

Supporting information

Asymmetric Aziridination of *N*-Sulphonyl Ketimines with Unfunctionalized Ketones: a One-pot Approach to Multi-substituted Fused Aziridines

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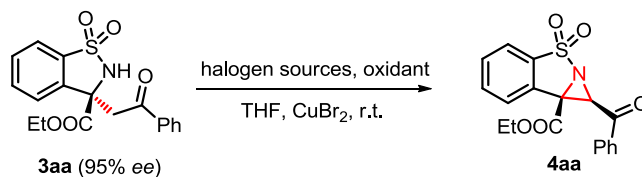
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Part I Experimental Section

1.1 Optimization of reaction conditions

Table S1. The effects of halogen sources and oxidants on the oxidative C-H amination process.^a

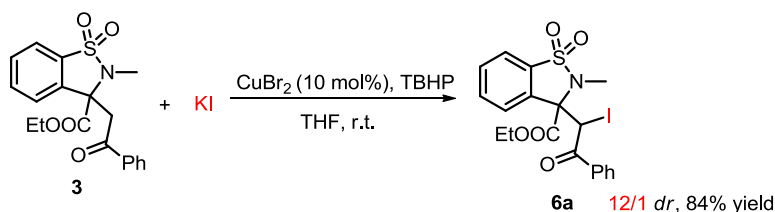


entry	Halogen sources	oxidant	yield (%) ^b	<i>ee</i> (%) ^c
1	KBr	TBHP	trace	n.d.
2	(<i>n</i> -Bu) ₄ NI	TBHP	76	94
3	NaI	TBHP	37	93
4	KI	TBHP	94	95
5	NIS	TBHP	trace	n.d.
6	KI	PhIO	trace	n.d.
7	KI	PhI(OAc) ₂	35	90

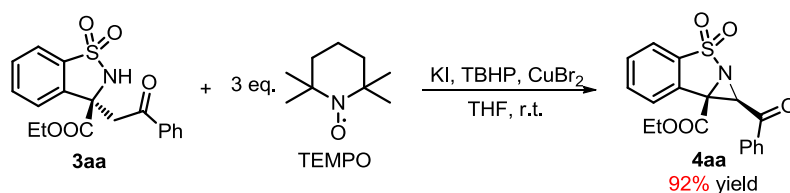
^a The reaction of **3aa** (0.1 mmol), halogen sources (0.2 mmol) with oxidants (0.3 mmol) was performed in the presence of CuBr₂ (10 mol %) in THF (1.0 mL) at room temperature for 4 h. ^b Yield of isolated product. ^c The *ee* value of the product was determined by HPLC on a chiral stationary phase.

1.2 Mechanism study on the intramolecular C-H amination

Control experiments:



First, the racemic methylated Mannich product **3** was prepared according to the previously reported method.¹ To the mixture of **3** (75 mg, 0.2 mmol) and KI (64 mg, 0.4 mmol) in 2 mL THF, was added CuBr₂ (4.4 mg, 0.02 mmol). After stirring the mixture at room temperature for 30 minutes, the oxidant TBHP (109 μ L, 5.5 mol/L in *n*-decane) was added in portions during 4 hours. After completion of the reaction (monitored by TLC), the solvent was evaporated in vacuo. Purification of the residue by column chromatography (PE/EA = 8/1-4/1) afforded an iodinated intermediate **6a** in 84% yield with 12/1 *dr*.



To the mixture of **3aa** (36 mg, 0.1 mmol) and KI (32 mg, 0.2 mmol) in 1 mL THF, was added CuBr₂ (2.2 mg, 0.01 mmol) and TEMPO (47 mg, 0.3 mmol). After stirring the mixture at room temperature for 30 minutes, the oxidant TBHP (55 μ L, 5.5 mol/L in *n*-decane) was added in portions during 4 hours. After completion of the reaction (monitored by TLC), the solvent was evaporated in vacuo. Purification of the residue by column chromatography (PE/EA = 8/1-4/1) afforded the product **4aa** in 92% yield.

The coordination between CuBr₂ and Mannich product 3aa:



Figure S1. **3aa** in THF

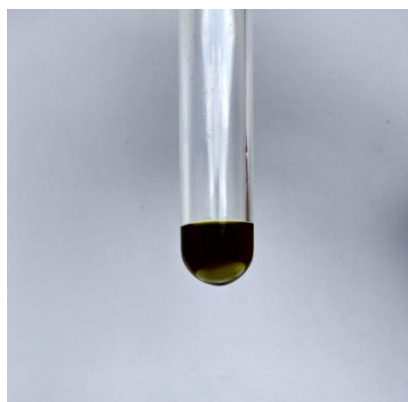
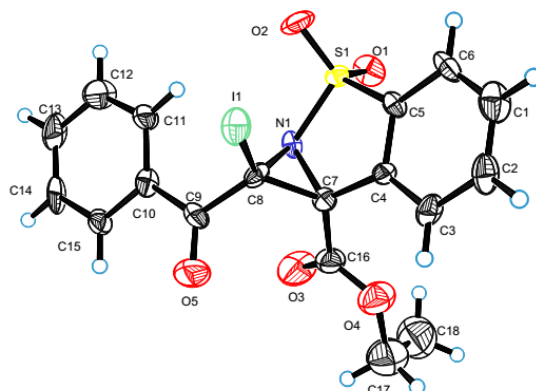


Figure S2. CuBr₂ and **3aa** in THF

As shown in the above figures, an obvious change in the solution color was detected. This observation suggested the coordination between CuBr₂ and Mannich product **3aa**. This coordination interaction was considered as an important role in inhibiting the racemization of the Mannich product **3aa** and the further iodination of the aziridine product **4aa**.

1.3 Determination of absolute configuration of the aziridine products

5aa



Chemical formula	C ₁₈ H ₁₄ INO ₅ S
Formula weight	483.26
Space group	P2 ₁ 2 ₁ 2 ₁
Z	4
a, Å	7.2554
b, Å	15.7659
c, Å	16.4944
α, °	90.00
β, °	90.00
γ, °	90.00
V, Å ³	1886.76
T, K	291 (2)
ρ, g/cm ³	1.701

Reflections collected / unique: 4432/3082 ($R_{int} = 0.0616$), number of observations [$I > 2 \sigma(I)$] 2990, parameters 236. Final R indices [$I > 2 \sigma(I)$]: $R_1 = 0.0842$, $wR_2 = 0.2177$; R indices (all data): $R_1 = 0.0852$, $wR_2 = 0.2203$; Flack parameter = 0.005(12).

Table S2 Crystal data and structure refinement for 5aa.

Identification code	5aa
Empirical formula	C ₁₈ H ₁₄ INO ₅ S
Formula weight	483.26
Temperature/K	291(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	7.25540(10)
b/Å	15.7659(3)
c/Å	16.4944(3)
α/°	90
β/°	90

$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	1886.76(6)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.701
μ/mm^{-1}	14.626
F(000)	952.0
Crystal size/ mm^3	$0.280 \times 0.220 \times 0.200$
Radiation	$\text{CuK}\alpha$ ($\lambda = 1.54184$)
2Θ range for data collection/ $^\circ$	7.758 to 142.364
Index ranges	$-8 \leq h \leq 8, -18 \leq k \leq 19, -11 \leq l \leq 19$
Reflections collected	4432
Independent reflections	3082 [$R_{\text{int}} = 0.0616, R_{\text{sigma}} = 0.0693$]
Data/restraints/parameters	3082/18/236
Goodness-of-fit on F^2	1.047
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0842, wR_2 = 0.2177$
Final R indexes [all data]	$R_1 = 0.0852, wR_2 = 0.2203$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	3.92/-3.14
Flack parameter	0.005(12)

Table S3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 5aa. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
I1	-2833.9(12)	414.3(6)	6569.1(5)	36.8(4)
S1	1803(4)	937.9(17)	7211.8(19)	23.8(7)
N1	1566(13)	411(7)	6316(5)	21(2)
O2	696(17)	1679(6)	7199(8)	43(3)
O1	3720(14)	1037(7)	7333(7)	42(3)
C7	1045(16)	-497(8)	6503(8)	25(2)
O4	2300(20)	-1853(8)	6381(8)	59(3)
C4	707(19)	-602(7)	7405(8)	24(3)
O5	-1010(30)	-714(7)	4903(8)	68(5)
C5	999(16)	138(8)	7842(7)	22(2)
C8	-240(20)	75(7)	6053(8)	27(3)
O3	2970(30)	-960(9)	5422(8)	68(4)
C14	70(20)	1256(12)	3266(8)	42(4)
C6	740(20)	196(11)	8669(8)	35(3)
C16	2210(30)	-1139(9)	6031(9)	40(3)
C10	-209(19)	721(9)	4628(8)	29(3)

C13	250(30)	2073(12)	3554(11)	53(5)
C12	280(40)	2198(11)	4376(10)	54(5)
C15	-190(20)	580(9)	3781(9)	34(3)
C11	30(30)	1541(9)	4915(8)	44(4)
C3	140(20)	-1328(9)	7811(9)	34(3)
C9	-510(30)	-29(9)	5147(8)	36(3)
C1	100(20)	-545(12)	9069(10)	46(4)
C2	-160(30)	-1278(11)	8643(9)	43(4)
C17	3310(40)	-2553(16)	6010(17)	76(6)
C18	5490(50)	-2390(20)	6114(19)	96(9)

Table S4 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 5aa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	23.5(5)	49.2(6)	37.6(5)	6.7(4)	-0.5(4)	2.7(3)
S1	22.5(14)	19.4(12)	29.5(15)	-1.5(11)	0.0(12)	-1.6(10)
N1	15(4)	36(5)	13(4)	4(4)	6(4)	1(4)
O2	49(6)	18(4)	63(7)	-5(4)	-6(6)	8(4)
O1	18(5)	56(6)	51(6)	-8(5)	-3(5)	-5(4)
C7	17(5)	30(6)	27(6)	-4(5)	0(5)	8(5)
O4	73(6)	47(5)	58(5)	0(4)	14(5)	9(5)
C4	25(6)	20(5)	26(6)	-2(5)	-3(5)	4(4)
O5	116(15)	31(5)	56(7)	0(6)	-18(9)	-15(7)
C5	18(5)	33(6)	16(5)	-2(5)	5(5)	-1(5)
C8	36(7)	19(5)	25(6)	8(5)	10(6)	4(5)
O3	88(11)	62(8)	55(7)	-2(6)	35(9)	25(8)
C14	40(8)	72(11)	14(6)	21(6)	4(6)	9(8)
C6	28(7)	56(8)	21(6)	-13(6)	-6(6)	8(6)
C16	54(9)	31(6)	34(7)	-4(5)	7(8)	4(7)
C10	28(6)	41(7)	18(6)	5(5)	10(5)	9(6)
C13	67(11)	53(9)	39(9)	27(8)	-5(9)	-1(8)
C12	87(15)	42(8)	34(8)	6(7)	14(10)	0(9)
C15	38(7)	40(8)	23(6)	-6(6)	-2(6)	10(6)
C11	80(13)	30(7)	22(6)	1(6)	-8(8)	1(8)
C3	38(7)	28(6)	36(7)	14(6)	2(7)	-7(6)
C9	54(9)	36(7)	19(6)	-4(5)	-6(7)	-1(7)
C1	39(8)	67(11)	31(7)	9(8)	15(7)	7(8)
C2	45(9)	53(9)	30(7)	18(7)	3(7)	-7(7)
C17	80(8)	68(7)	81(8)	-6(6)	6(6)	4(6)
C18	98(13)	102(13)	87(12)	-7(10)	-7(11)	23(11)

