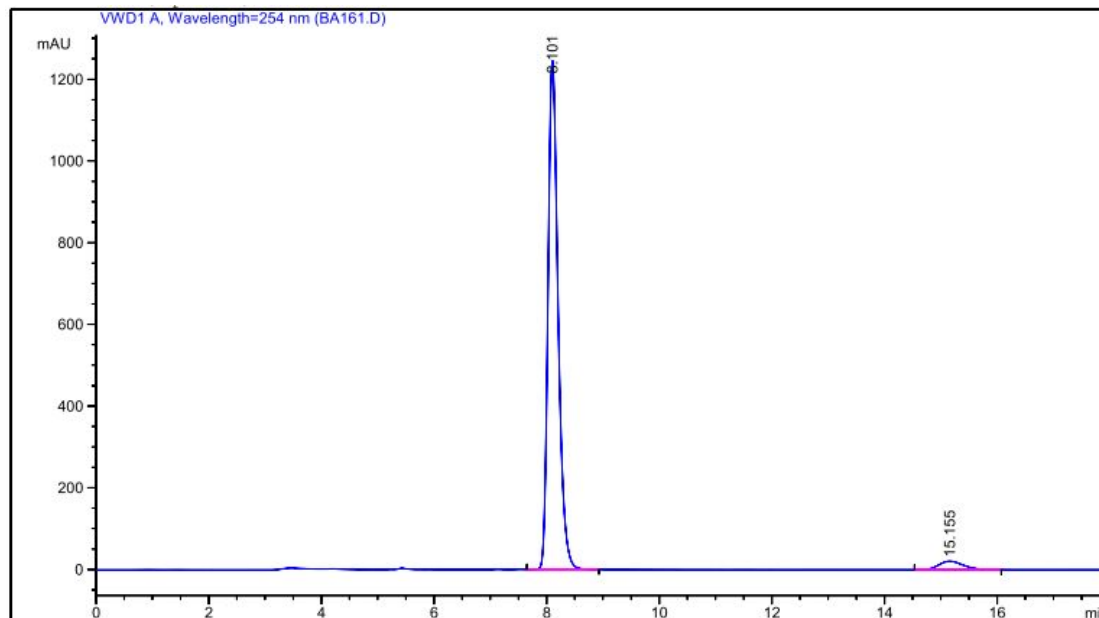
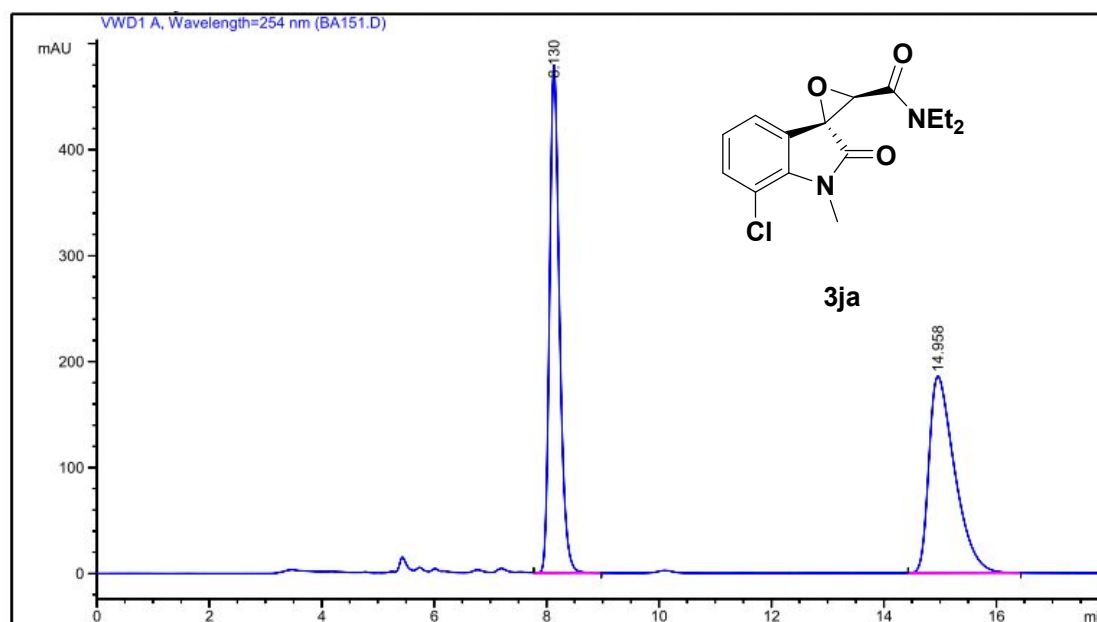
(3*R*,3'*R*)-6-bromo-*N,N*-diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (**3ha**):



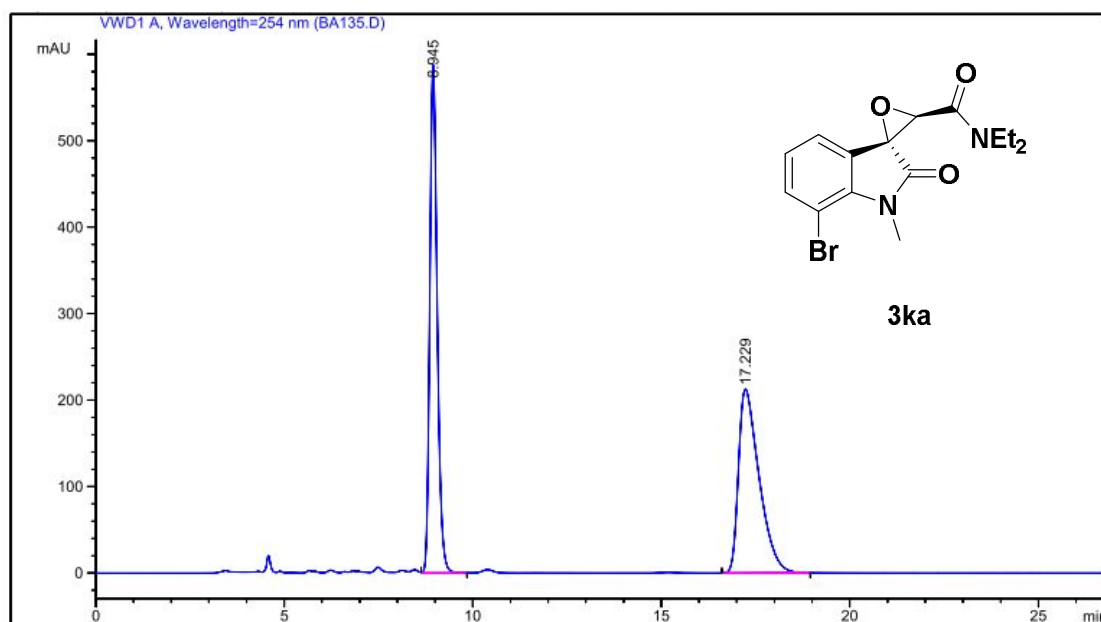
(3*R*,3'*R*)-*N,N*-diethyl-7-fluoro-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (**3ia**):



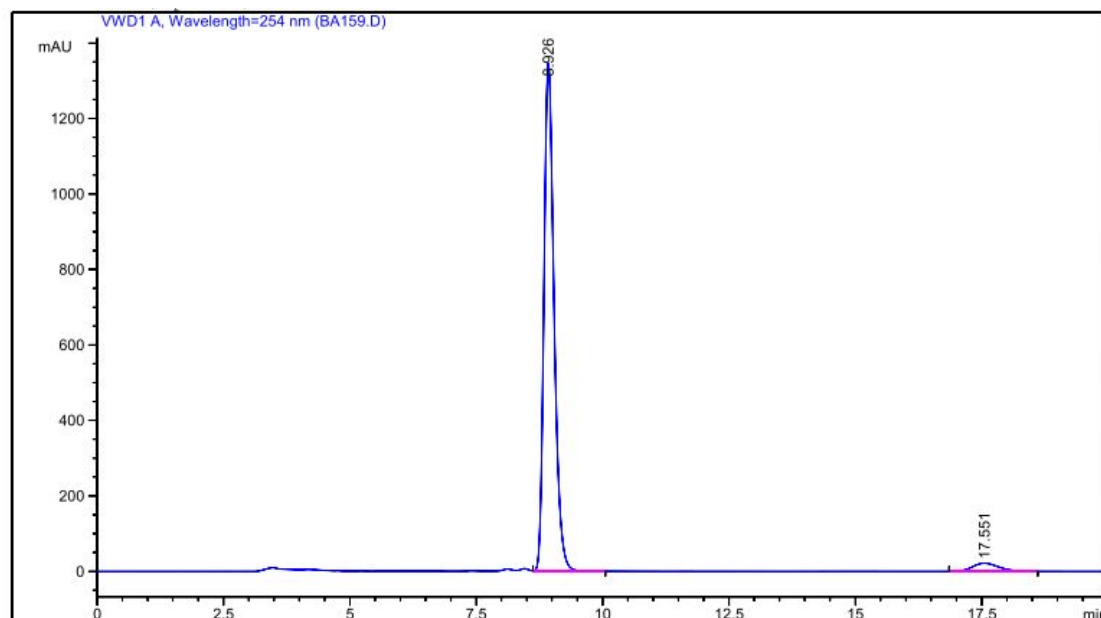
(3*R*,3'*R*)-7-chloro-*N,N*-diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3ja):



(3*R*,3'*R*)-7-bromo-*N,N*-diethyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (3ka):

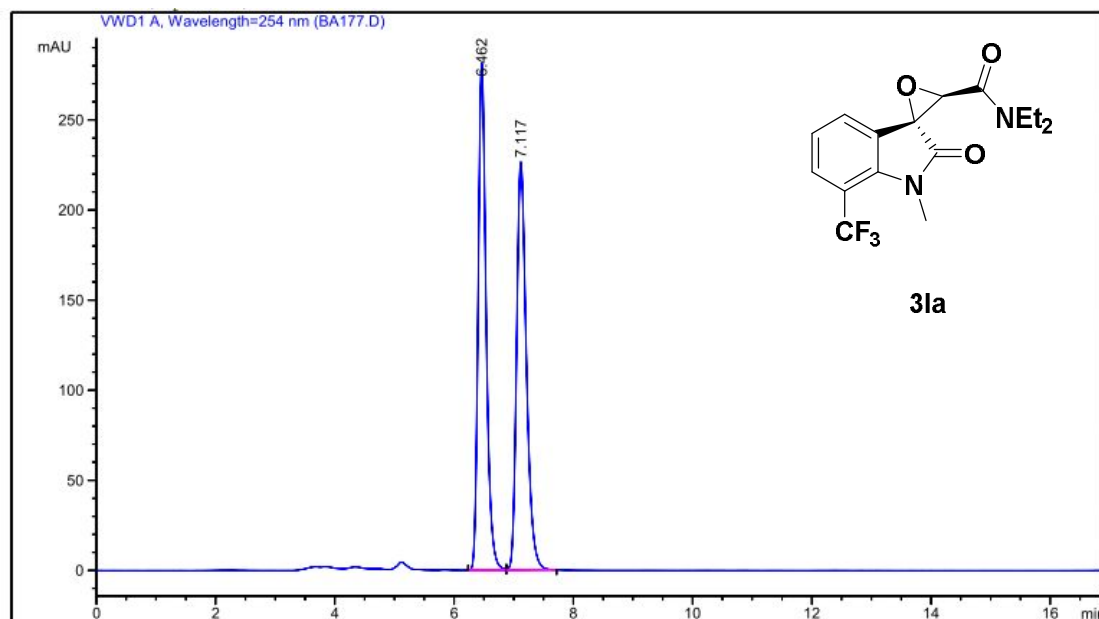


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	8.945	VB	0.2104	8025.78174	587.41980	49.8165
2	17.229	BB	0.5690	8084.89990	212.52249	50.1835

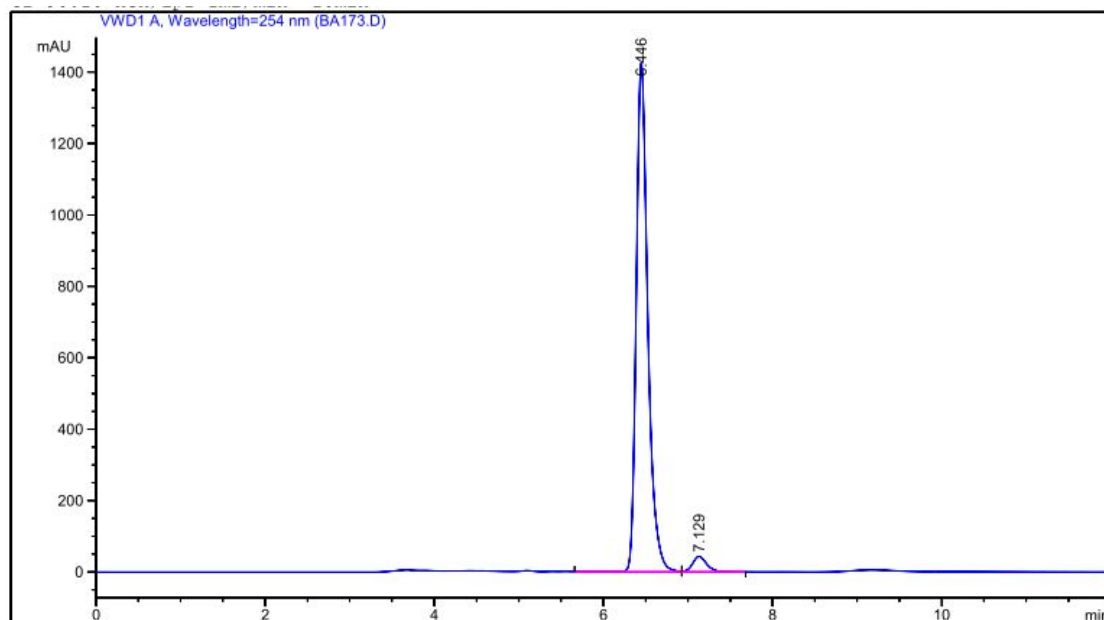


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	8.926	VB	0.2135	1.87471e4	1345.82178	95.9405
2	17.551	BB	0.5646	793.23975	21.78641	4.0595

(3*R*,3'*R*)-*N,N*-diethyl-1-methyl-2-oxo-7-(trifluoromethyl)spiro[indoline-3,2'-oxirane]-3'-carboxamide (**3la**)

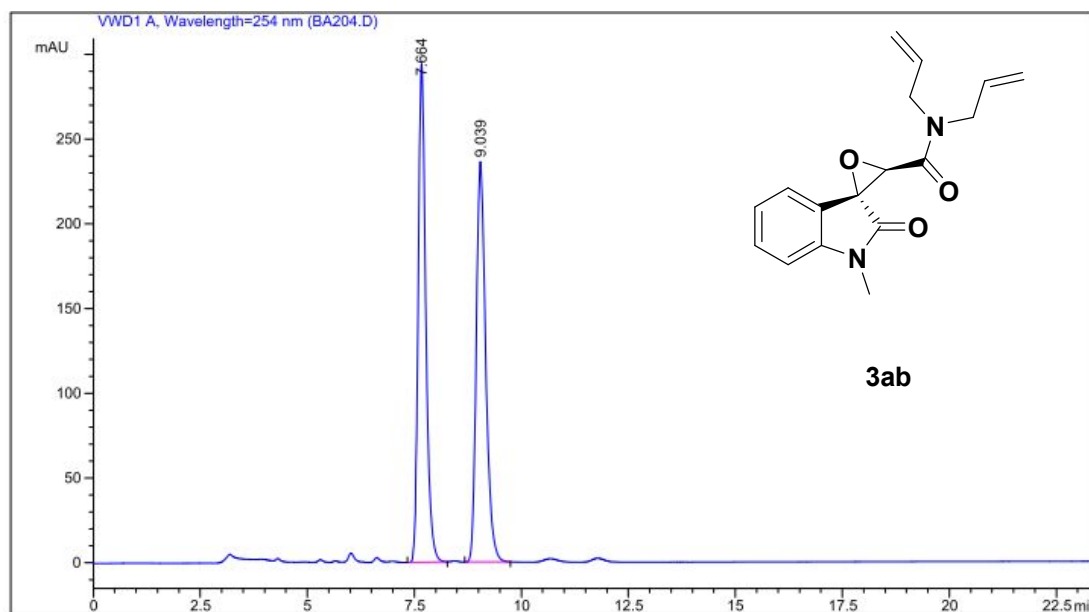


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	6.462	BV	0.1419	2615.68652	281.43369	50.2960
2	7.117	VB	0.1739	2584.89673	226.57855	49.7040

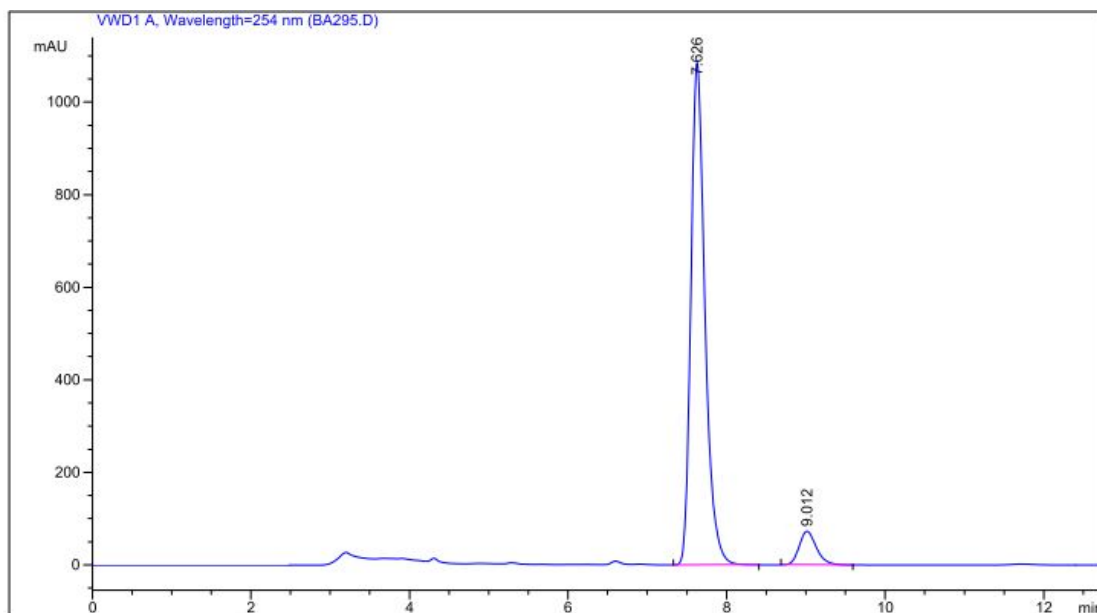


Peak #	RetTime [min]	Type	Width [min]	Area mAU*s	Height [mAU]	Area %
1	6.446	VV	0.1448	1.36054e4	1425.85474	96.3487
2	7.129	VB	0.1803	515.60114	43.57608	3.6513

(3*R*,3'*R*)-*N,N*-diallyl-1-methyl-2-oxospiro[indoline-3,2'-oxirane]-3'-carboxamide (**3ab**):

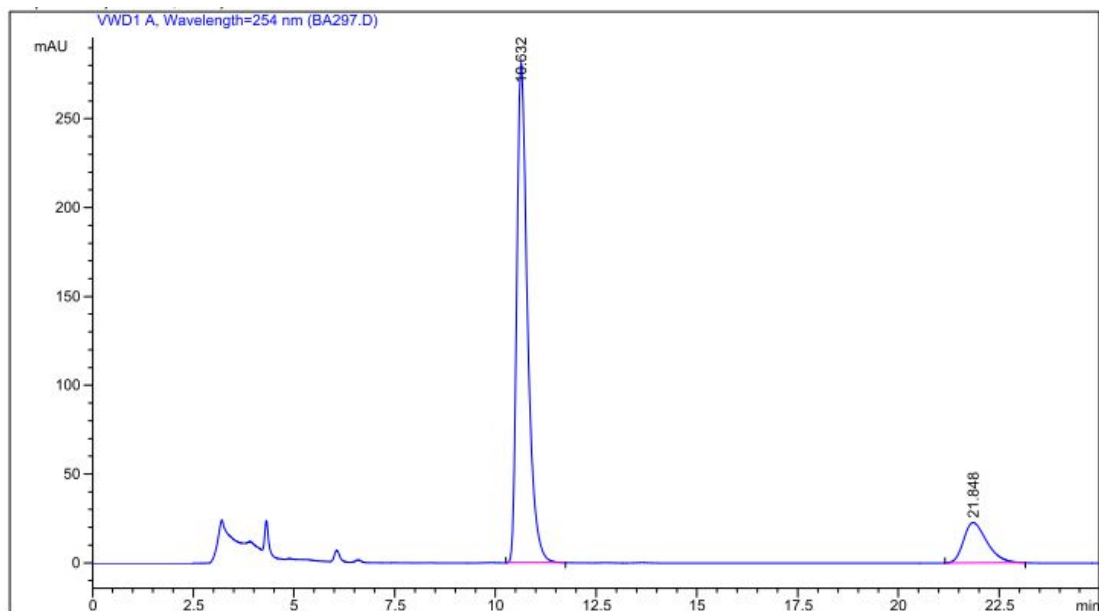
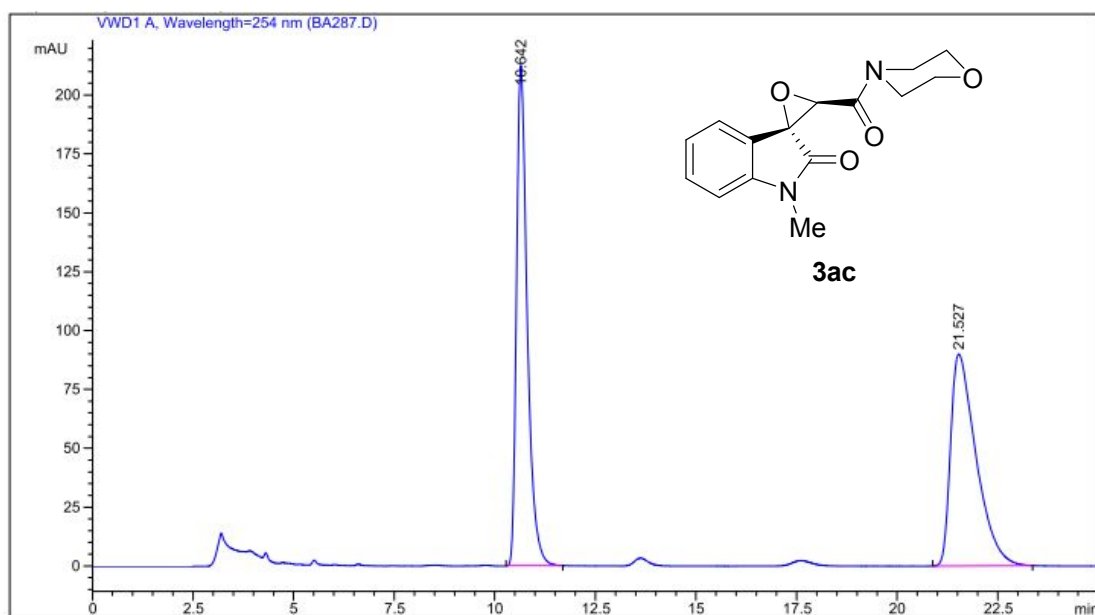


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.664	VB	0.1890	3629.54272	294.33792	49.9953
2	9.039	VB	0.2345	3630.22388	236.42465	50.0047



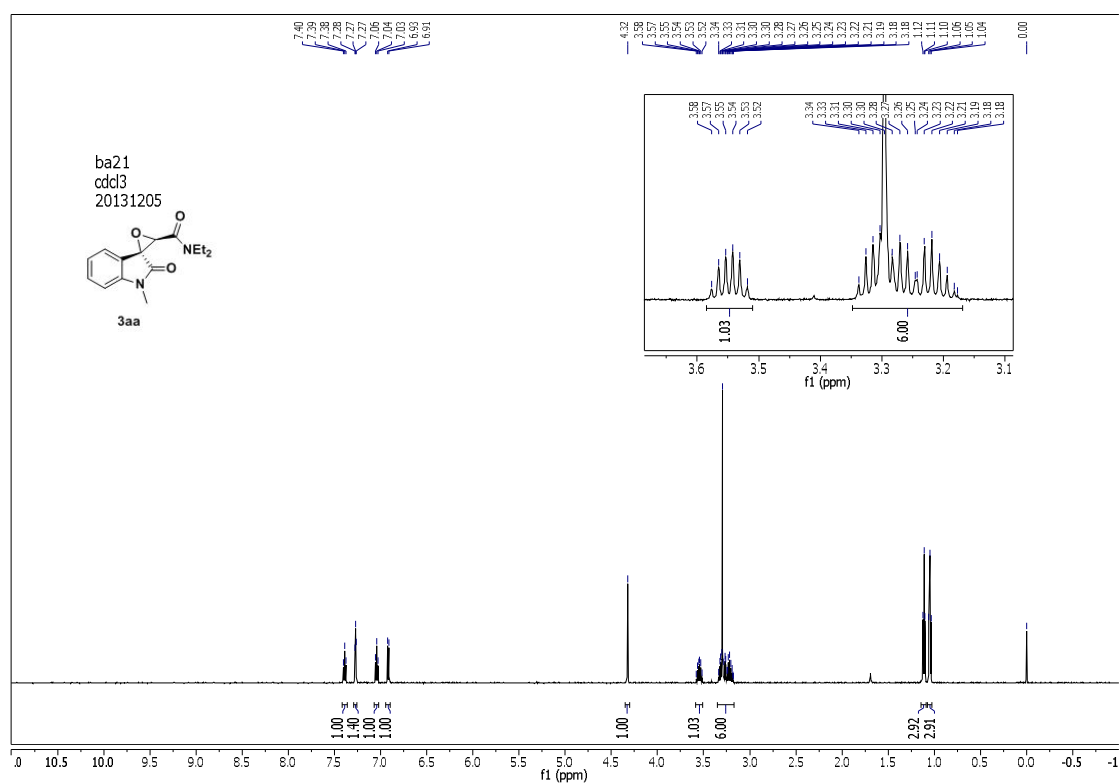
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.626	PB	0.1890	1.33766e4	1084.45508	92.4271
2	9.012	BB	0.2316	1095.99915	72.52859	7.5729

(3*R*,3'*R*)-1-methyl-3'-(morpholine-4-carbonyl)spiro[indoline-3,2'-oxiran]-2-one (3ac):

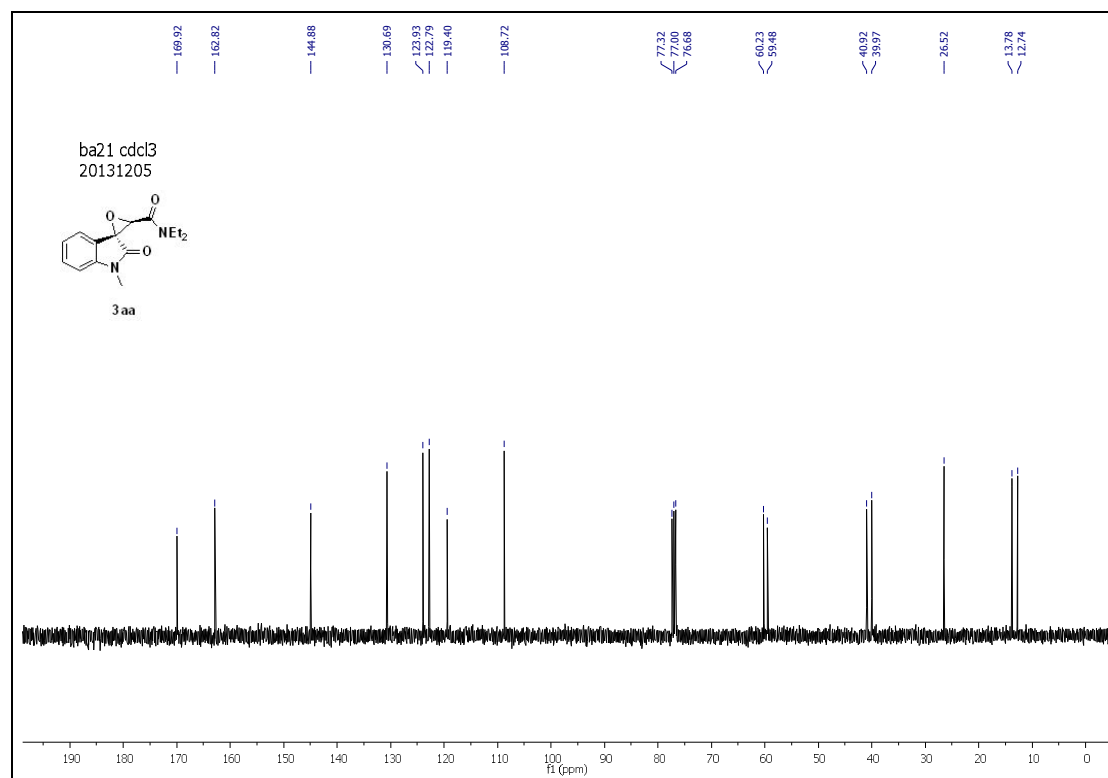


6. Copies of ^1H NMR and ^{13}C NMR Spectra

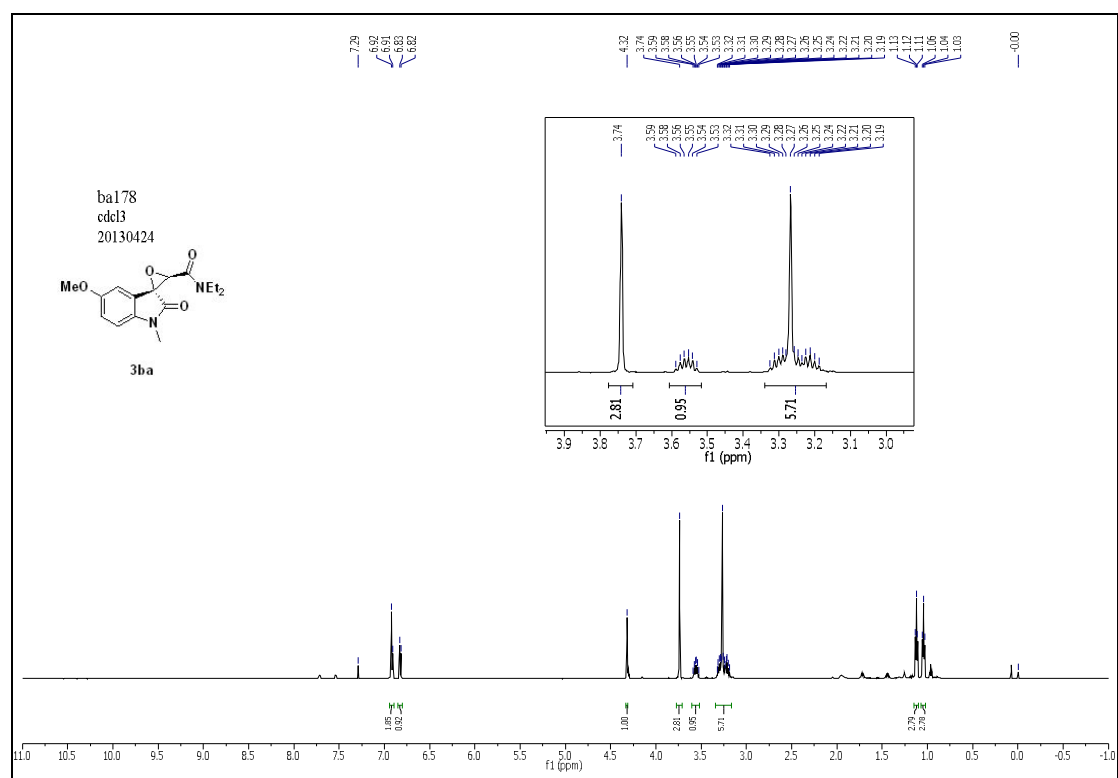
^1H NMR (600 MHz, CDCl_3) spectrum of 3aa