Table S5 Bond Lengths for 5aa.**Atom Atom Length/Å**

I1	C8	2.135(13)
S1	O1	1.414(10)
S1	O2	1.419(10)
S1	N1	1.704(10)
S1	C5	1.736(12)
N1	C8	1.477(17)
N1	C7	1.512(16)
C7	C8	1.494(17)
C7	C4	1.517(18)
C7	C16	1.533(18)
O4	C16	1.27(2)
O4	C17	1.46(3)
C4	C3	1.387(18)
C4	C5	1.387(17)
O5	C9	1.208(19)

Atom Atom Length/Å

C5	C6	1.380(18)
C8	C9	1.517(18)
O3	C16	1.18(2)
C14	C15	1.38(2)
C14	C13	1.38(3)
C6	C1	1.42(2)
C10	C11	1.39(2)
C10	C15	1.415(19)
C10	C9	1.48(2)
C13	C12	1.37(3)
C12	C11	1.38(2)
C3	C2	1.39(2)
C1	C2	1.37(3)
C17	C18	1.61(5)

Table S6 Bond Angles for 5aa.**Atom Atom Atom Angle/°**

O1	S1	O2	117.9(7)
O1	S1	N1	106.0(6)
O2	S1	N1	109.4(6)
O1	S1	C5	109.0(7)
O2	S1	C5	114.7(7)
N1	S1	C5	97.5(5)
C8	N1	C7	59.9(7)
C8	N1	S1	121.3(8)
C7	N1	S1	108.1(7)
C8	C7	N1	58.8(8)
C8	C7	C4	116.9(10)
N1	C7	C4	110.1(10)
C8	C7	C16	119.3(12)
N1	C7	C16	112.5(11)
C4	C7	C16	121.1(11)
C16	O4	C17	120.3(16)
C3	C4	C5	119.2(12)
C3	C4	C7	127.6(12)
C5	C4	C7	113.1(11)
C6	C5	C4	123.3(13)

Atom Atom Atom Angle/°

C7	C8	C9	120.5(11)
N1	C8	I1	125.1(8)
C7	C8	I1	120.2(8)
C9	C8	I1	107.7(10)
C15	C14	C13	121.7(13)
C5	C6	C1	116.7(14)
O3	C16	O4	125.4(15)
O3	C16	C7	122.2(13)
O4	C16	C7	112.4(13)
C11	C10	C15	118.8(13)
C11	C10	C9	124.6(12)
C15	C10	C9	116.6(13)
C12	C13	C14	118.5(15)
C13	C12	C11	121.9(17)
C14	C15	C10	119.2(14)
C12	C11	C10	119.8(14)
C4	C3	C2	118.4(14)
O5	C9	C10	124.6(13)
O5	C9	C8	117.7(13)
C10	C9	C8	117.7(12)

C6	C5	S1	126.1(11)
C4	C5	S1	110.6(9)
N1	C8	C7	61.2(8)
N1	C8	C9	116.5(11)

C2	C1	C6	120.2(14)
C1	C2	C3	122.2(15)
O4	C17	C18	109(2)

Table S7 Torsion Angles for 5aa.

A	B	C	D	Angle/°
O1	S1	N1	C8	170.2(9)
O2	S1	N1	C8	-61.6(11)
C5	S1	N1	C8	57.9(10)
O1	S1	N1	C7	105.0(8)
O2	S1	N1	C7	-126.9(8)
C5	S1	N1	C7	-7.4(8)
S1	N1	C7	C8	116.3(9)
C8	N1	C7	C4	-110.0(11)
S1	N1	C7	C4	6.2(11)
C8	N1	C7	C16	111.7(13)
S1	N1	C7	C16	-132.1(10)
C8	C7	C4	C3	113.2(16)
N1	C7	C4	C3	177.6(13)
C16	C7	C4	C3	-48(2)
C8	C7	C4	C5	-66.1(15)
N1	C7	C4	C5	-1.7(14)
C16	C7	C4	C5	132.4(14)
C3	C4	C5	C6	-1(2)
C7	C4	C5	C6	178.7(13)
C3	C4	C5	S1	177.0(11)
C7	C4	C5	S1	-3.6(14)
O1	S1	C5	C6	74.4(14)
O2	S1	C5	C6	-60.3(15)
N1	S1	C5	C6	-175.7(12)
O1	S1	C5	C4	-103.2(10)
O2	S1	C5	C4	122.1(10)
N1	S1	C5	C4	6.7(10)
S1	N1	C8	C7	-93.9(9)
C7	N1	C8	C9	-111.9(12)
S1	N1	C8	C9	154.2(10)
C7	N1	C8	I1	108.3(10)
S1	N1	C8	I1	14.5(13)
C4	C7	C8	N1	98.2(12)

A	B	C	D	Angle/°
N1	C7	C8	I1	-116.0(10)
C4	C7	C8	I1	-17.8(16)
C16	C7	C8	I1	144.0(11)
C4	C5	C6	C1	-2(2)
S1	C5	C6	C1	-178.9(11)
C17	O4	C16	O3	-3(3)
C17	O4	C16	C7	178.5(18)
C8	C7	C16	O3	43(2)
N1	C7	C16	O3	-23(2)
C4	C7	C16	O3	-156.0(18)
C8	C7	C16	O4	-138.8(15)
N1	C7	C16	O4	155.4(14)
C4	C7	C16	O4	22(2)
C15	C14	C13	C12	4(3)
C14	C13	C12	C11	-3(4)
C13	C14	C15	C10	-2(3)
C11	C10	C15	C14	0(2)
C9	C10	C15	C14	179.3(15)
C13	C12	C11	C10	1(4)
C15	C10	C11	C12	0(3)
C9	C10	C11	C12	-179.0(19)
C5	C4	C3	C2	2(2)
C7	C4	C3	C2	-177.4(14)
C11	C10	C9	O5	168(2)
C15	C10	C9	O5	-12(3)
C11	C10	C9	C8	-10(2)
C15	C10	C9	C8	170.4(13)
N1	C8	C9	O5	127.0(18)
C7	C8	C9	O5	56(2)
I1	C8	C9	O5	-86.7(19)
N1	C8	C9	C10	-54.8(18)
C7	C8	C9	C10	-125.5(14)
I1	C8	C9	C10	91.5(15)

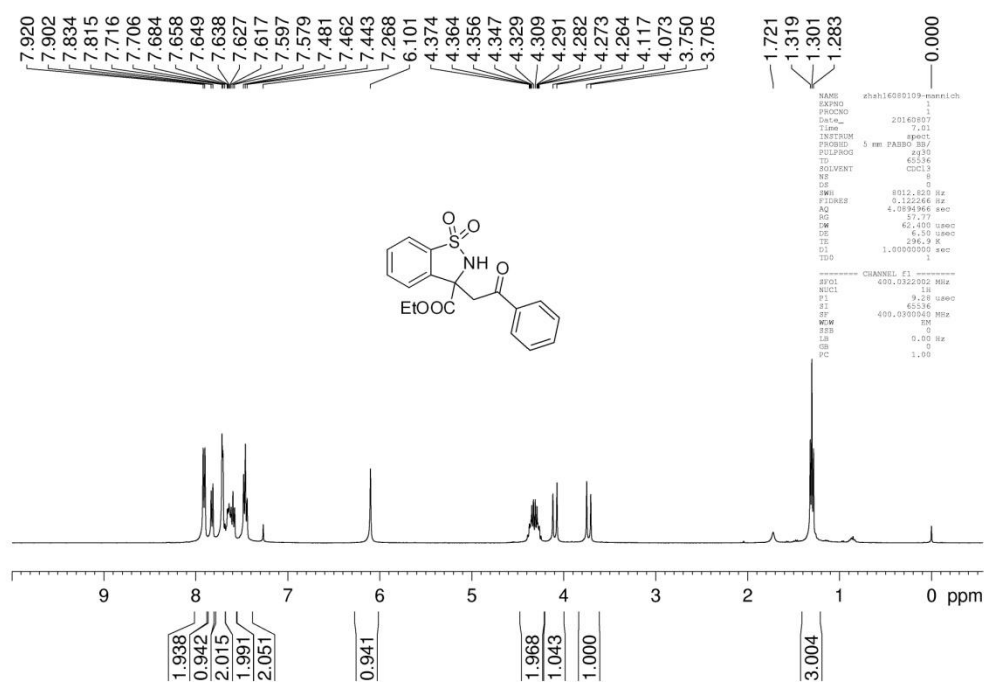
C16C7C8N1 -99.9(13)	C5 C6 C1 C2 3(2)
N1 C7C8C9 105.5(14)	C6 C1 C2 C3 -2(3)
C4 C7C8C9 -156.3(12)	C4 C3 C2 C1 -1(3)
C16C7C8C9 6(2)	C16O4 C17C1875(3)

Table S8 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 5aa.

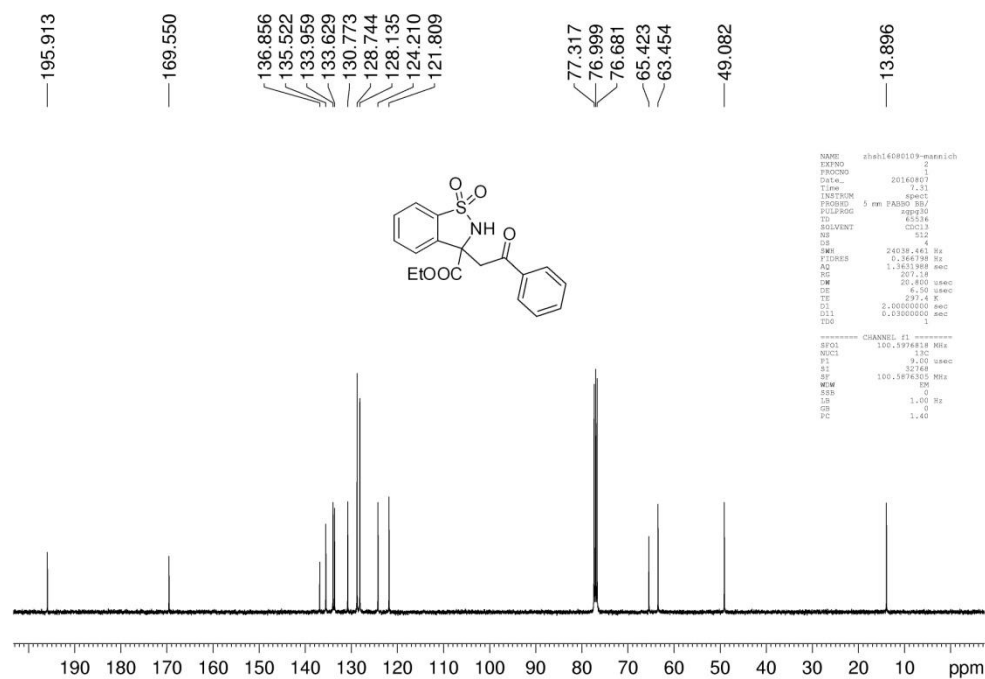
Atom	x	y	z	U(eq)
H14	121	1160	2710	50
H6	975	696	8950	42
H13	359	2528	3198	64
H12	471	2743	4576	65
H15	-350	36	3574	41
H11	31	1646	5469	53
H3	-26	-1835	7533	41
H1	-145	-531	9622	55
H2	-553	-1760	8918	51
H17A	3005	-2594	5439	92
H17B	2979	-3083	6269	92
H18A	6071	-2385	5590	144
H18B	6022	-2826	6442	144
H18C	5683	-1846	6371	144