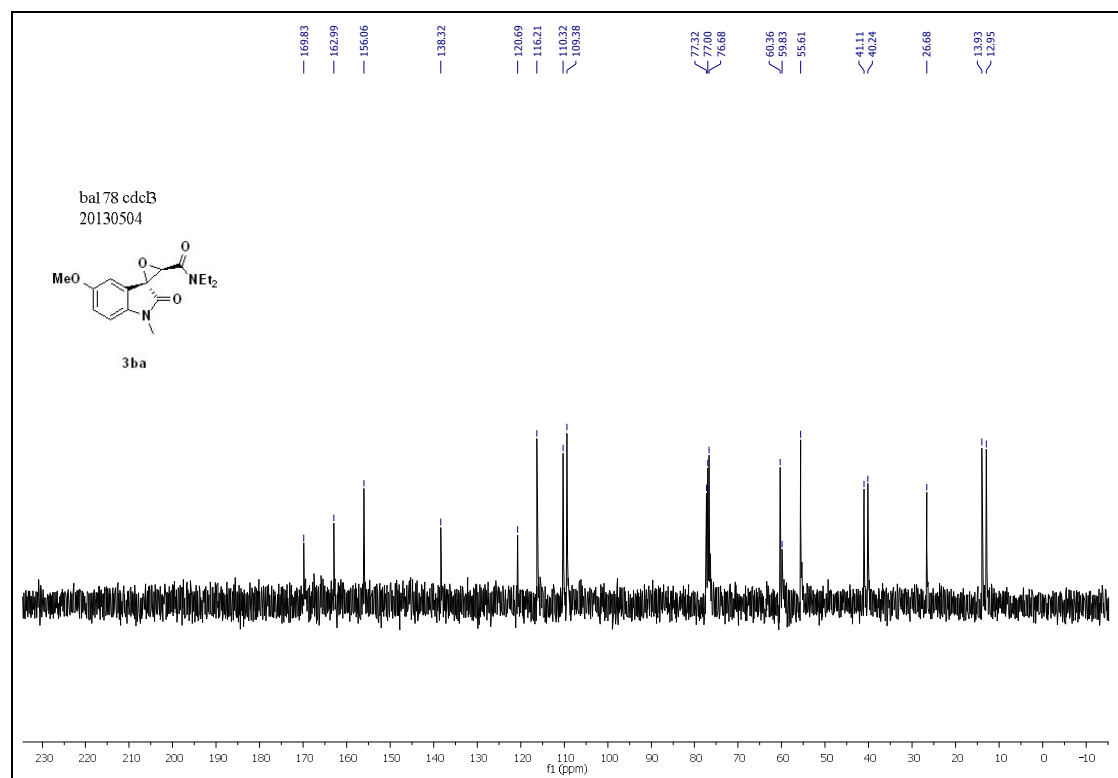
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3aa



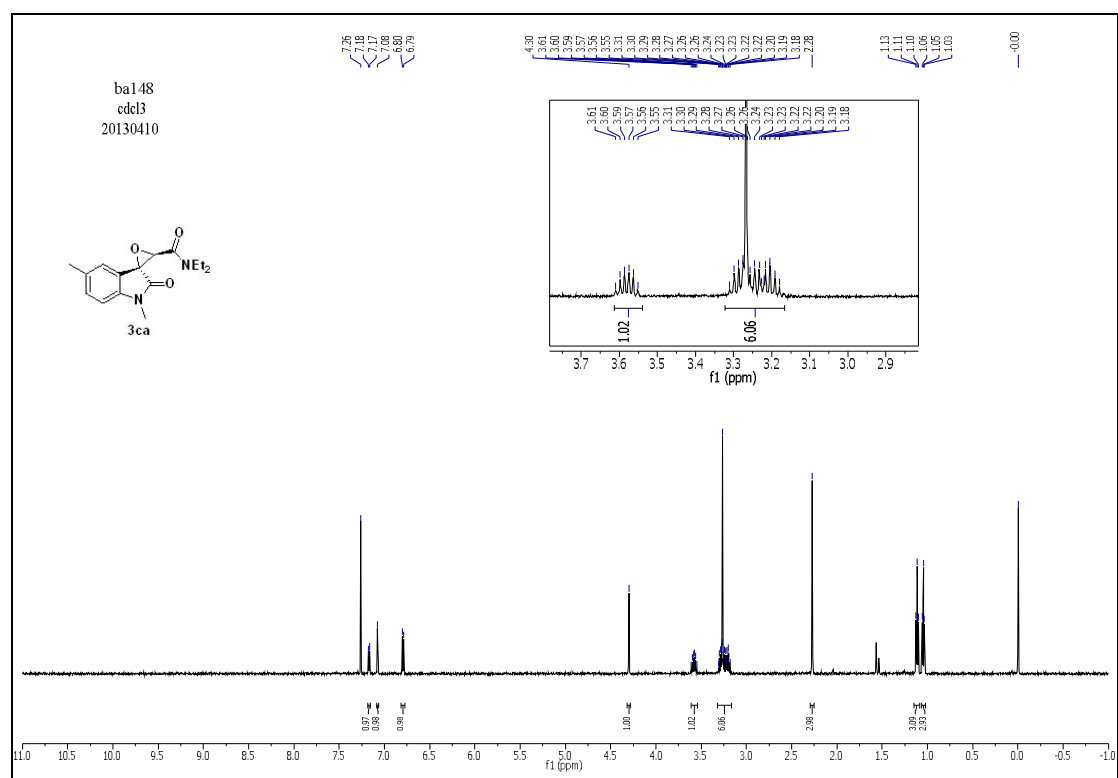
¹H NMR (600 MHz, CDCl₃) spectrum of 3ba



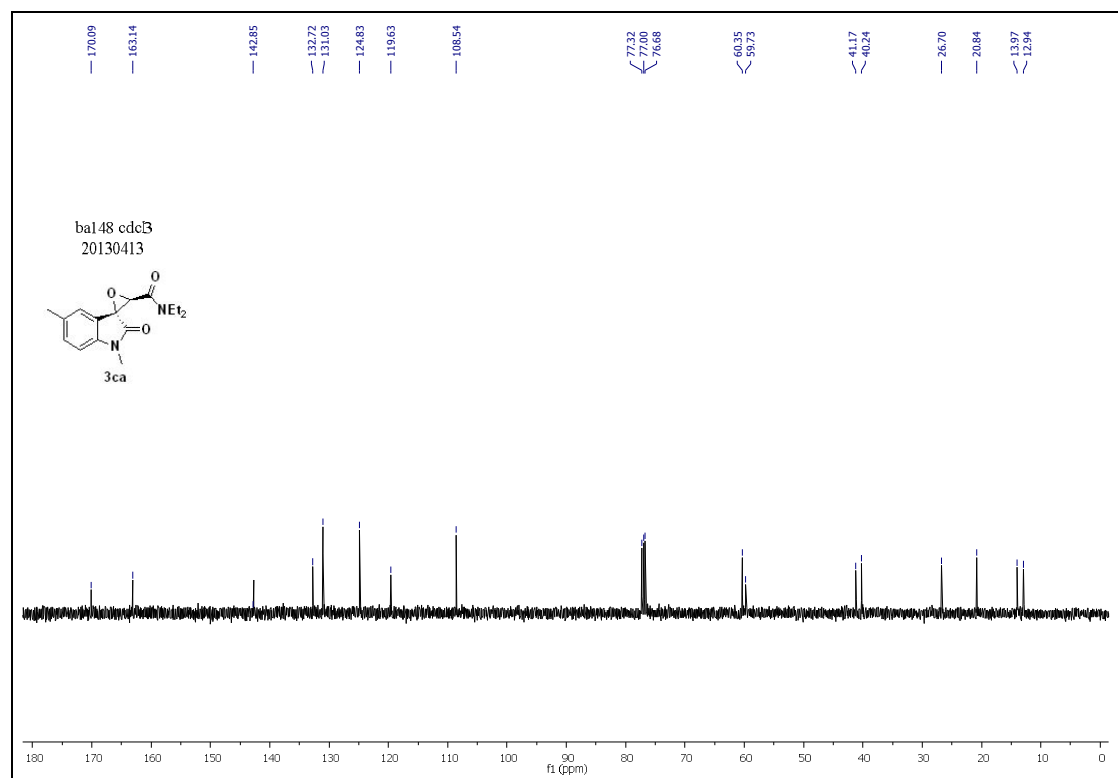
¹³C NMR (100 MHz, CDCl₃) spectrum of 3ba



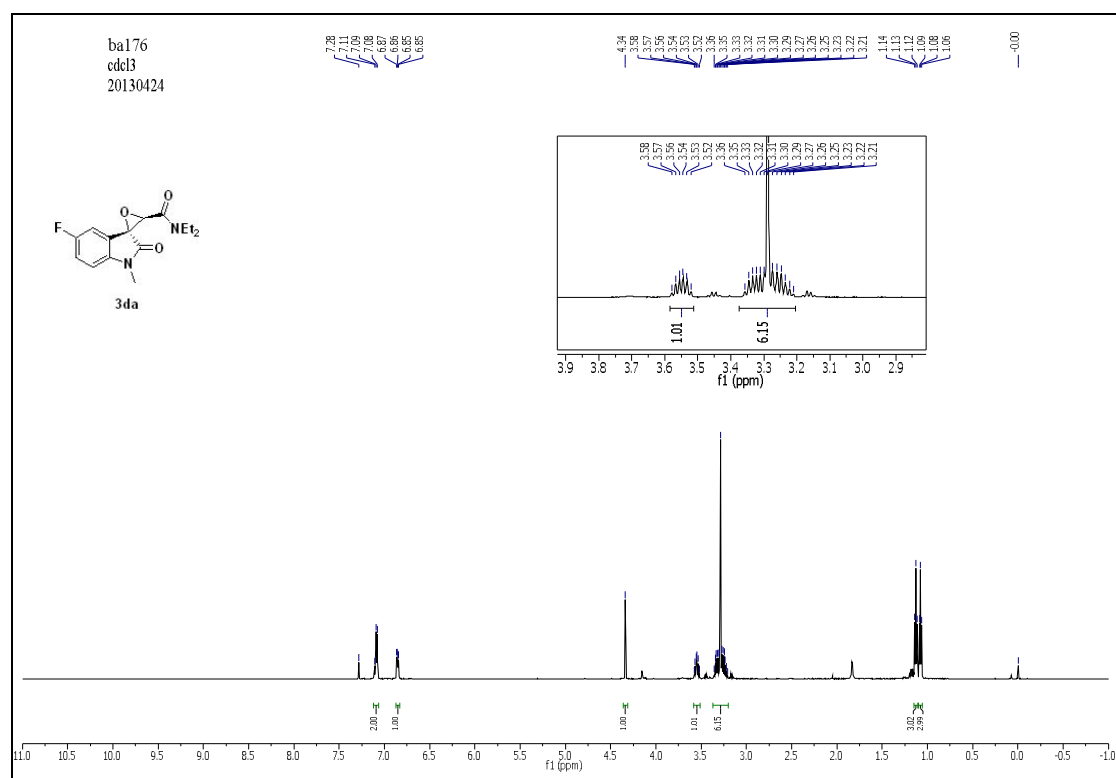
¹H NMR (600 MHz, CDCl₃) spectrum of 3ca



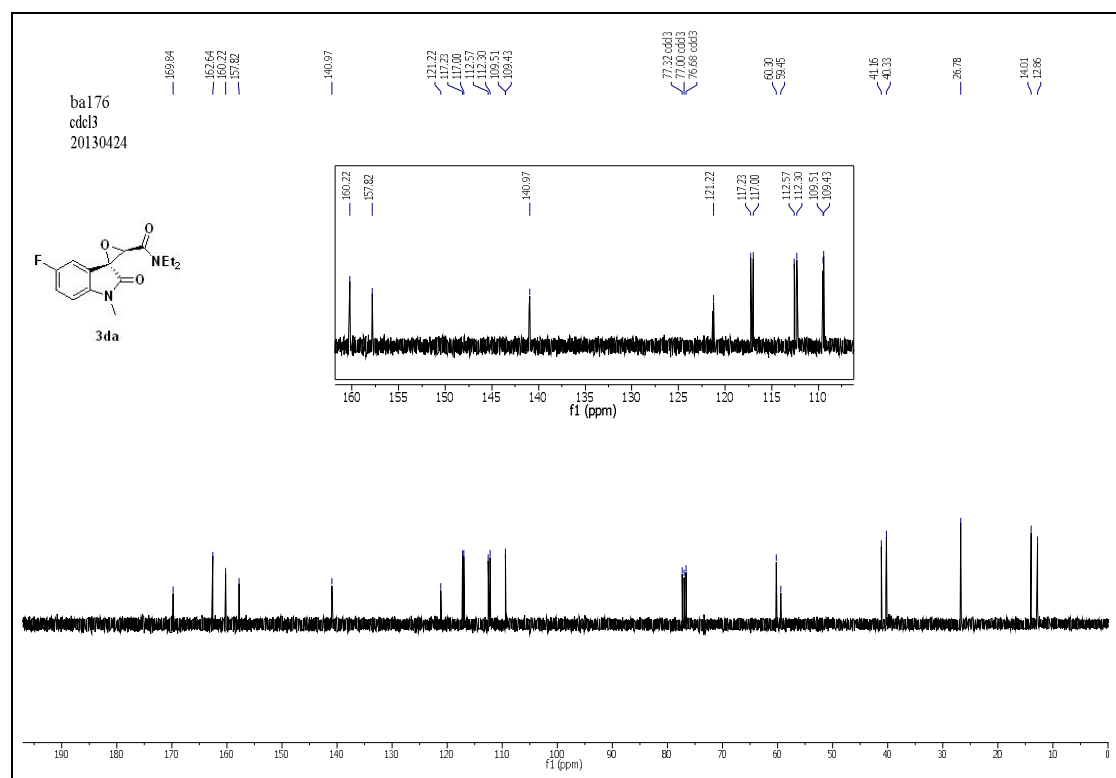
¹³C NMR (100 MHz, CDCl₃) spectrum of 3ca



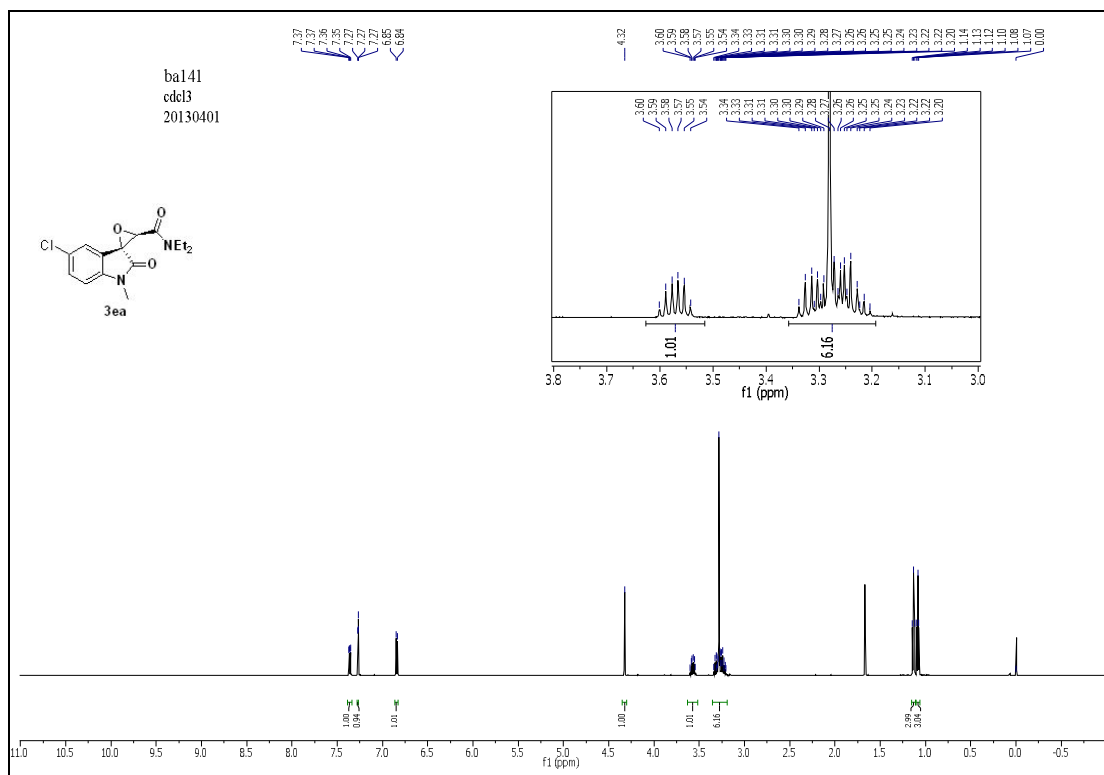
^1H NMR (600 MHz, CDCl_3) spectrum of 3da



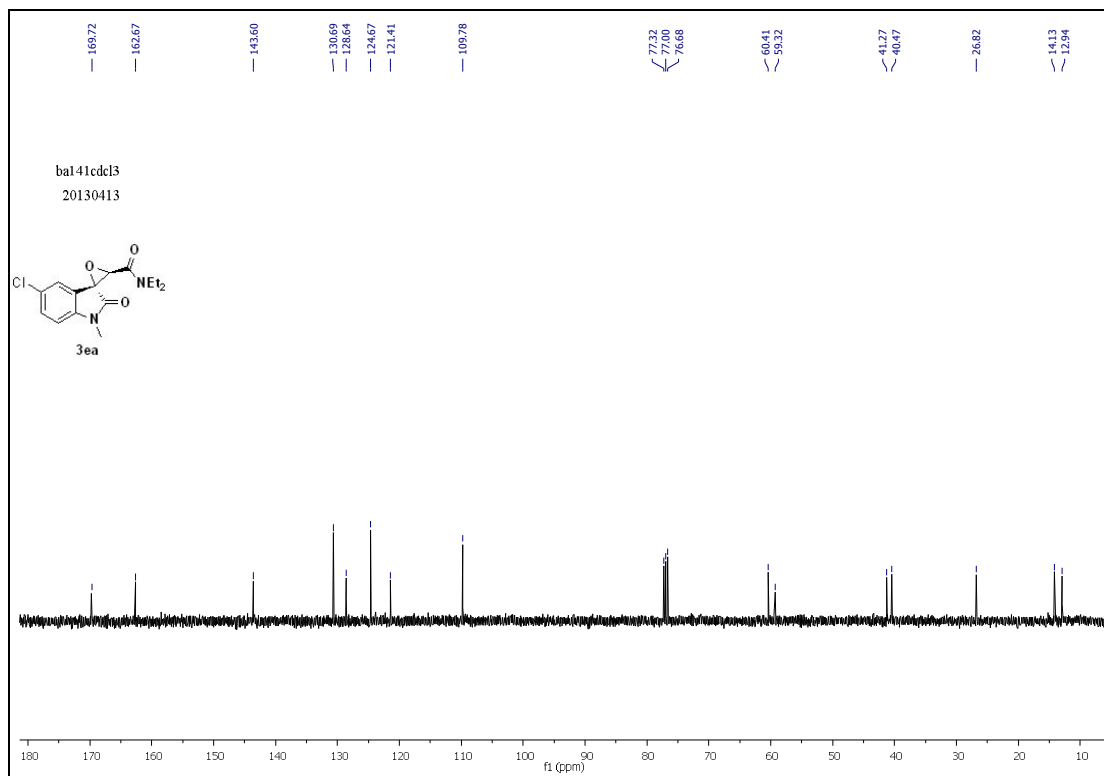
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3da



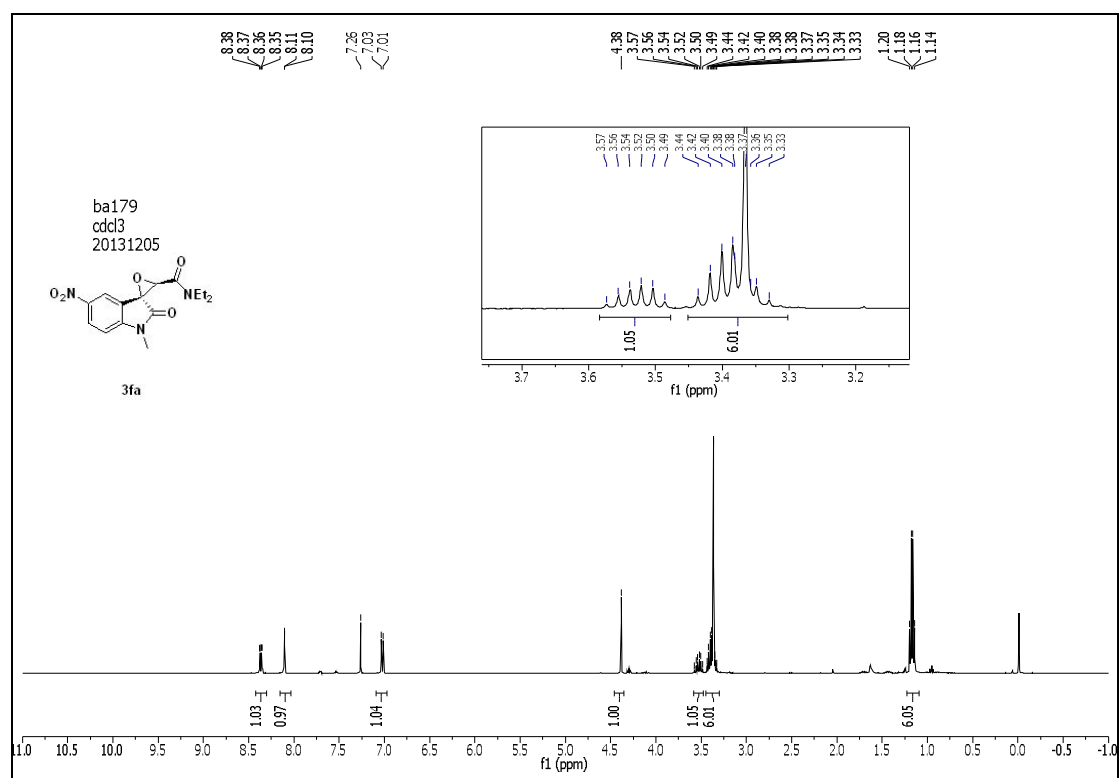
^1H NMR (600 MHz, CDCl_3) spectrum of 3ea



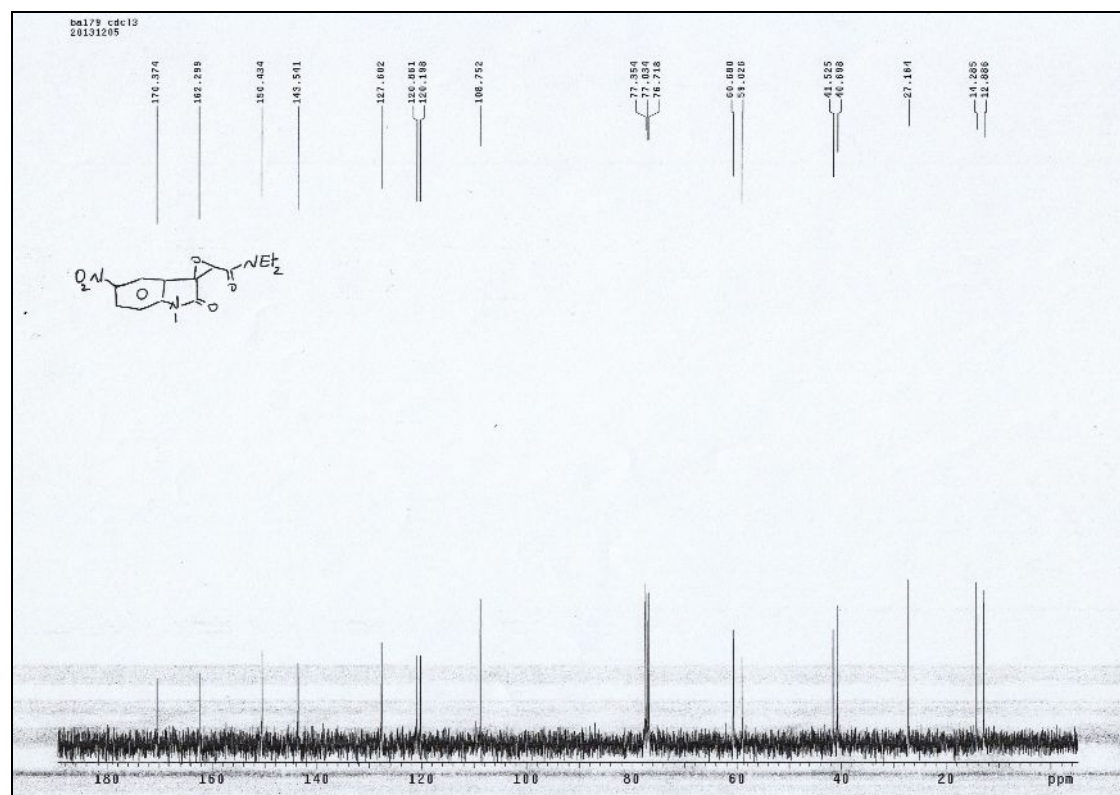
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3ea



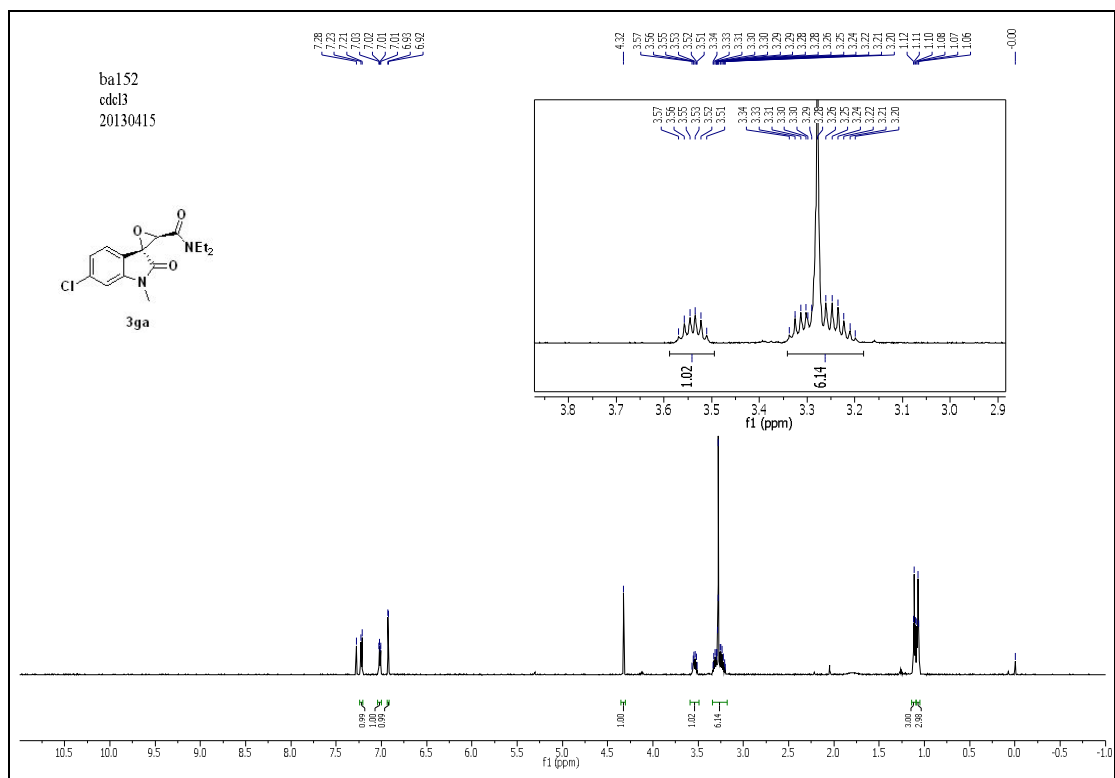
¹H NMR (600 MHz, CDCl₃) spectrum of 3fa



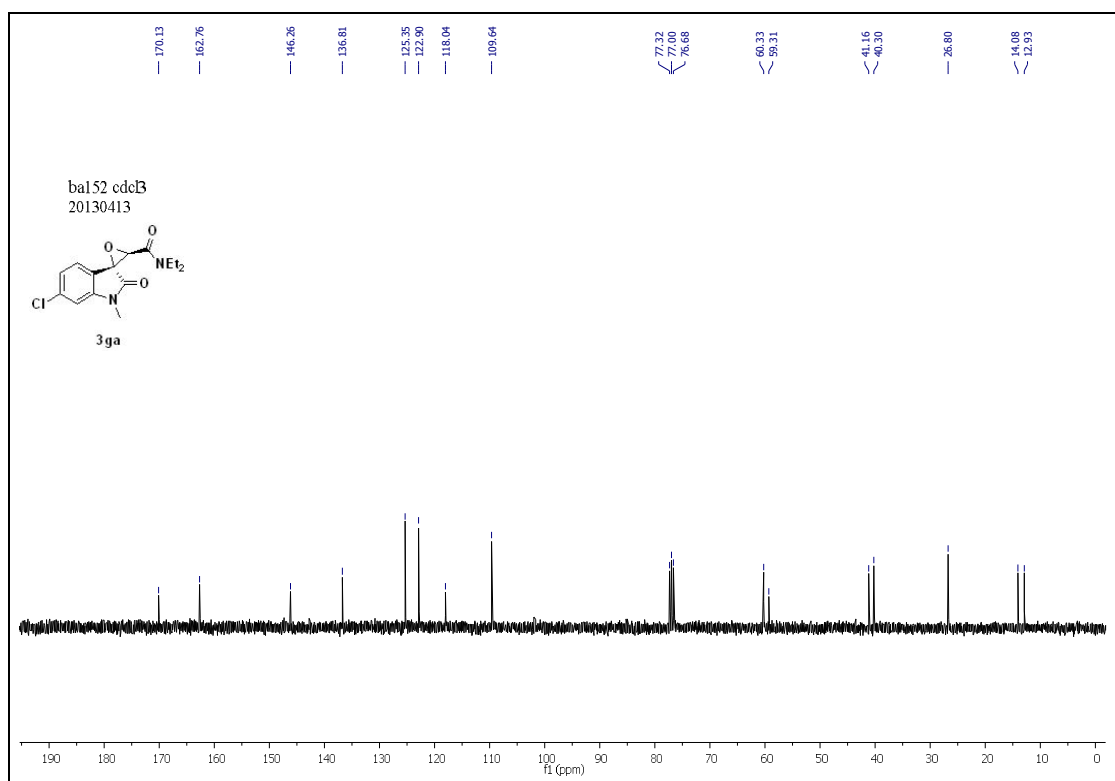
¹³C NMR (100 MHz, CDCl₃) spectrum of 3fa



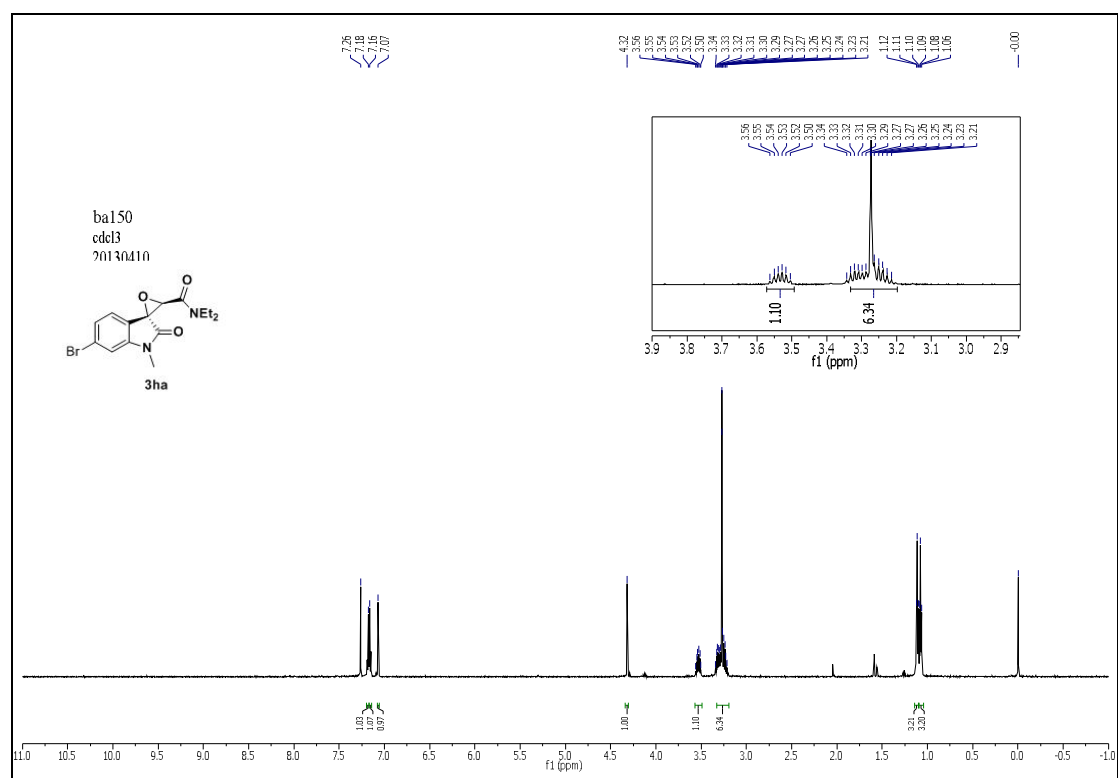
^1H NMR (600 MHz, CDCl_3) spectrum of 3ga