Part II NMR Spectra

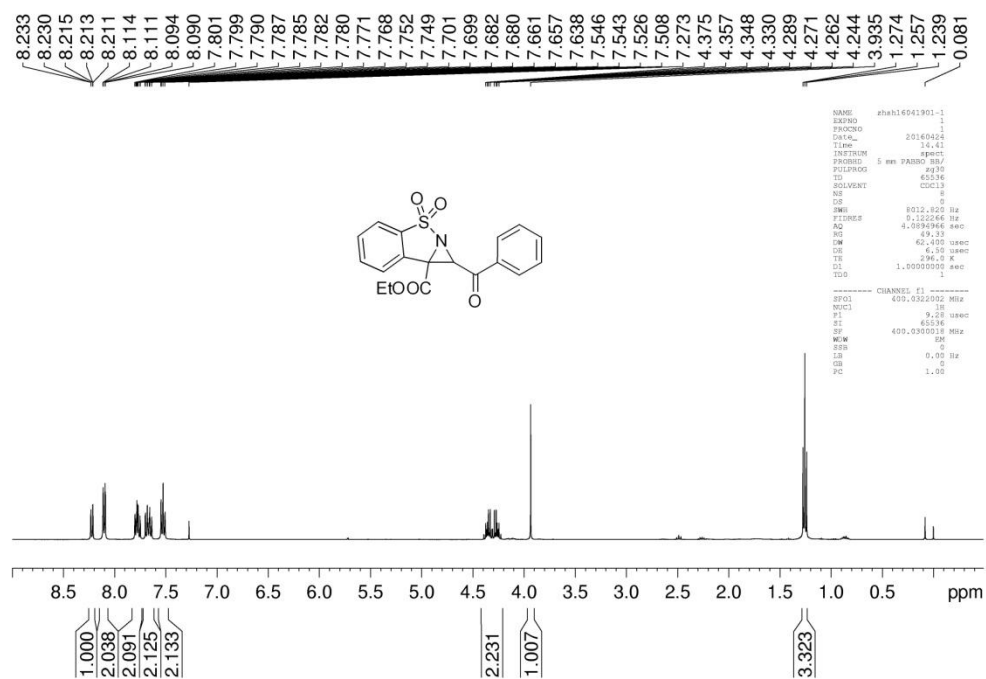
3aa ¹H NMR



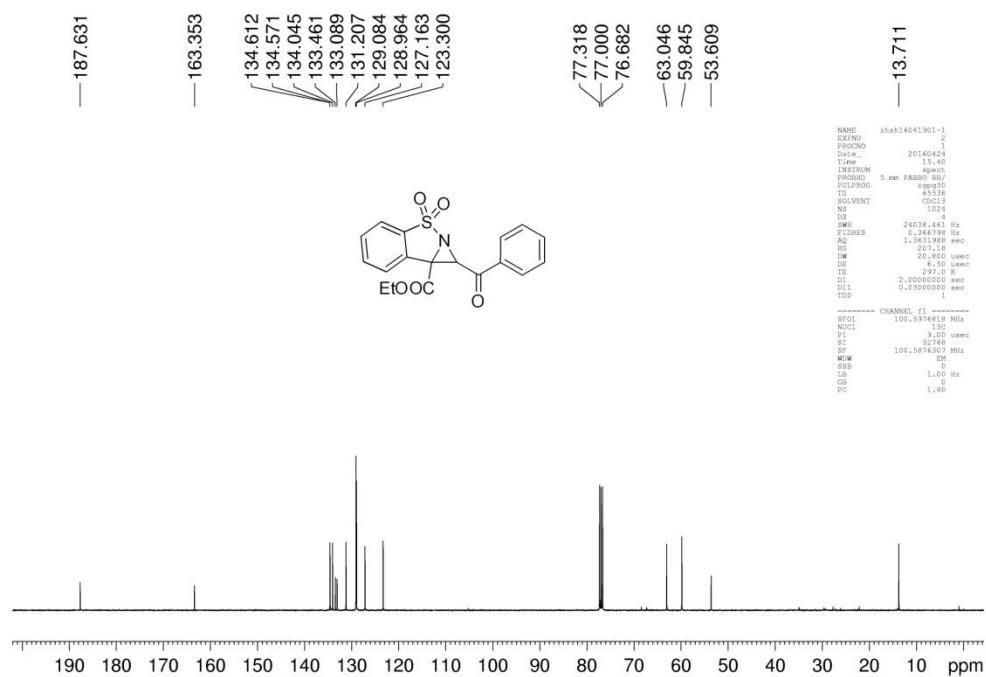
3aa ¹³C NMR



4aa ¹H NMR



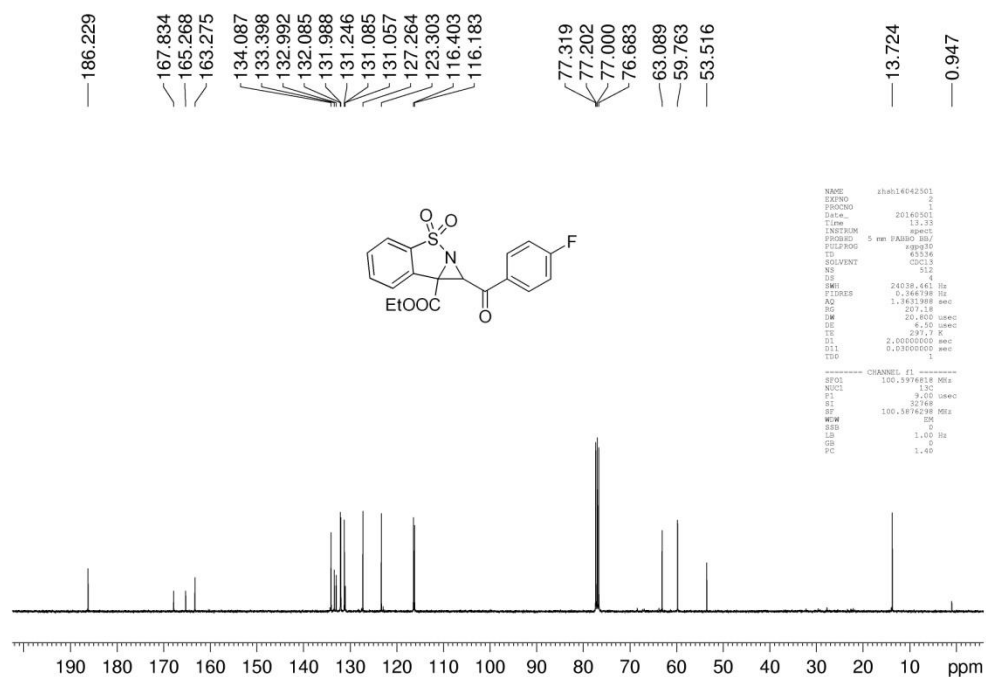
4aa ¹³C NMR



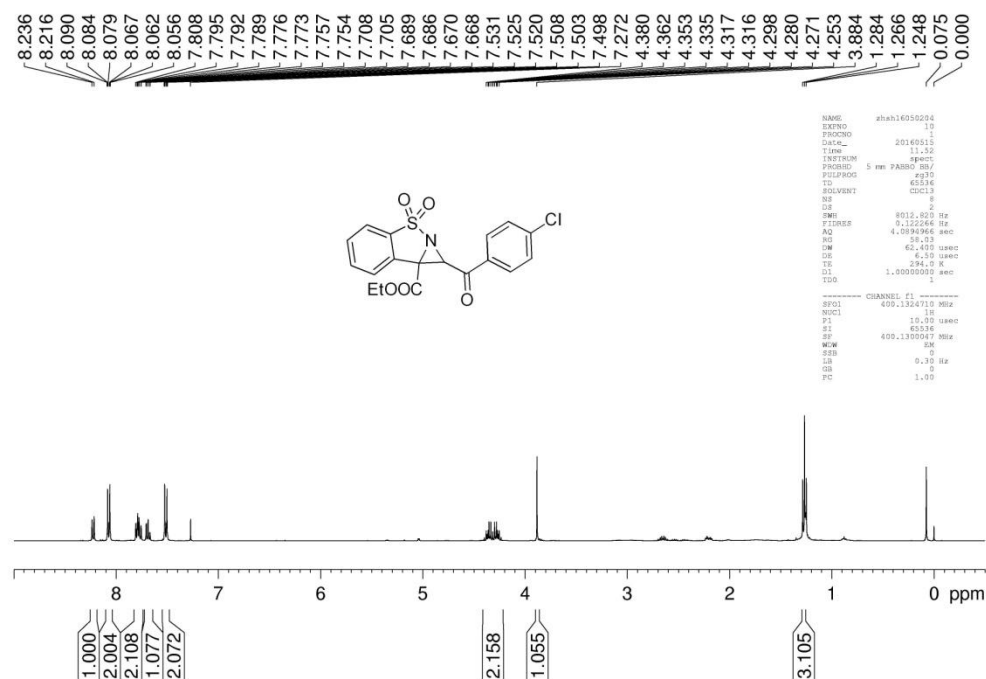
4ab ¹H NMR



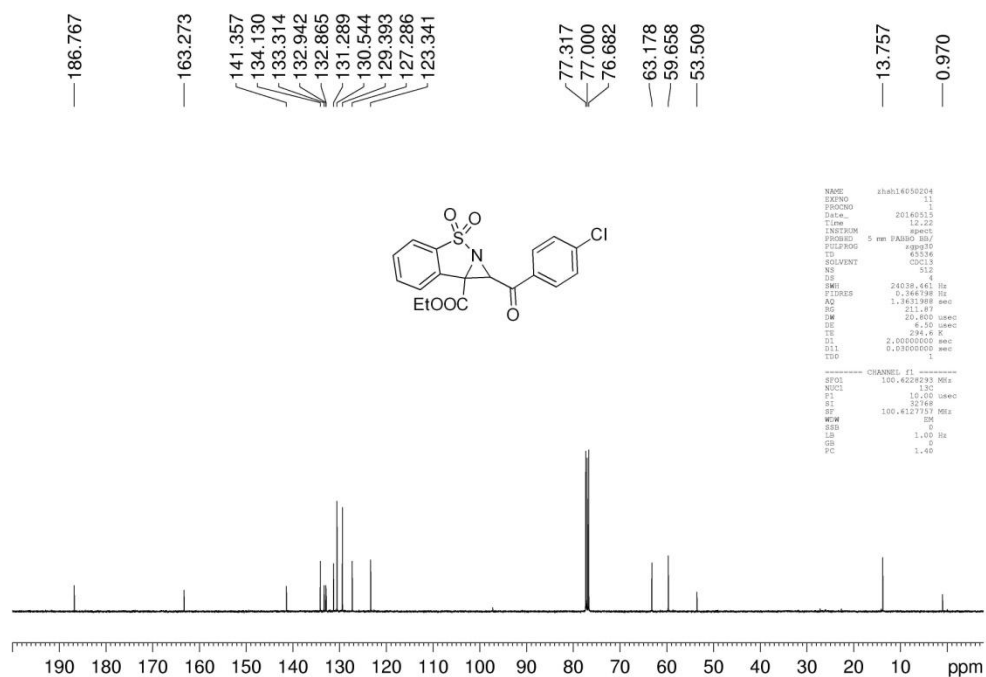
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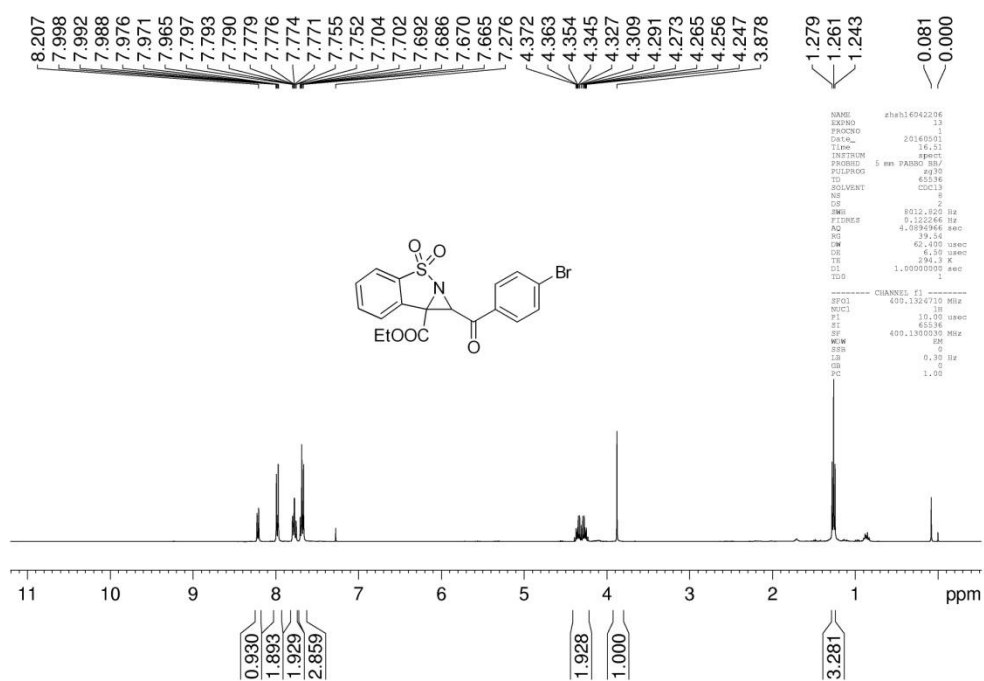
4ac ¹H NMR