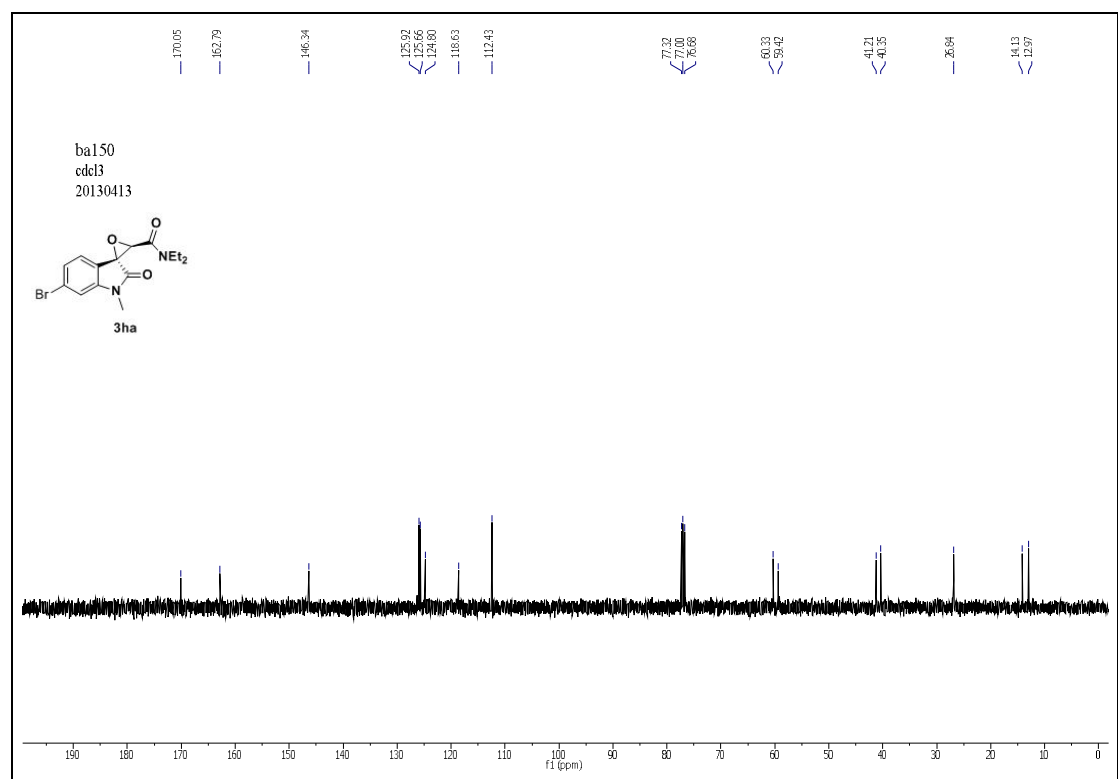
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3ga



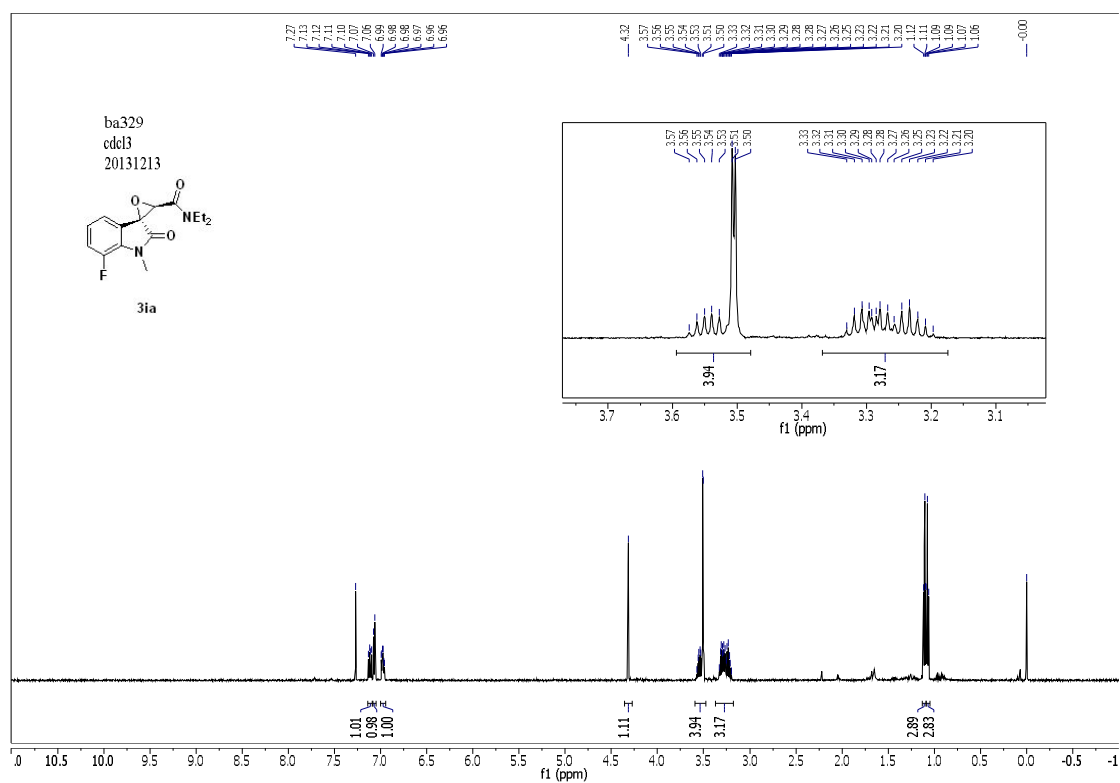
¹H NMR (600 MHz, CDCl₃) spectrum of 3ha



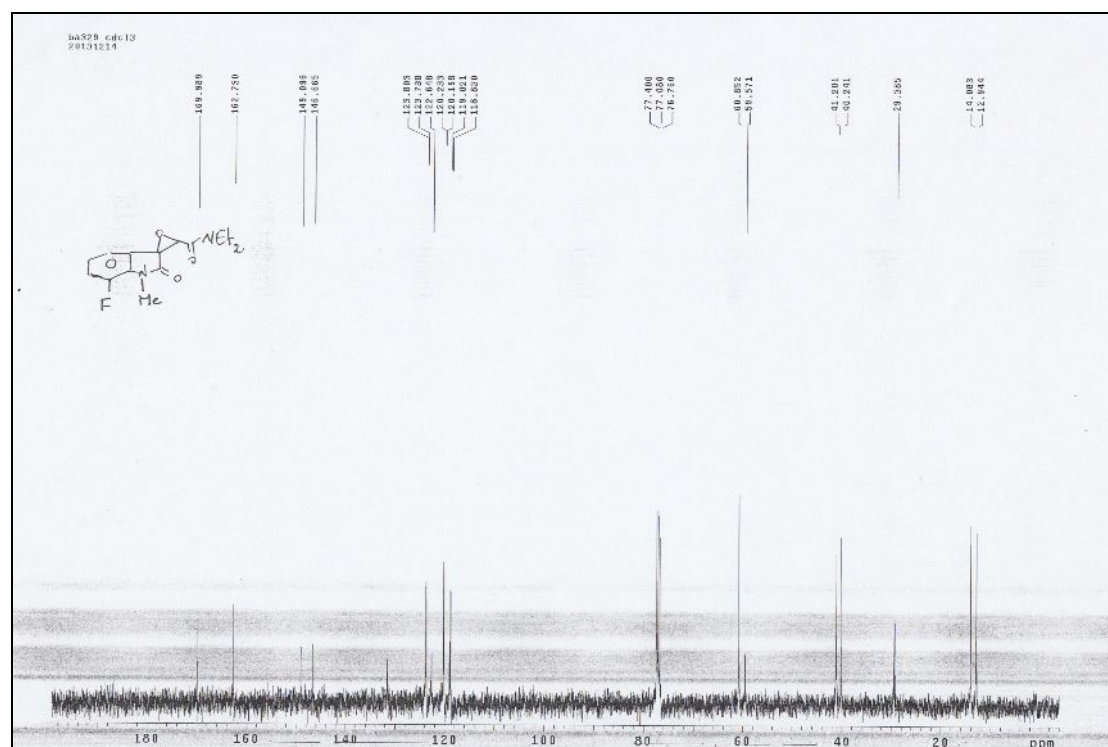
¹³C NMR (100 MHz, CDCl₃) spectrum of 3ha



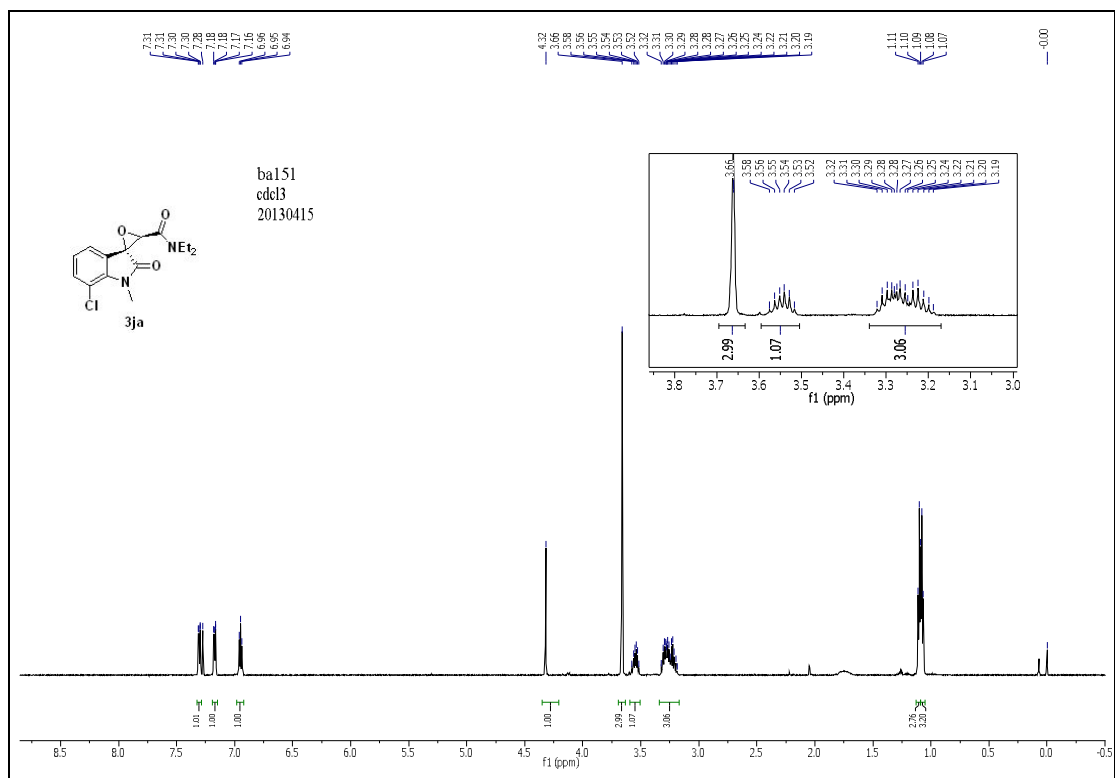
¹H NMR (600 MHz, CDCl₃) spectrum of 3ia



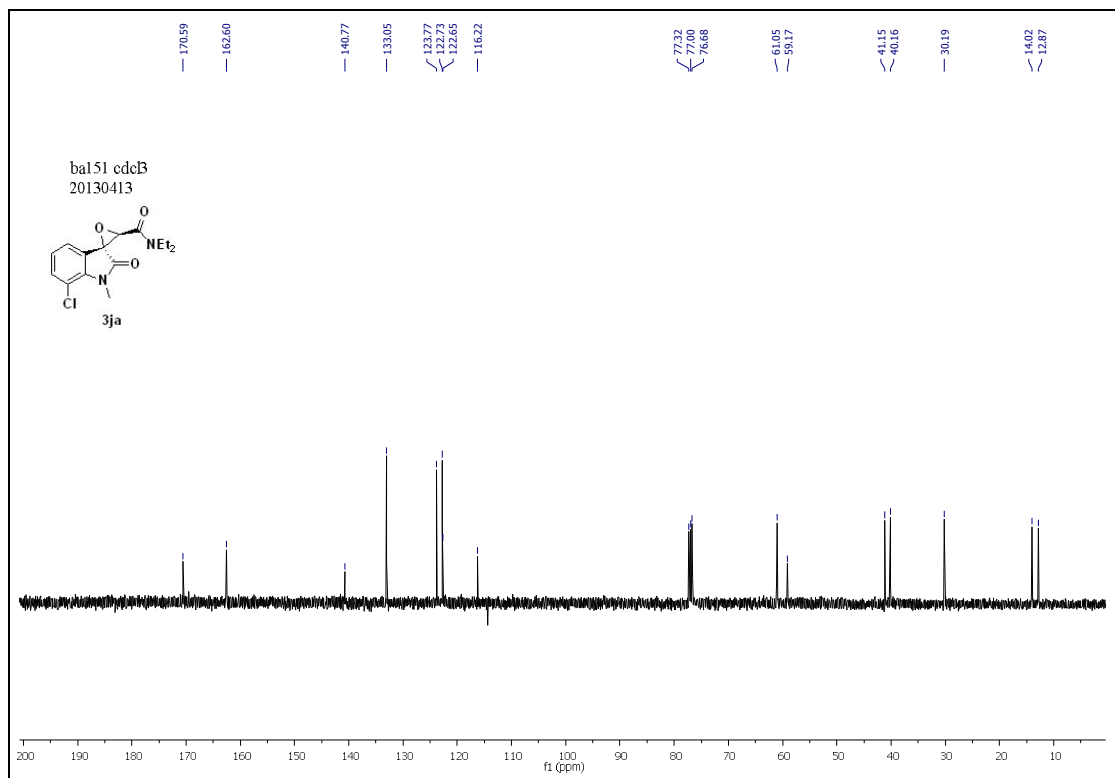
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3ia