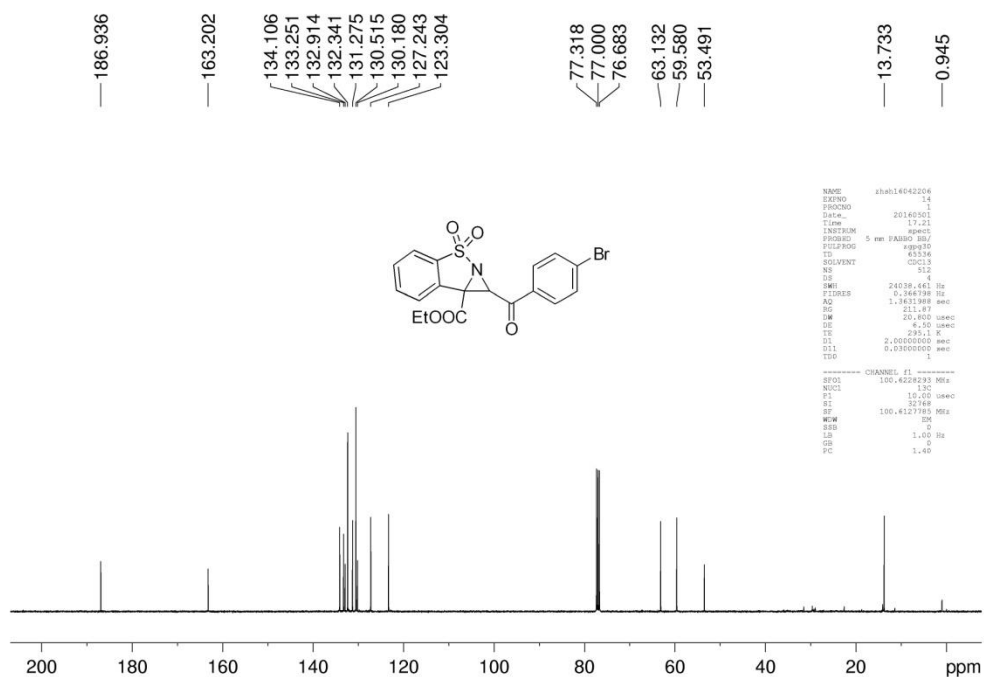
4ac ¹³C NMR



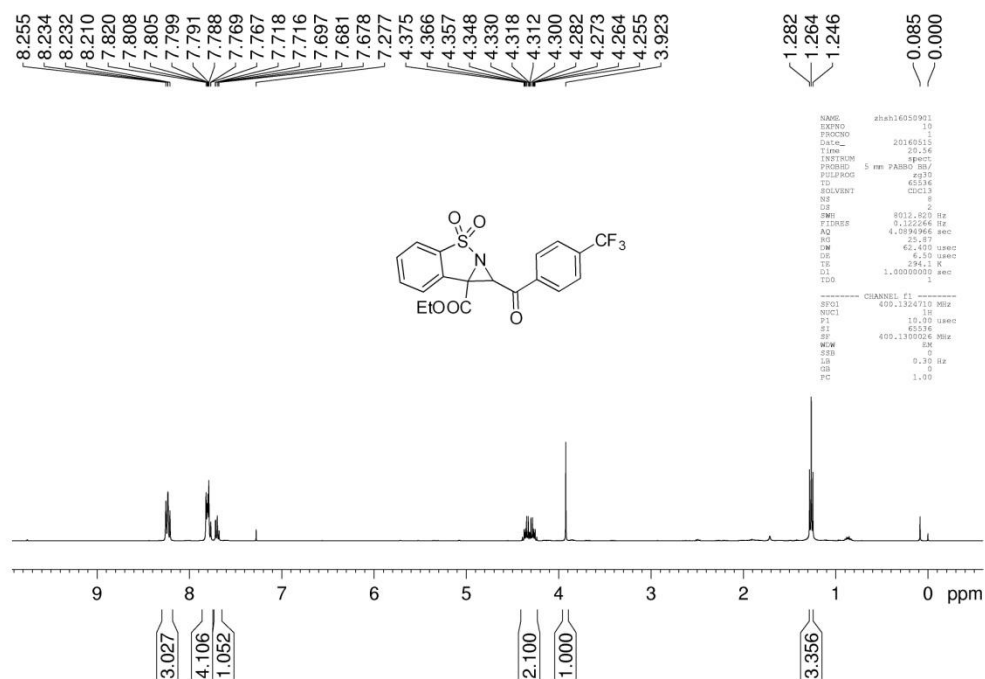
4ad ¹H NMR



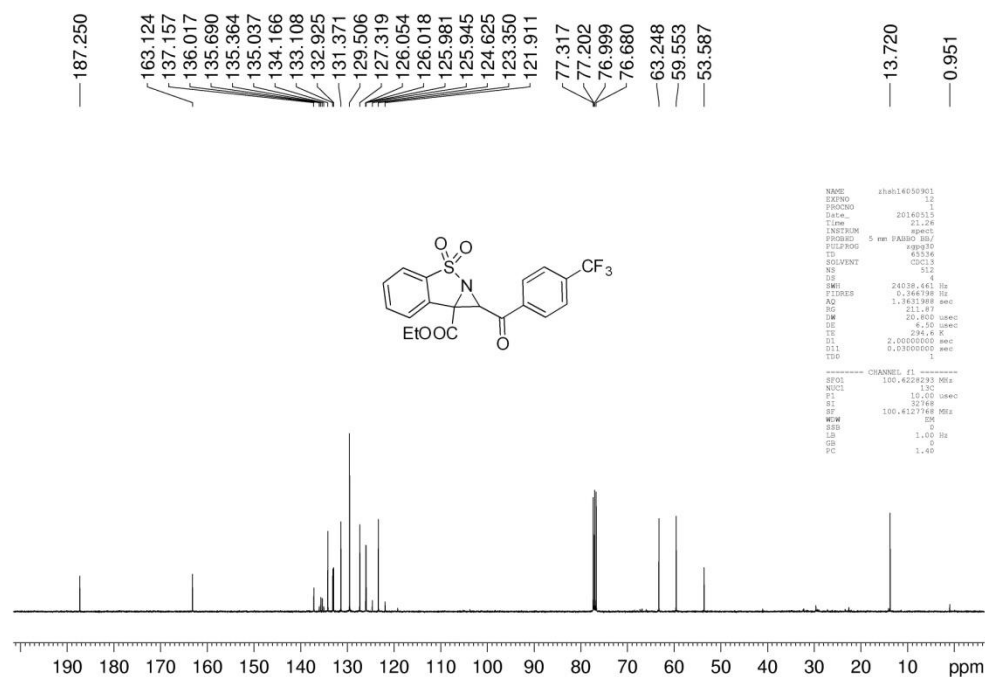
4ad ¹³C NMR



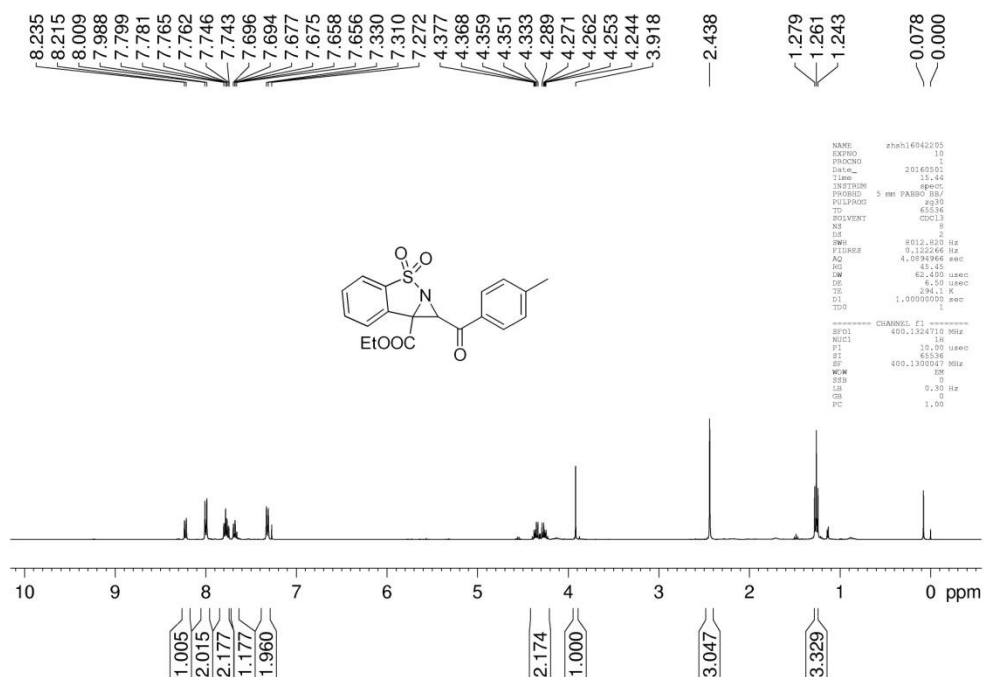
4ae ¹H NMR



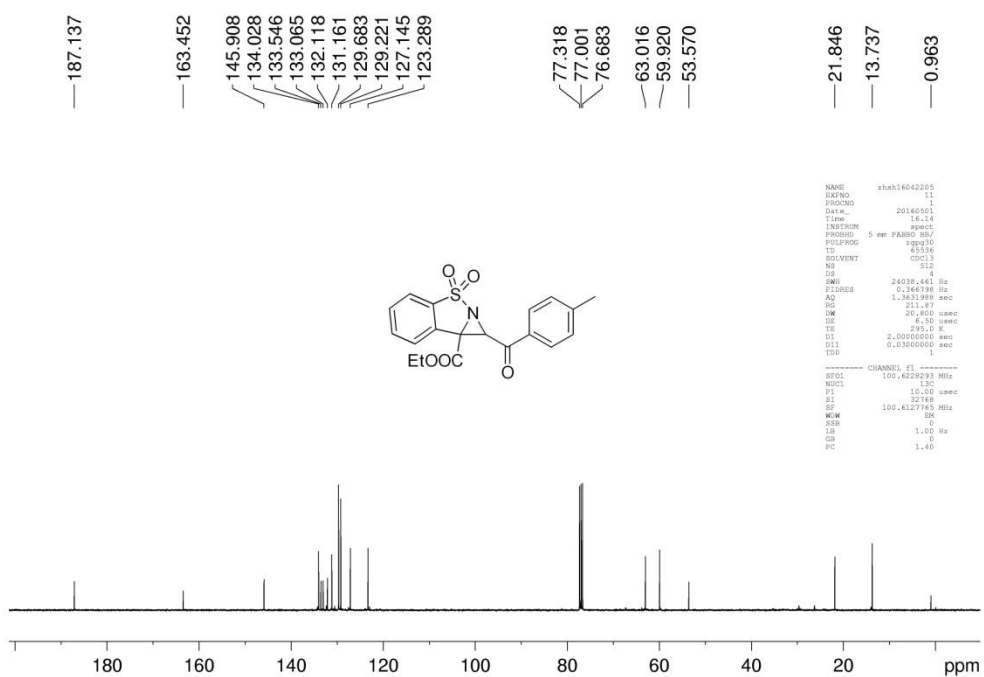
4ae ¹³C NMR



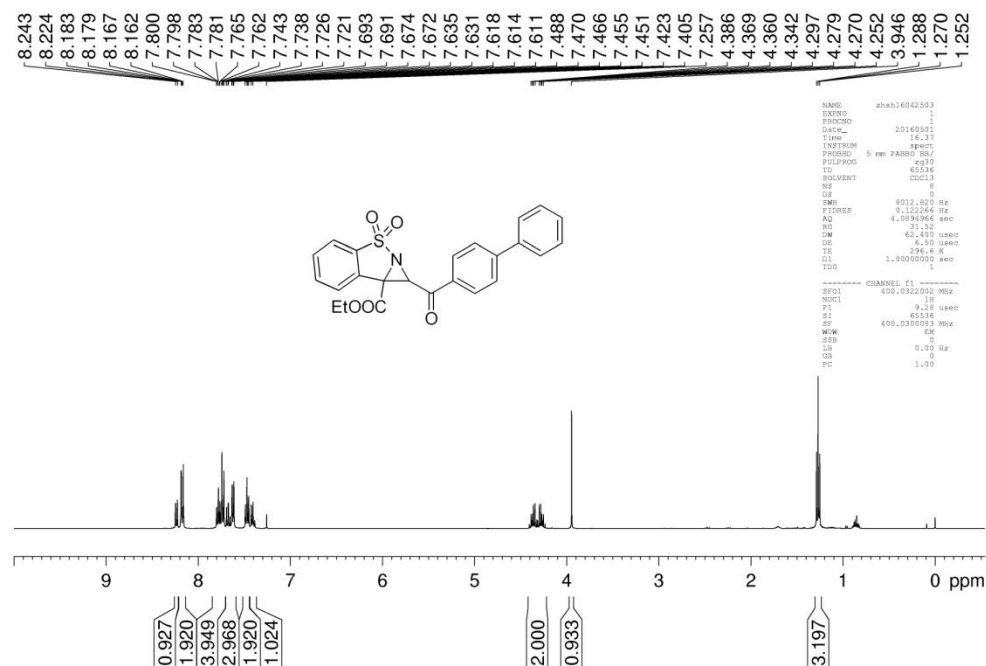
4af ¹H NMR



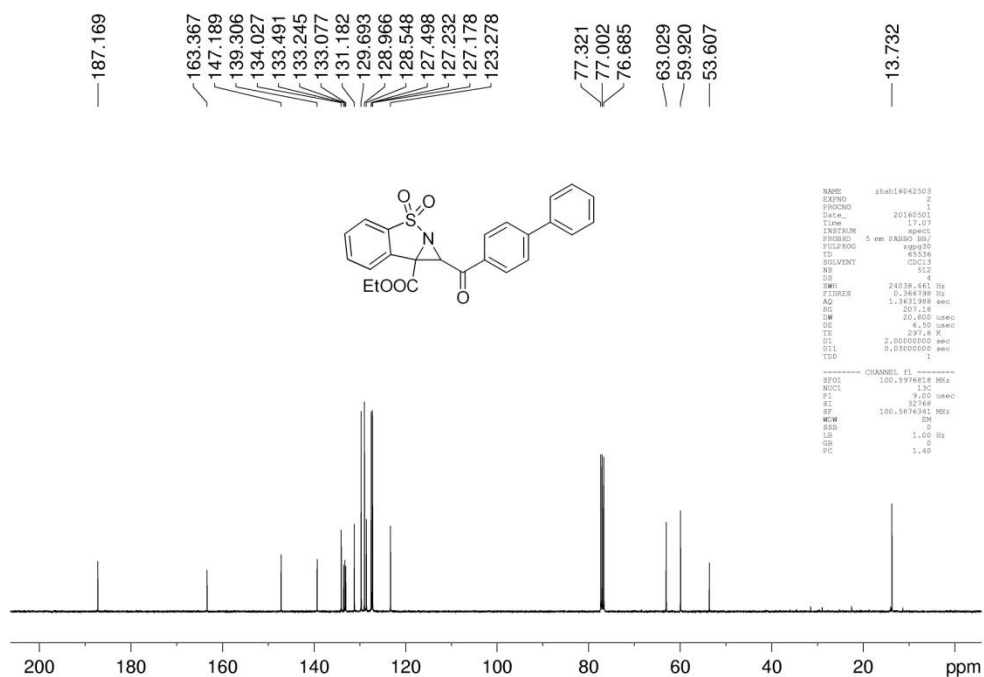
4af ¹³C NMR



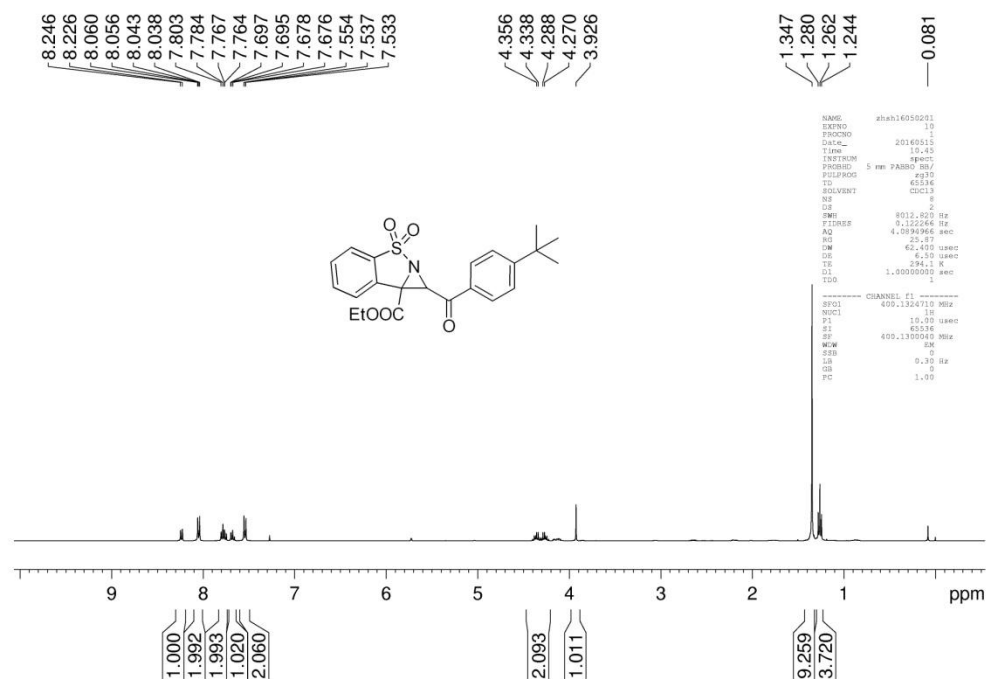
4ag ¹H NMR



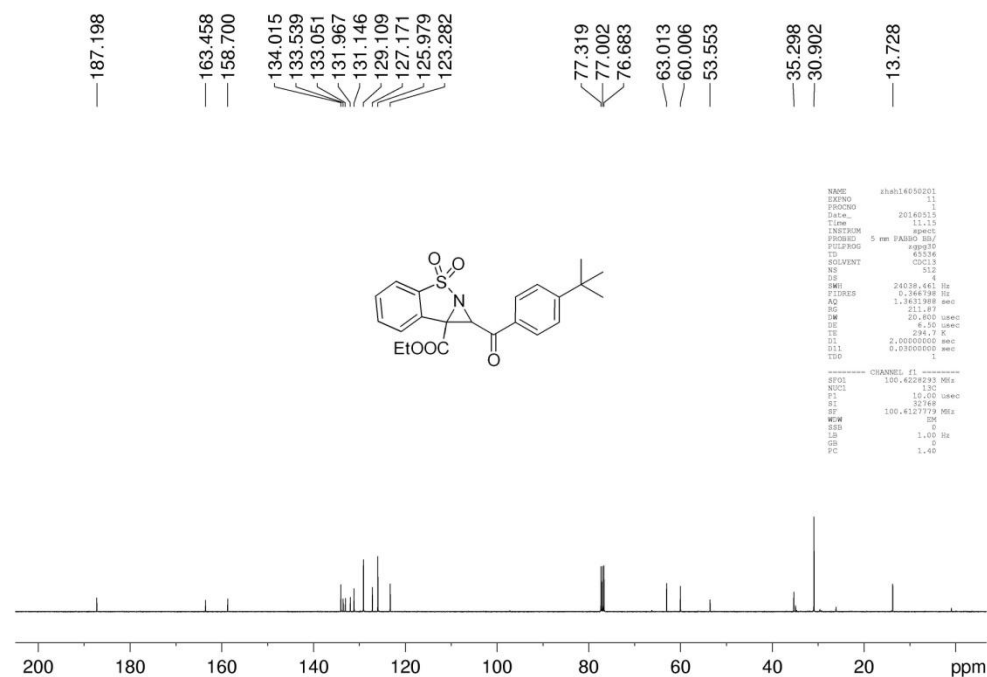
4ag ¹³C NMR