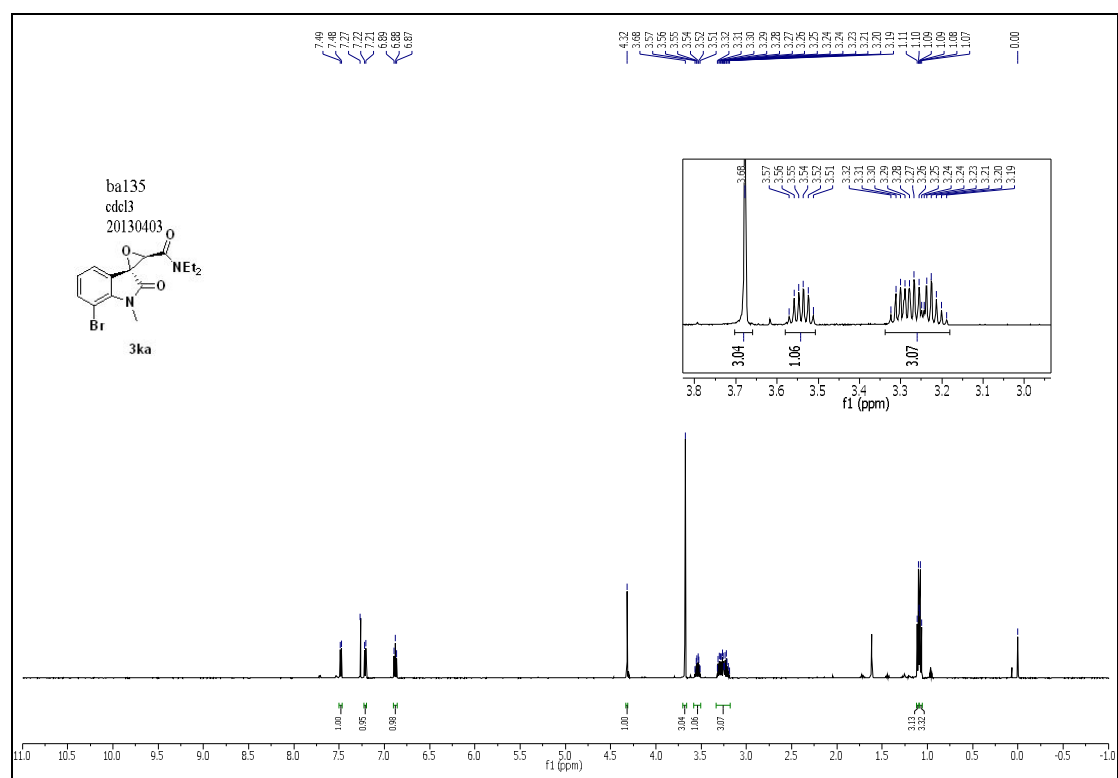
^1H NMR (600 MHz, CDCl_3) spectrum of 3ja



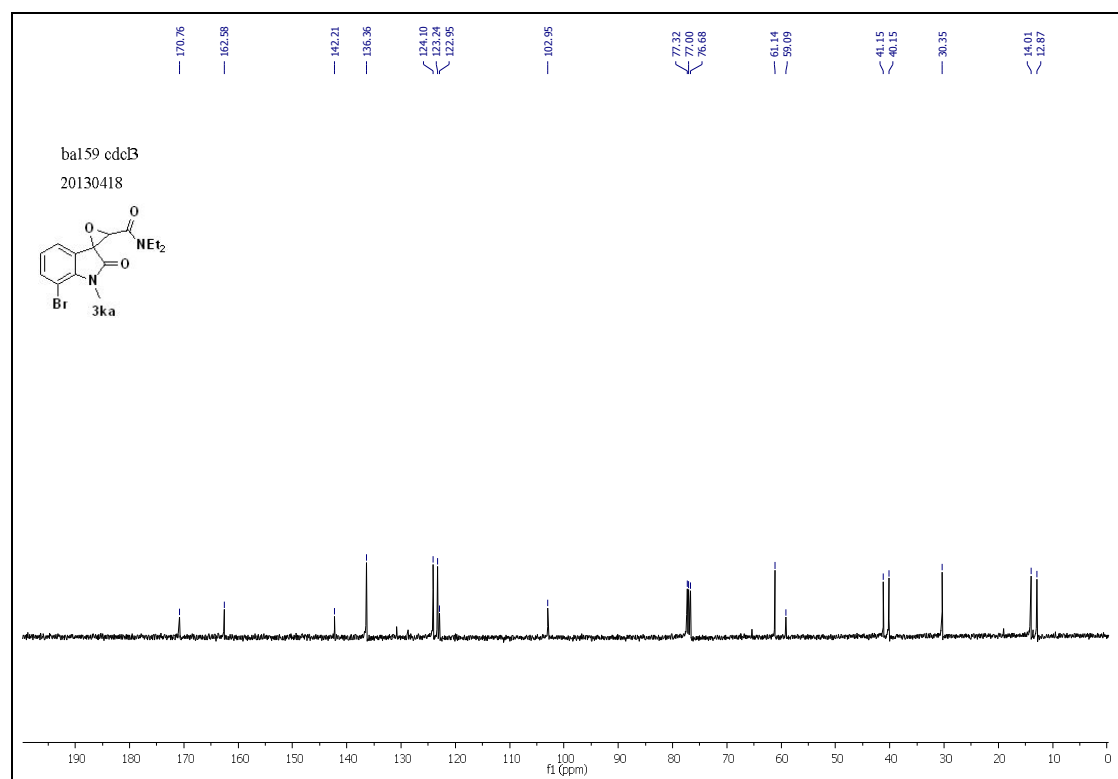
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3ja



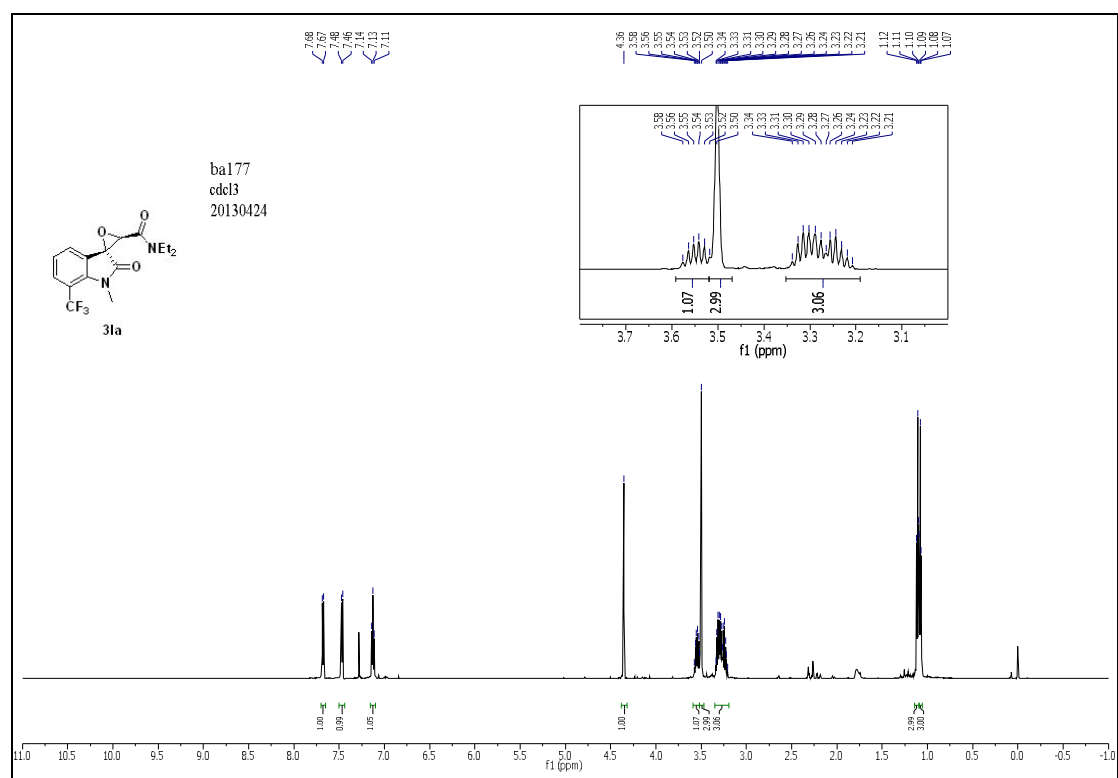
¹H NMR (600 MHz, CDCl₃) spectrum of 3ka



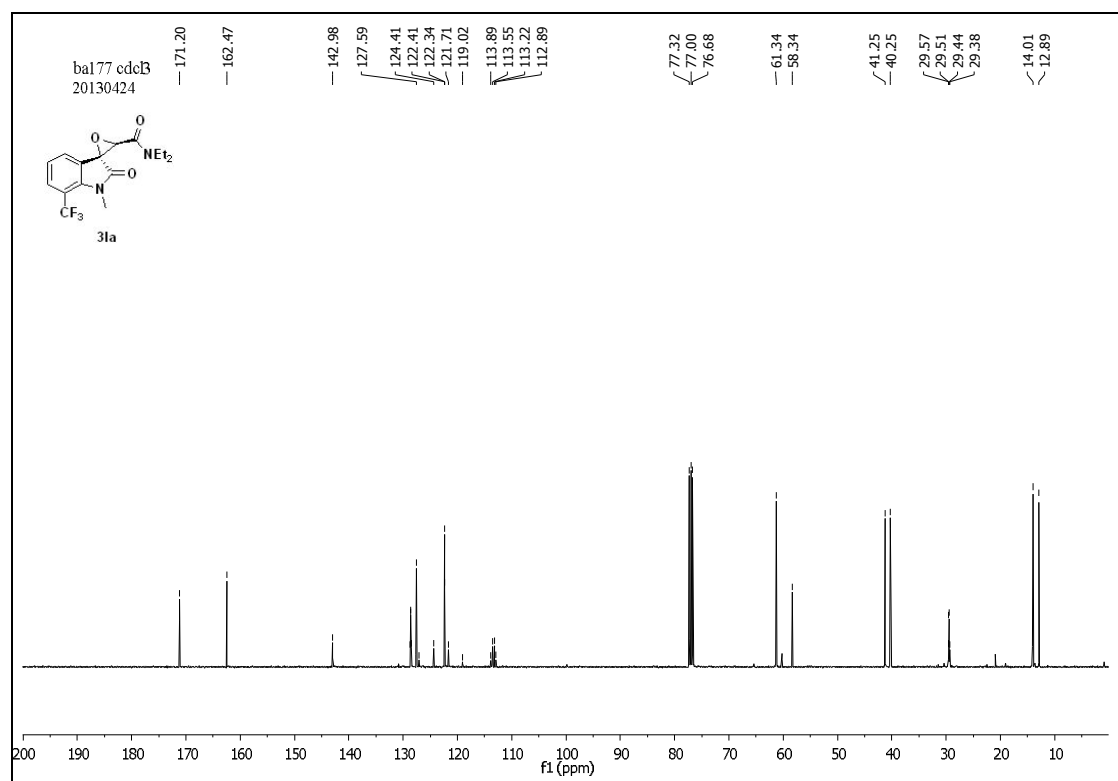
¹³C NMR (100 MHz, CDCl₃) spectrum of 3ka



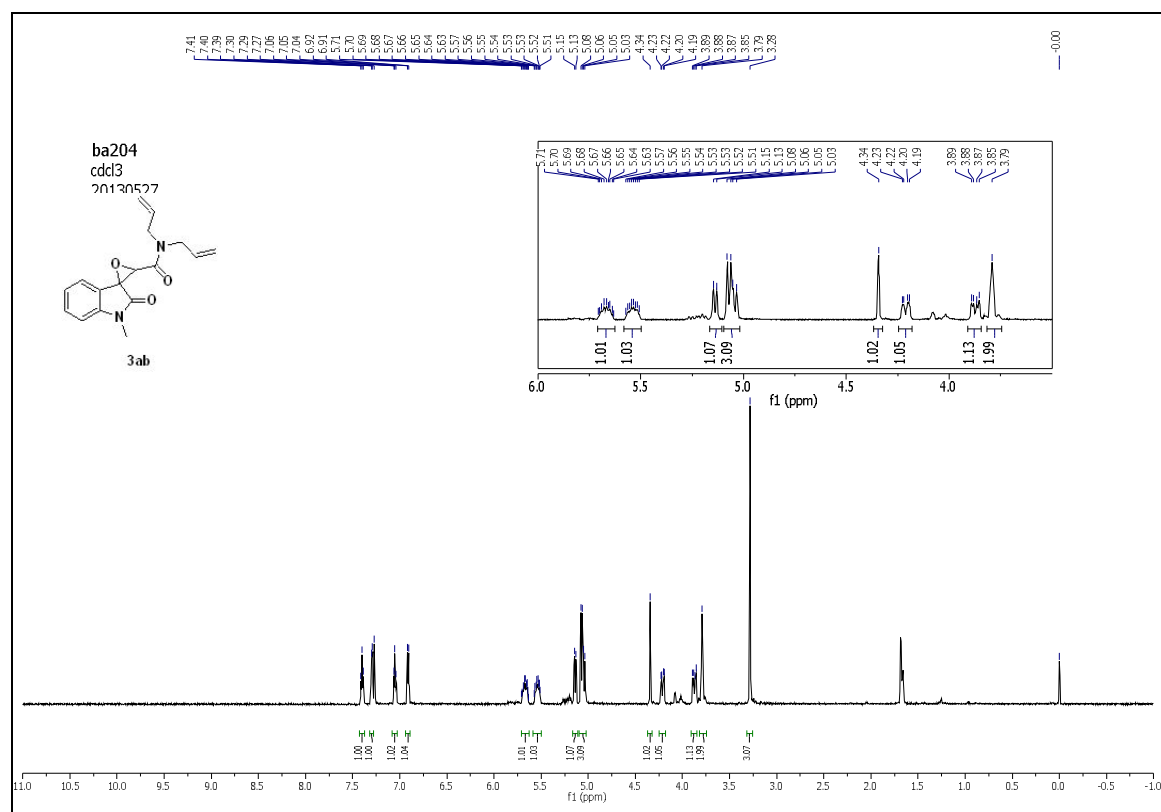
¹H NMR (600 MHz, CDCl₃) spectrum of 3la



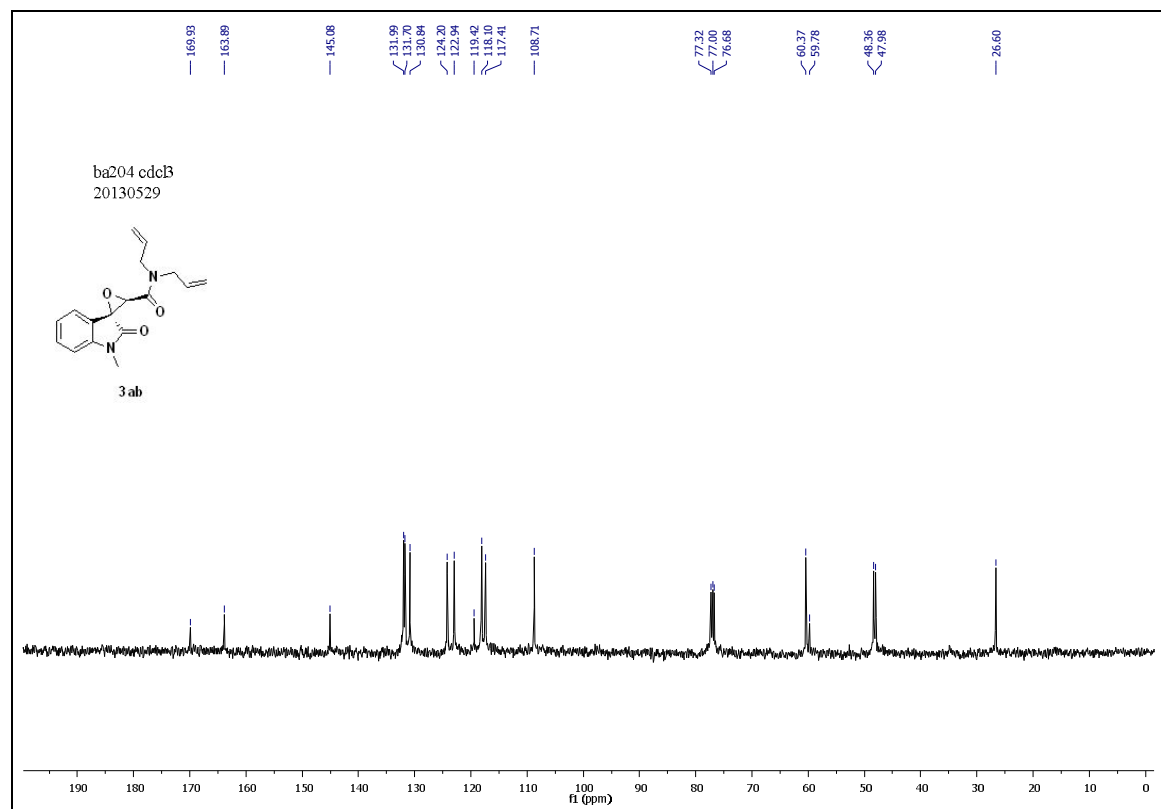
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3la