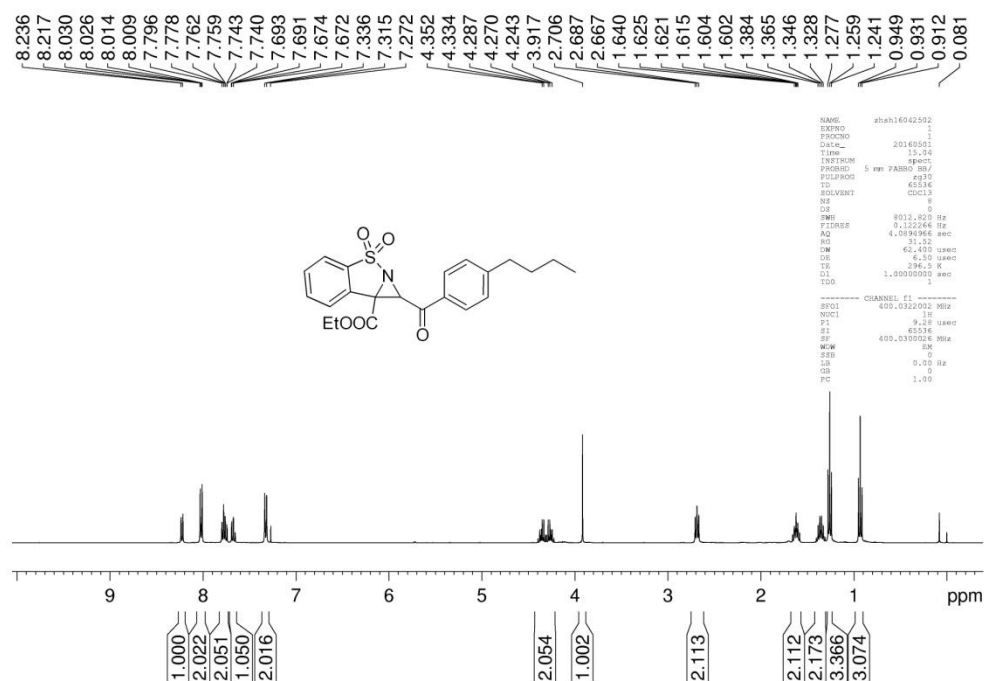
4ah ¹H NMR



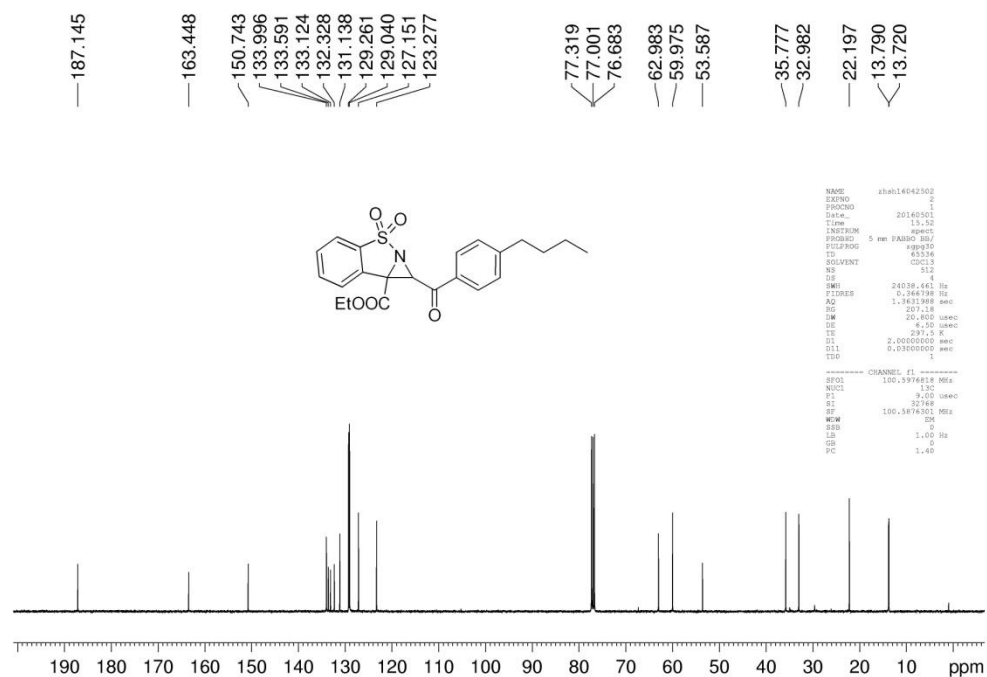
4ah ¹³C NMR



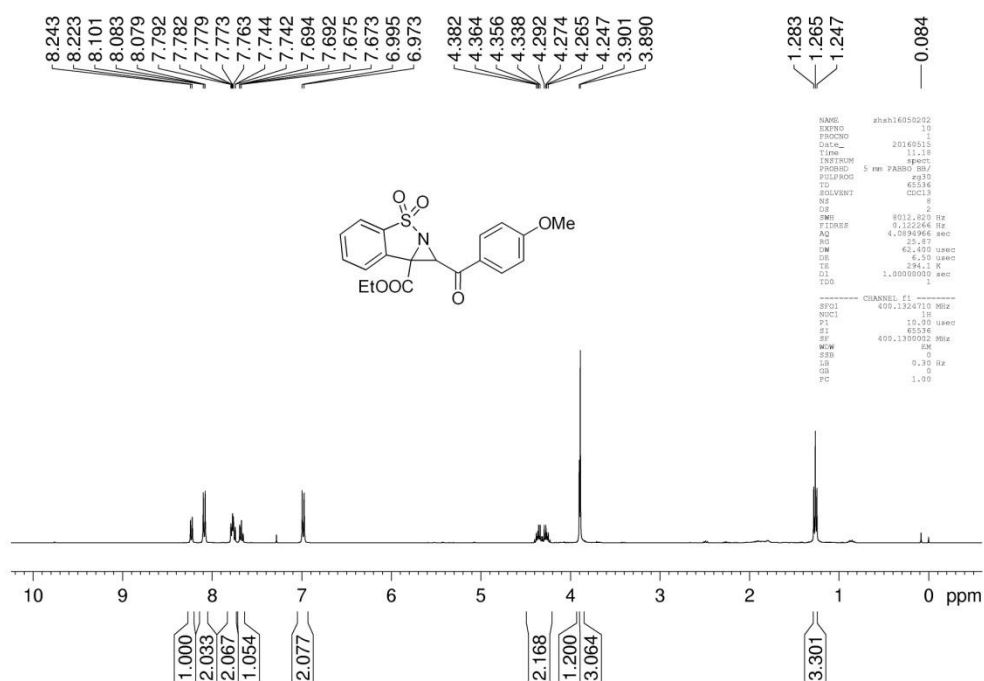
4ai ¹H NMR



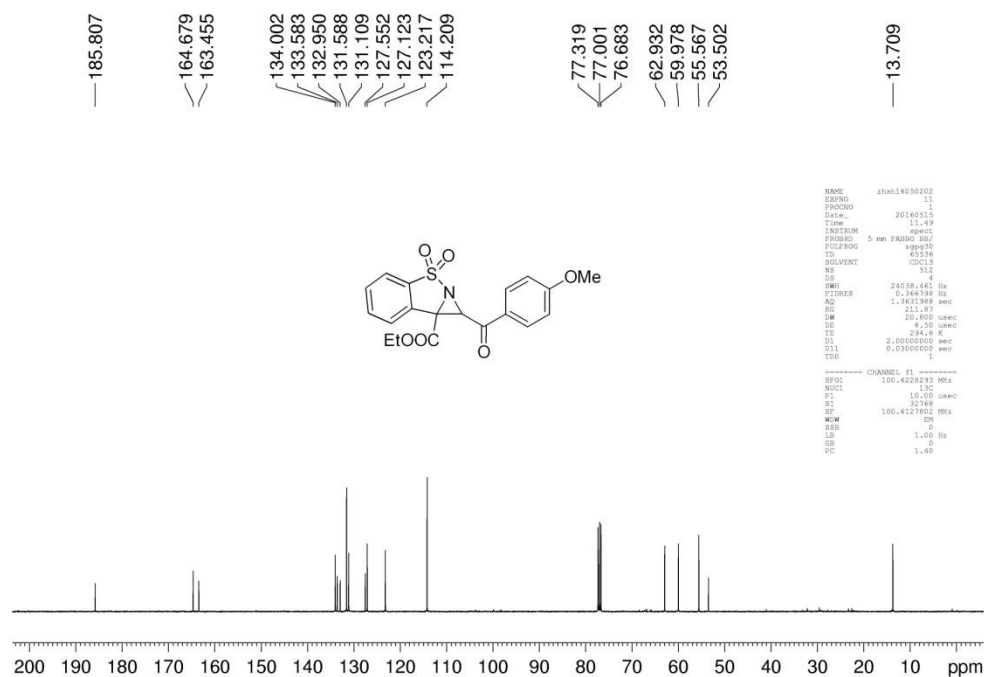
4ai ¹³C NMR



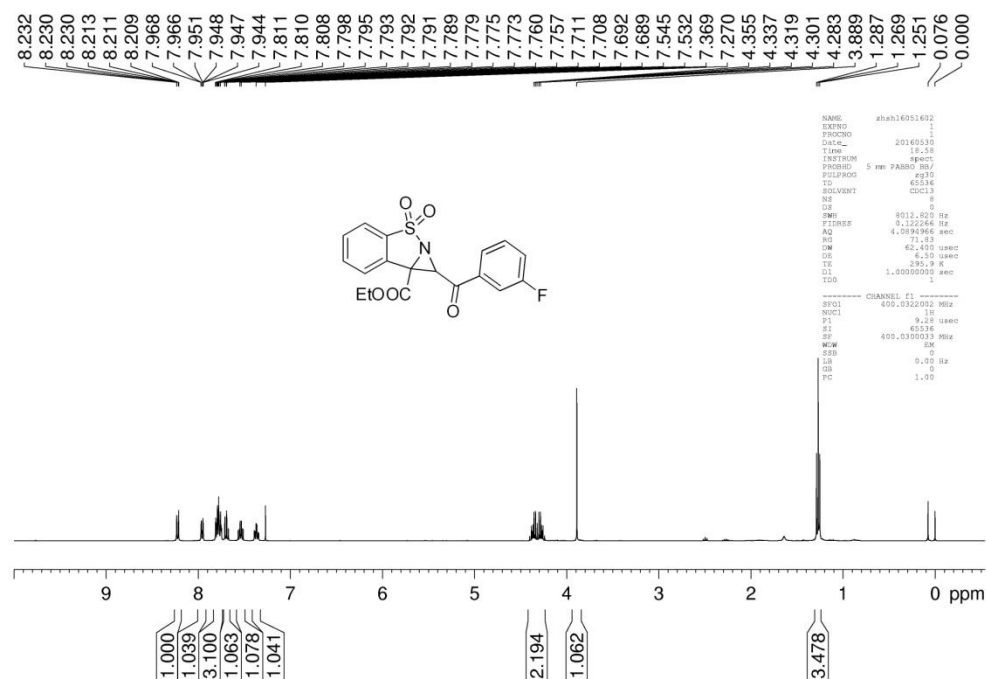
4aj ¹H NMR



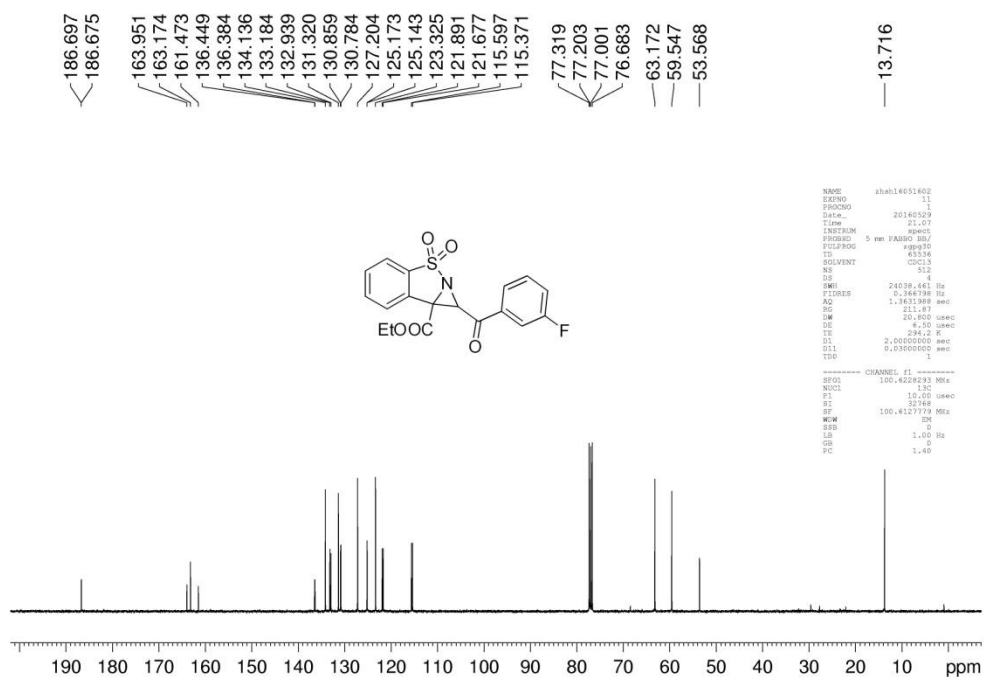
4aj ¹³C NMR



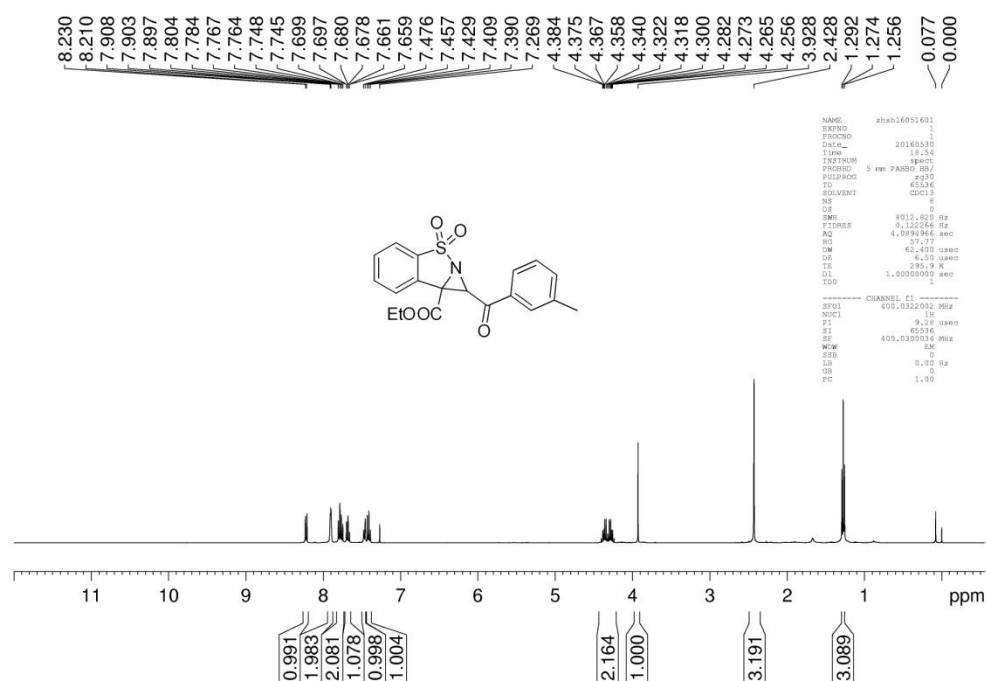
4ak ¹H NMR



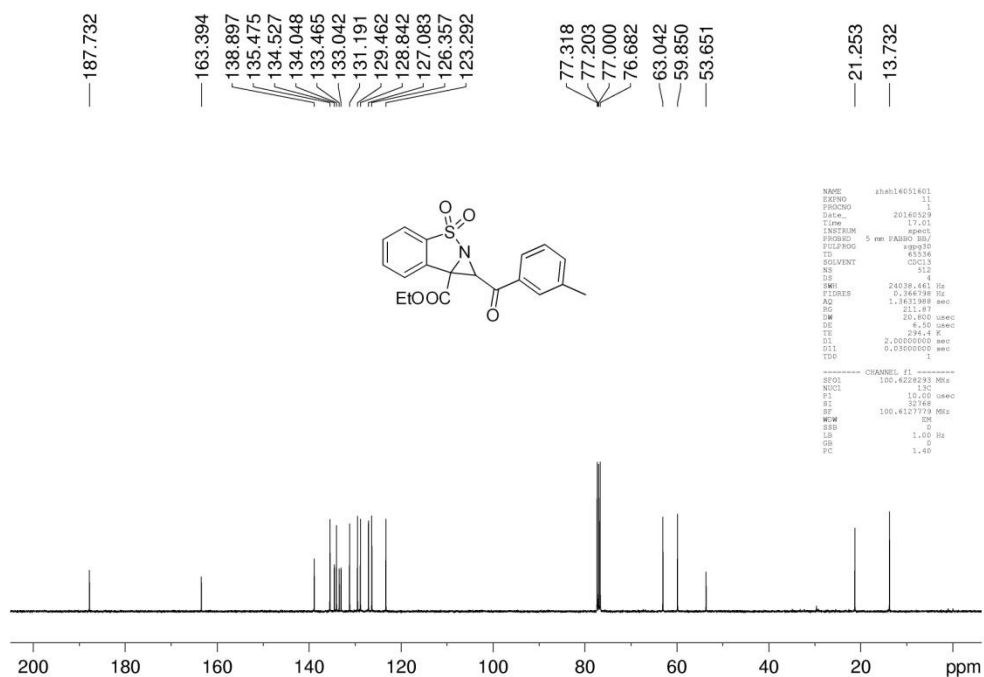
4ak ¹³C NMR



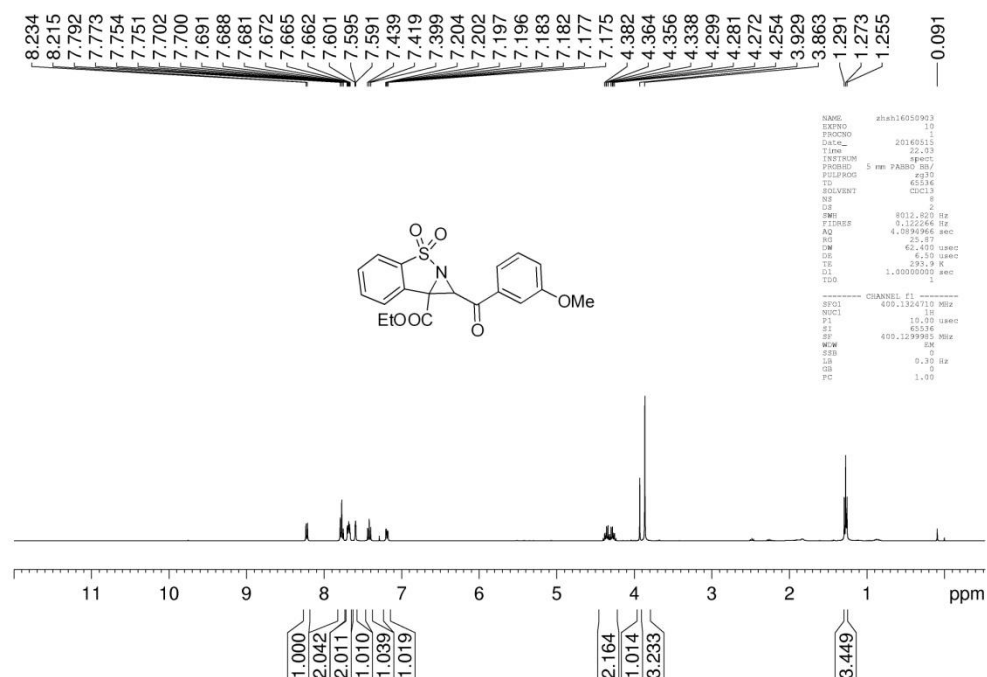
4al ¹H NMR



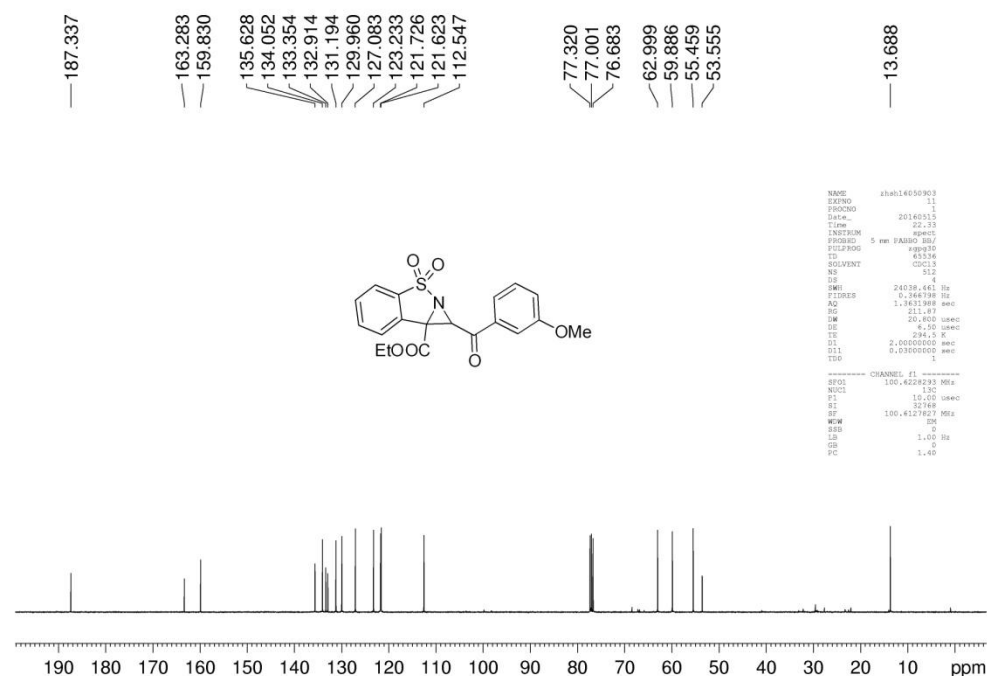