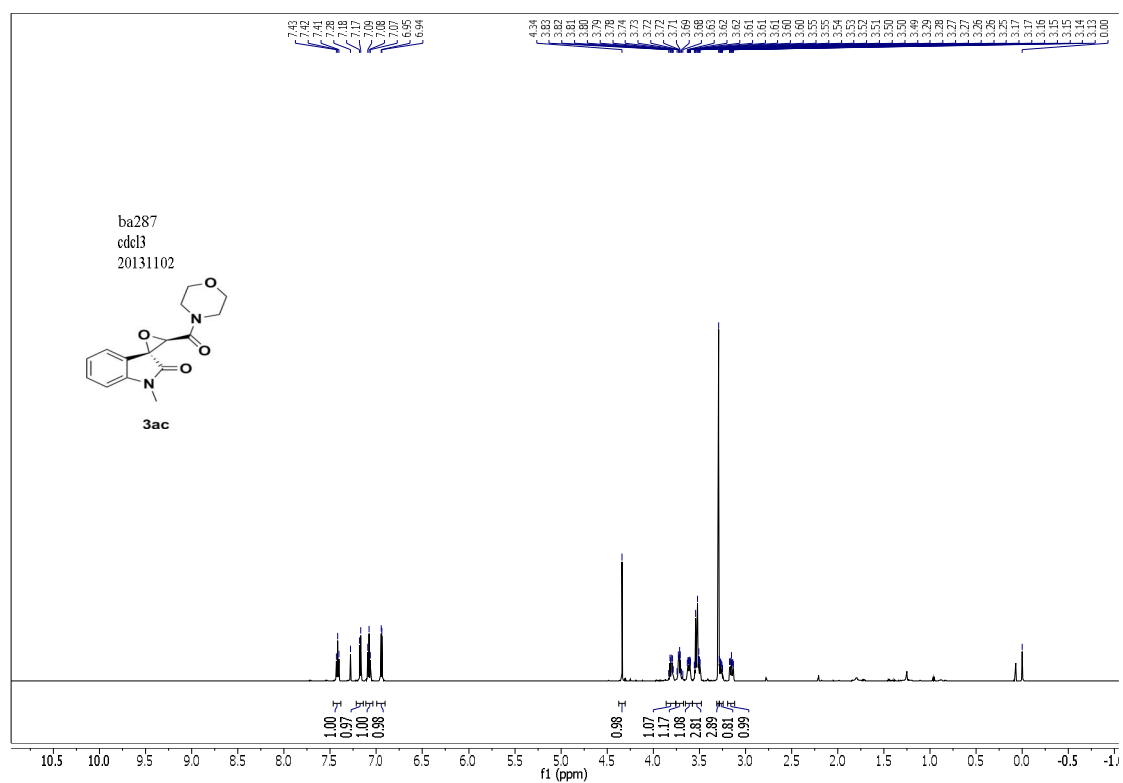
^1H NMR (600 MHz, CDCl_3) spectrum of 3ab



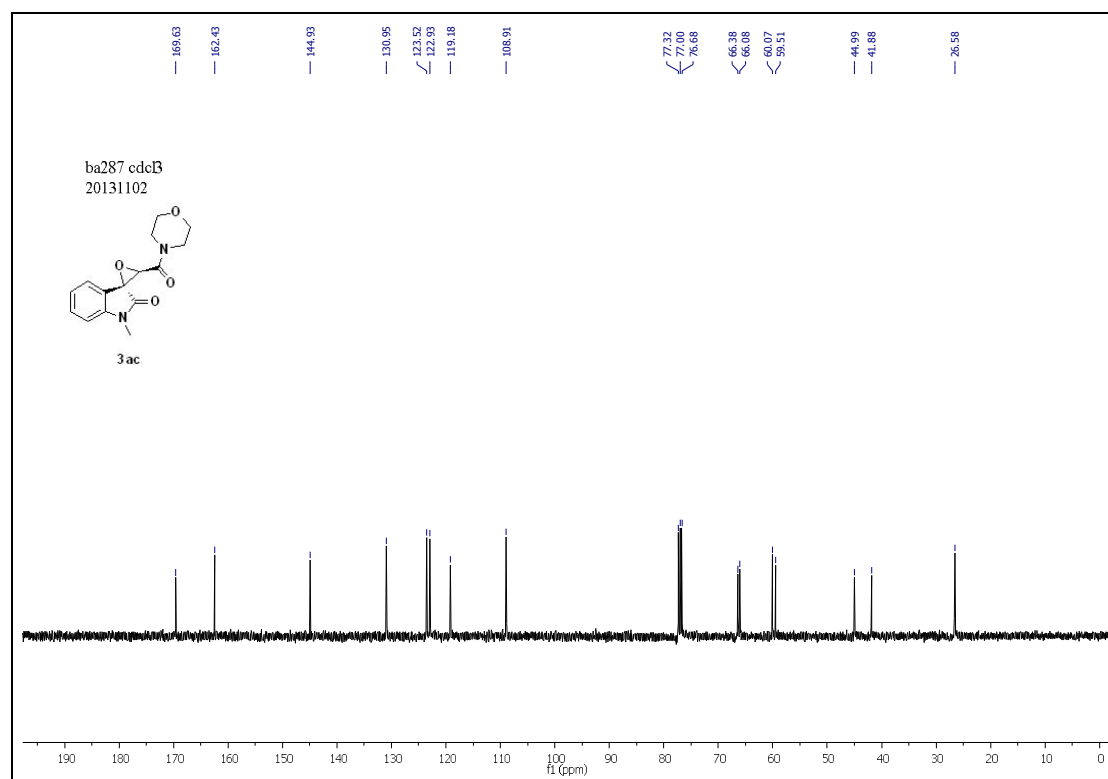
^{13}C NMR (100 MHz, CDCl_3) spectrum of 3ab



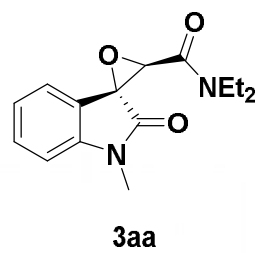
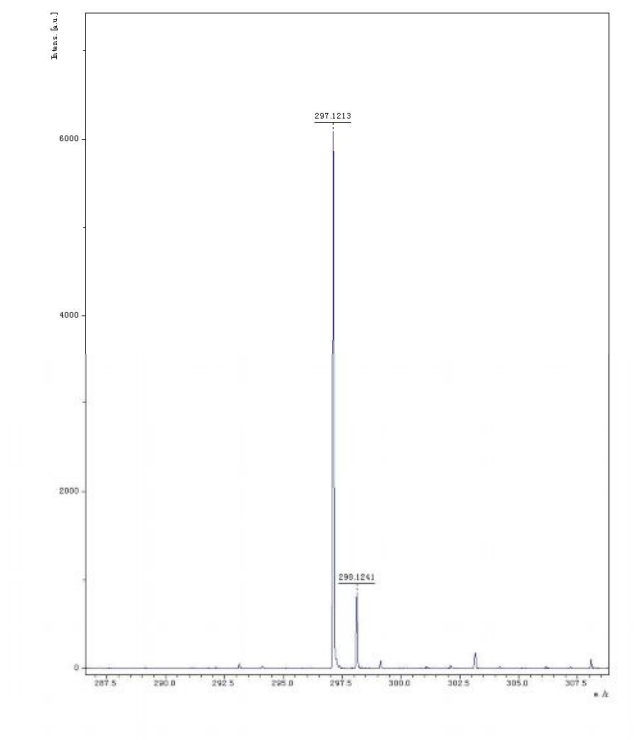
¹H NMR (400 MHz, CDCl₃) spectrum of 3ac



¹³C NMR (100 MHz, CDCl₃) spectrum of 3ac



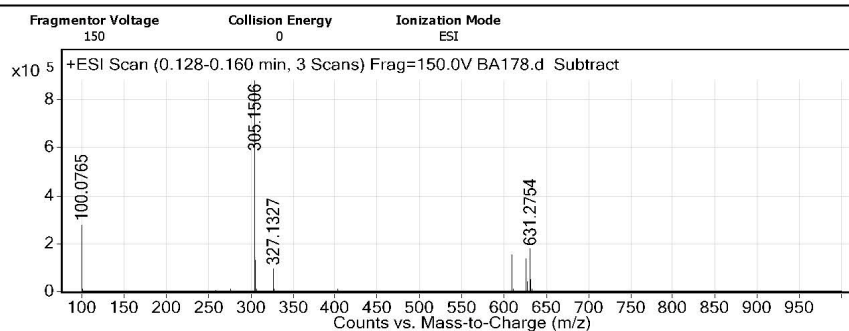
7. Copies of HRMS for Products



**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

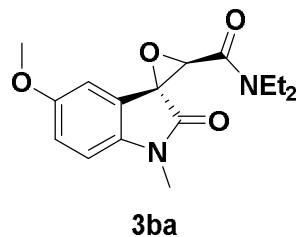
Data Filename BA178.d
Sample Name BA178
User Name
Acquired Time 2013-7-2 4:38:40 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0765		277261.6		
305.1506	1	879340.1	C ₁₆ H ₂₁ N ₂ O ₄	(M+H) ⁺
306.1539	1	135058.7	C ₁₆ H ₂₁ N ₂ O ₄	(M+H) ⁺
327.1327		94423.9		
609.2935	1	156016.6		
610.2966	1	45728.5		
626.32		136804.2		
631.2754	1	176156.4		
632.2787	1	52075.8		



Formula Calculator Results

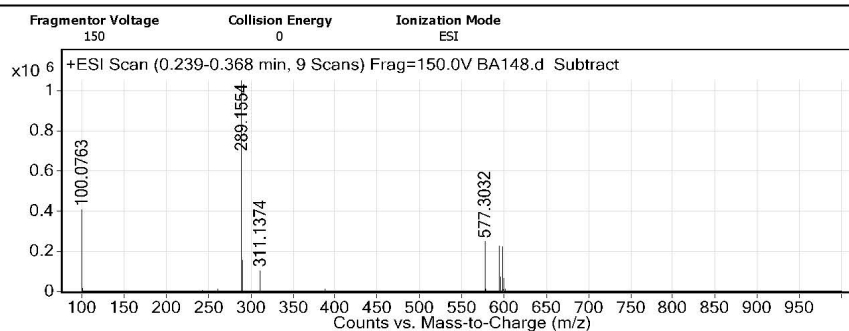
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C ₁₆ H ₂₁ N ₂ O ₄	305.1506	305.1496	-3.49	93.76

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

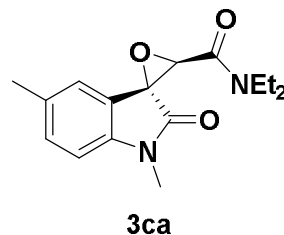
Data Filename BA148.d
Sample Name BA148
User Name
Acquired Time 2013-7-2 4:22:09 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0763		403949.3		
289.1554	1	1070810.2	C ₁₆ H ₂₁ N ₂ O ₃	(M+H) ⁺
290.1587	1	158554.3	C ₁₆ H ₂₁ N ₂ O ₃	(M+H) ⁺
311.1374		105200.2		
577.3032	1	252285		
578.3064	1	74778.6		
594.3297	1	236103.3		
595.3329	1	70959.9		
599.2852	1	222354.9		
600.2884	1	66177		



Formula Calculator Results

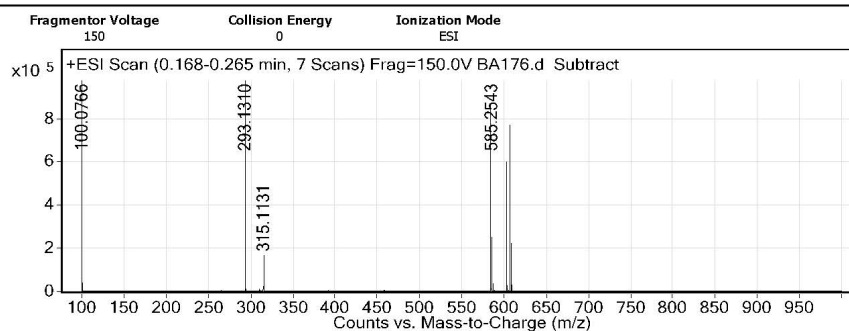
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C ₁₆ H ₂₁ N ₂ O ₃	289.1554	289.1547	-2.62	94.71

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

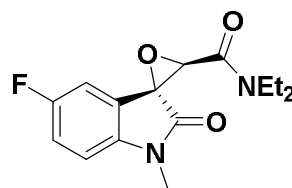
Data Filename BA176.d
Sample Name BA176
User Name
Acquired Time 2013-7-2 4:31:31 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0766		1100025.9		
293.131	1	1016995.7	C ₁₅ H ₁₈ F N ₂ O ₃	(M+H) ⁺
294.1343	1	134483.1	C ₁₅ H ₁₈ F N ₂ O ₃	(M+H) ⁺
315.1131		171895.7		
585.2543	1	889360.2		
586.2575	1	262501.6		
602.2809	1	608126.7		
603.284	1	175976.8		
607.2363	1	768032.1		
608.2395	1	224540.2		



3da

Formula Calculator Results

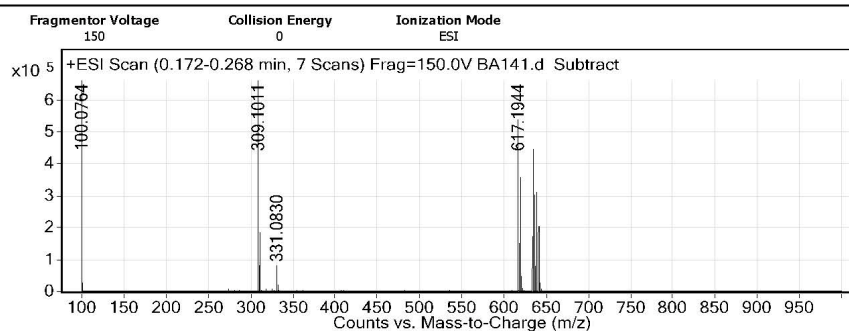
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C ₁₅ H ₁₈ F N ₂ O ₃	293.131	293.1296	-4.95	88.79
C ₂₃ H ₁₇	293.131	293.1325	4.91	73.45

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

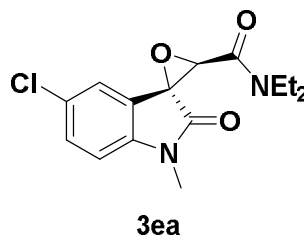
Data Filename BA141.d
Sample Name BA141
User Name
Acquired Time 2013-7-2 4:19:49 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0764		726937.2		
309.1011	1	668157.1	C15 H18 Cl N2 O3	(M+H)+
311.0987	1	187492.4	C15 H18 Cl N2 O3	(M+H)+
617.1944	1	542824.4		
618.1975	1	151482.2		
619.1923	1	359439		
634.2209	1	455370.7		
636.2188	1	301264.8		
639.1766	1	311672		
641.1743	1	203496.3		



Formula Calculator Results

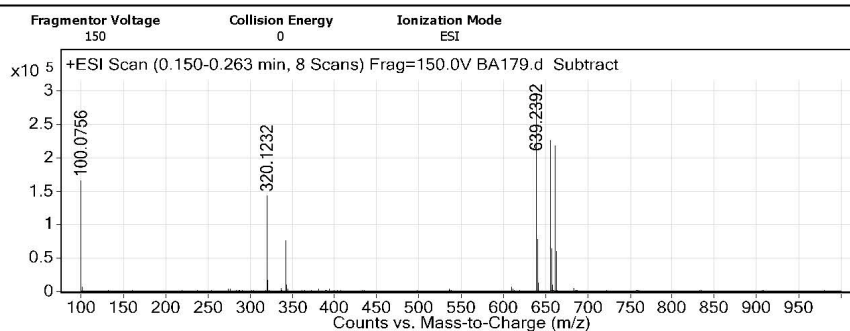
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H18 Cl N2 O3	309.1011	309.1	-3.33	90.93

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

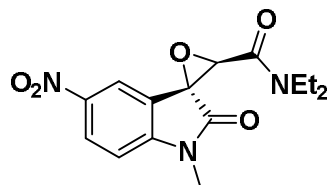
Data Filename BA179.d
Sample Name BA179
User Name
Acquired Time 2013-7-4 11:47:37 AM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0756		170739.7		
320.1232	1	143616.7	C15 H18 N3 O5	(M+H)+
321.1263	1	16348.5	C15 H18 N3 O5	(M+H)+
342.105		76754.7		
639.2392	1	287272.1		
640.2423	1	79493.2		
656.2657	1	228442.5		
657.2686	1	62696.6		
661.2211	1	219302.1		
662.2241	1	59898.2		



3fa

Formula Calculator Results

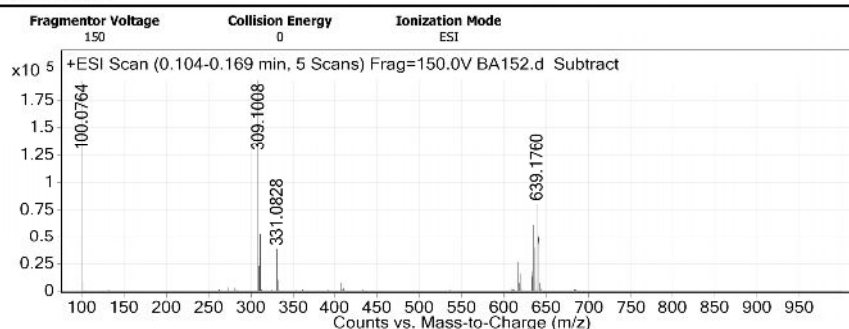
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H18 N3 O5	320.1232	320.1241	2.95	87.86

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

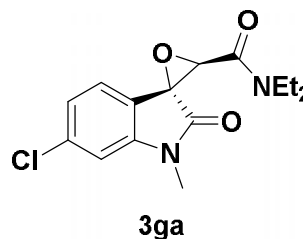
Data Filename BA152.d
Sample Name BA152
User Name
Acquired Time 2013-7-2 4:33:52 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0764		238432		
309.1008	1	194076.7	C ₁₅ H ₁₈ Cl N ₂ O ₃	(M+H) ⁺
310.1039	1	22772.3	C ₁₅ H ₁₈ Cl N ₂ O ₃	(M+H) ⁺
311.0983	1	53252.1	C ₁₅ H ₁₈ Cl N ₂ O ₃	(M+H) ⁺
331.0828		38838.3		
617.1938		25824.6		
634.2204	1	60870		
636.2185	1	38783.2		
639.176	1	79859		
641.1737	1	51613.6		



Formula Calculator Results

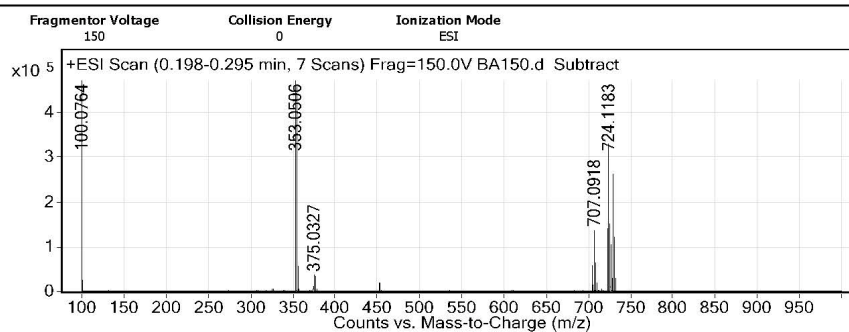
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C ₁₅ H ₁₈ Cl N ₂ O ₃	309.1008	309.1	-2.53	91.24

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report**

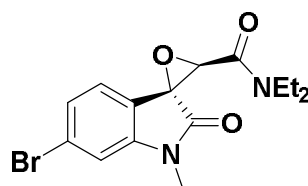
Data Filename BA150.d
Sample Name BA150
User Name
Acquired Time 2013-7-2 4:26:49 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0764		654172		
353.0506	1	484564.9	C15 H18 Br N2 O3	(M+H)+
355.0487	1	478998	C15 H18 Br N2 O3	(M+H)+
707.0918	1	139177.7		
722.1202	1	141129.8		
724.1183	1	331119		
726.1169	1	155355.5		
727.0833		105515.4		
729.0738	1	266800.6		
731.0726	1	121722.8		

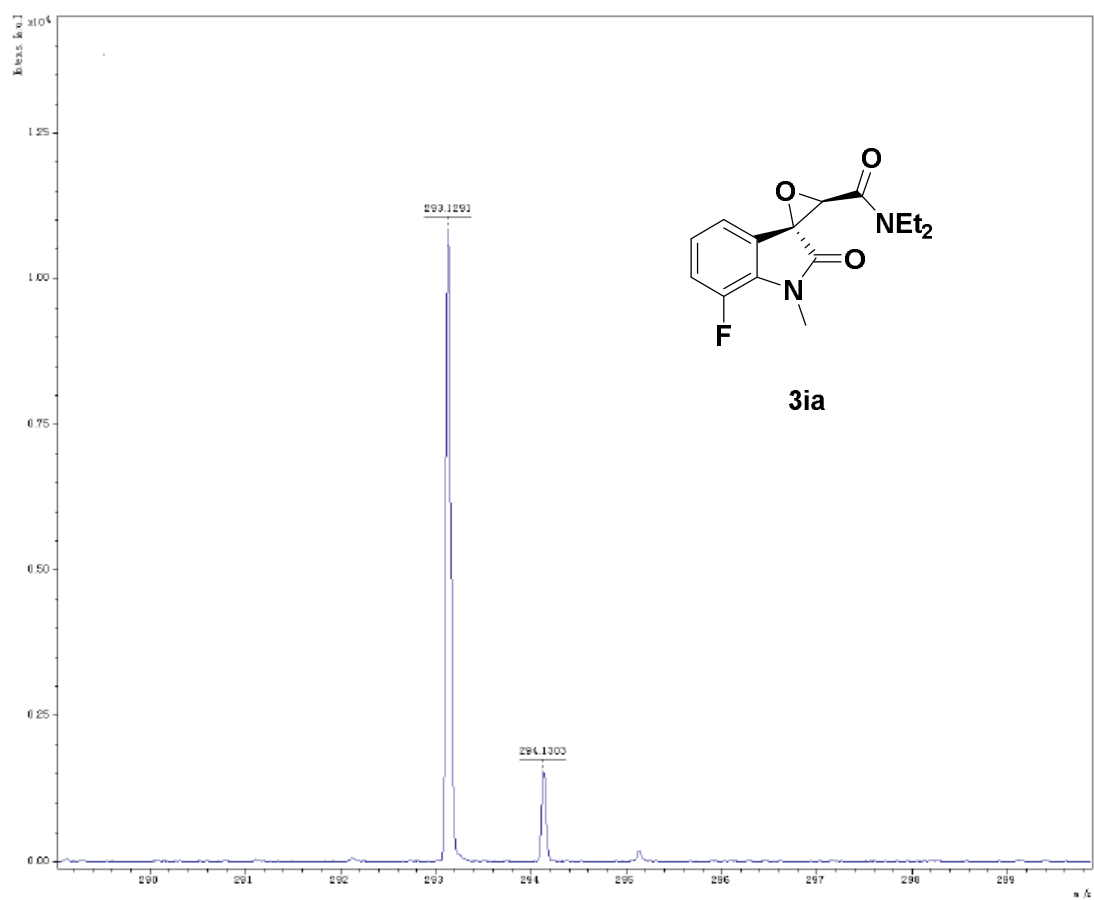


3ha

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H18 Br N2 O3	353.0506	353.0495	-3.13	90.43

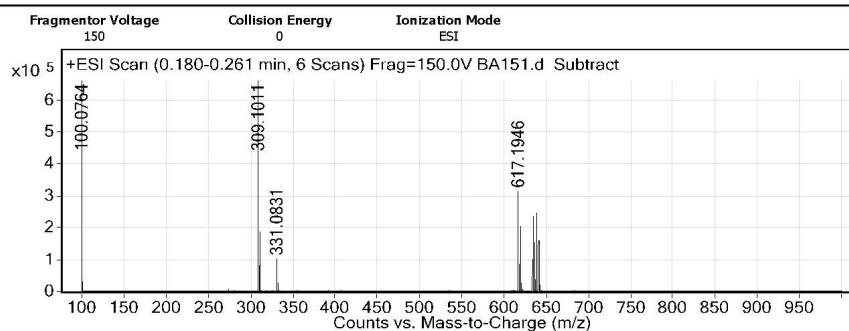
--- End Of Report ---



**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

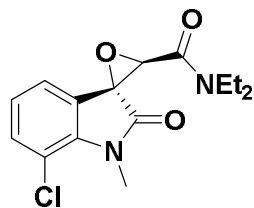
Data Filename BA151.d
Sample Name BA151
User Name
Acquired Time 2013-7-2 4:29:10 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0764		836449.1		
309.1011	1	668120.8	C15 H18 Cl N2 O3	(M+H)+
311.0987	1	188953.8	C15 H18 Cl N2 O3	(M+H)+
331.0831		102747.8		
617.1946	1	315645		
619.1926	1	204178		
634.2211	1	237406.3		
636.219	1	153852.9		
639.1768	1	246283.4		
641.1746	1	158945.3		



3ja

Formula Calculator Results

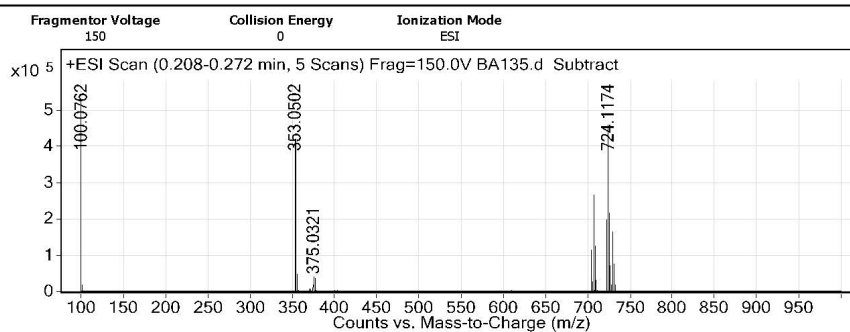
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H18 Cl N2 O3	309.1011	309.1	-3.46	91.01

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

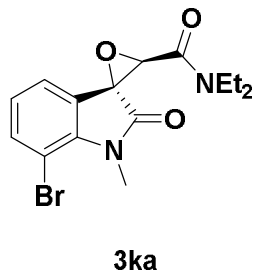
Data Filename BA135.d
Sample Name BA135
User Name
Acquired Time 2013-7-2 4:17:34 PM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0762		532544.6		
353.0502	1	437669.8	C15 H18 Br N2 O3	(M+H)+
355.0483	1	429076.6	C15 H18 Br N2 O3	(M+H)+
707.0908	1	269067.2		
709.0896	1	124711		
722.1191	1	202321.3		
724.1174	1	466676.9		
725.1202	1	128373.4		
726.116	1	223146		
729.0728	1	164418.7		



Formula Calculator Results

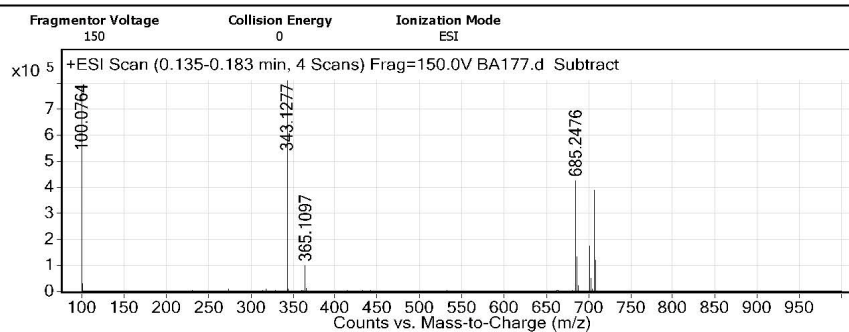
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H18 Br N2 O3	353.0502	353.0495	-1.75	92.54

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report**

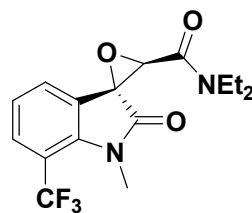
Data Filename BA177.d
Sample Name Unavailable
User Name Unavailable
Acquired Time Unavailable
Instrument Agilent Technologies 6224 TOF LC/MS

User Spectra



Peak List

m/z	z	Abund	Formula	Ion
100.0764		788661.4		
343.1277	1	838479.9	C ₁₆ H ₁₈ F ₃ N ₂ O ₃	(M+H) ⁺
344.131	1	120262.6	C ₁₆ H ₁₈ F ₃ N ₂ O ₃	(M+H) ⁺
365.1097		100931.1		
685.2476	1	431358.5		
686.2508	1	133469.2		
702.2741	1	174963.3		
703.2773	1	50926.1		
707.2297	1	409489.6		
708.2328	1	125239.6		



3la

Formula Calculator Results

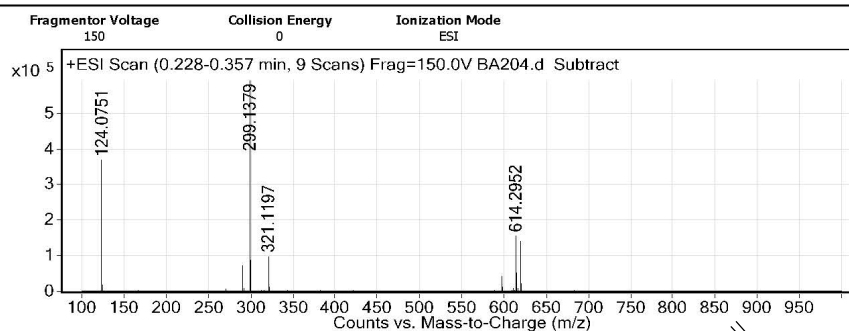
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C ₁₆ H ₁₈ F ₃ N ₂ O ₃	343.1277	343.1264	-3.72	91.18
C ₁₈ H ₁₉ N ₂ O ₅	343.1277	343.1288	3.42	87.37
C ₂₄ H ₁₇ F ₂	343.1277	343.1293	4.7	73.46

--- End Of Report ---

**State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Data Report**

Data Filename BA204.d
Sample Name BA204
User Name
Acquired Time 2013-7-4 11:56:58 AM
Instrument
 Agilent Technologies 6224 TOF LC/MS

User Spectra

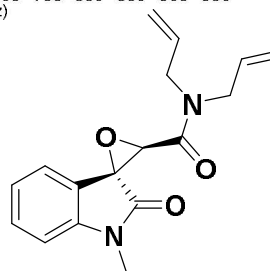


Peak List

m/z	z	Abund	Formula	Ion
124.0751		383962		
291.1692		72389		
299.1379	1	596994.5	C17 H19 N2 O3	(M+H)+
300.1411	1	88633.5	C17 H19 N2 O3	(M+H)+
321.1197		100653.1		
597.2686		44059.9		
614.2952	1	161628.6		
615.2983	1	51202.1		
619.2505	1	146088.6		
620.2538	1	45971.2		

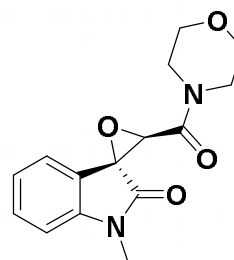
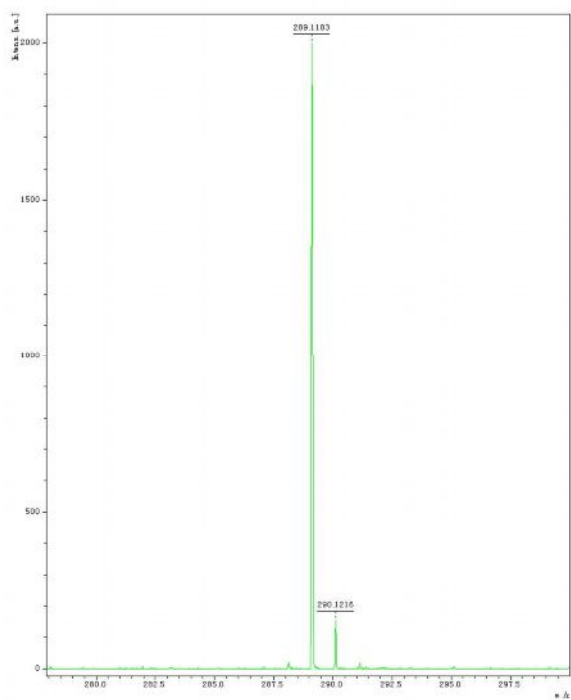
Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C17 H19 N2 O3	299.1379	299.139	3.91	90.39



3ab

--- End Of Report ---



3ac