4al ¹³C NMR



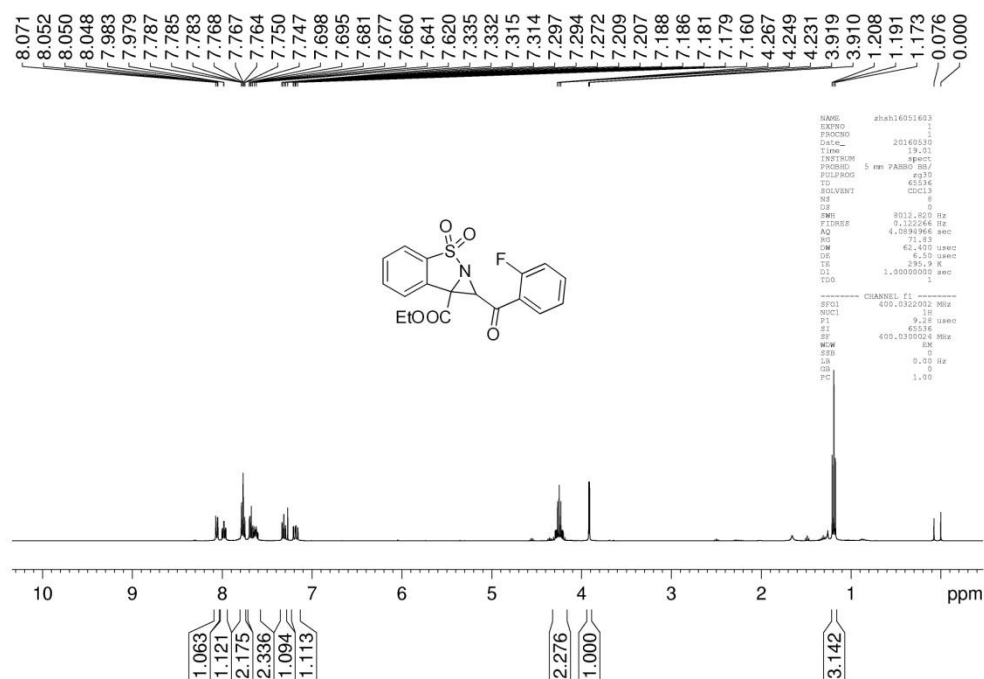
4am ¹H NMR



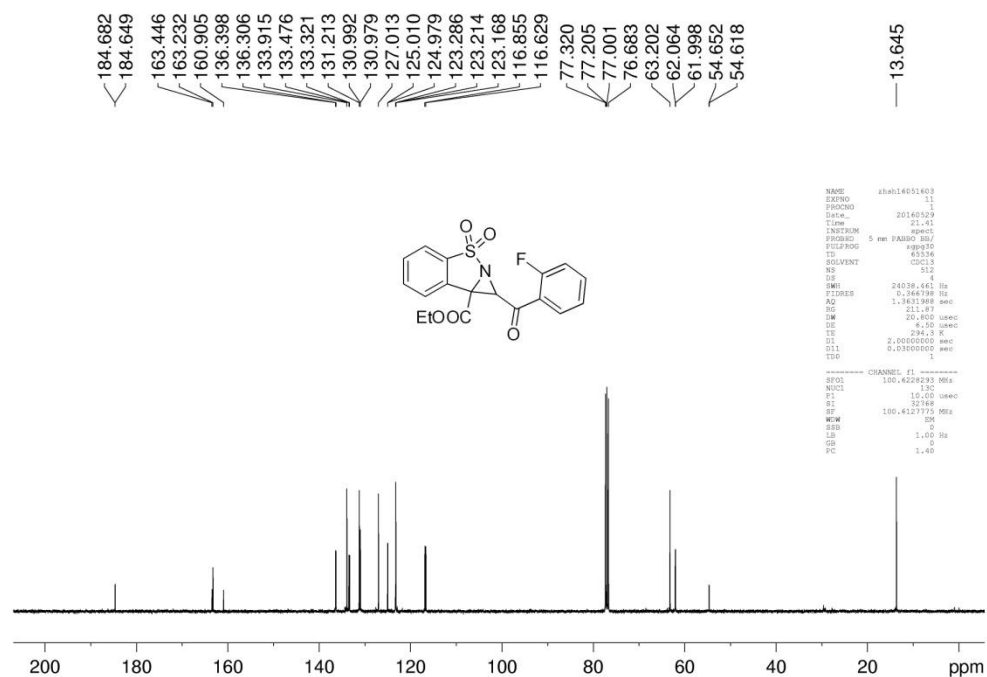
4am ¹³C NMR



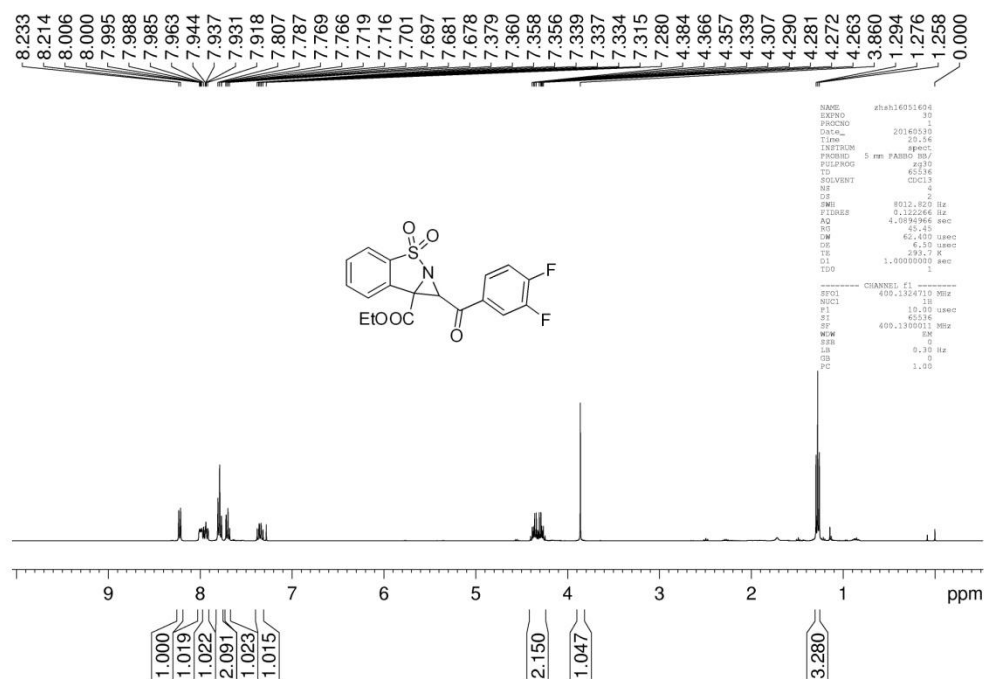
4an ¹H NMR



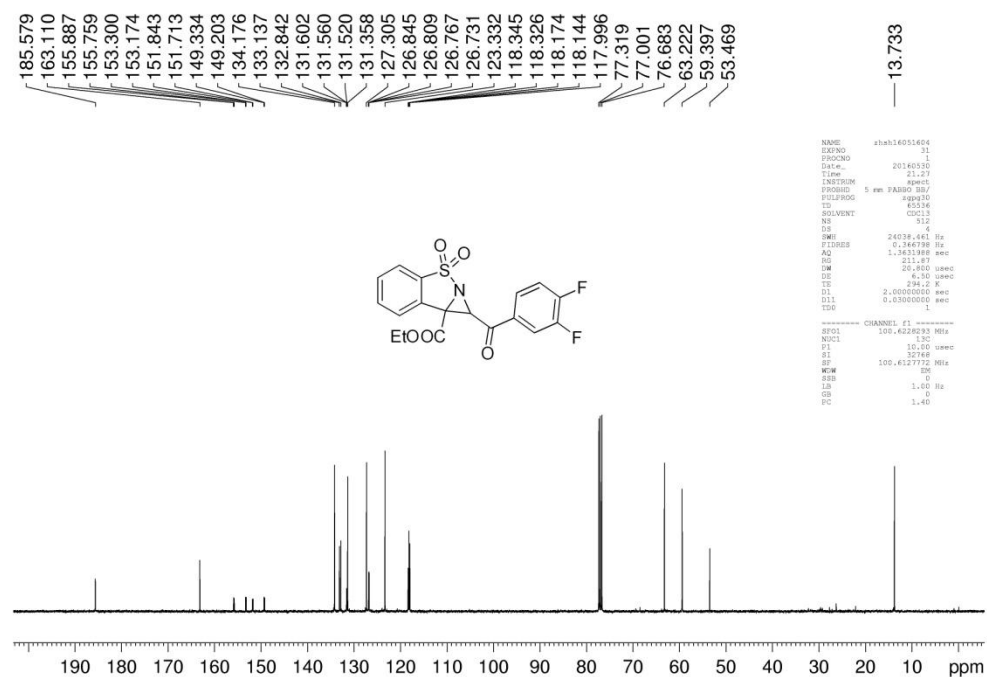
4an ¹³C NMR



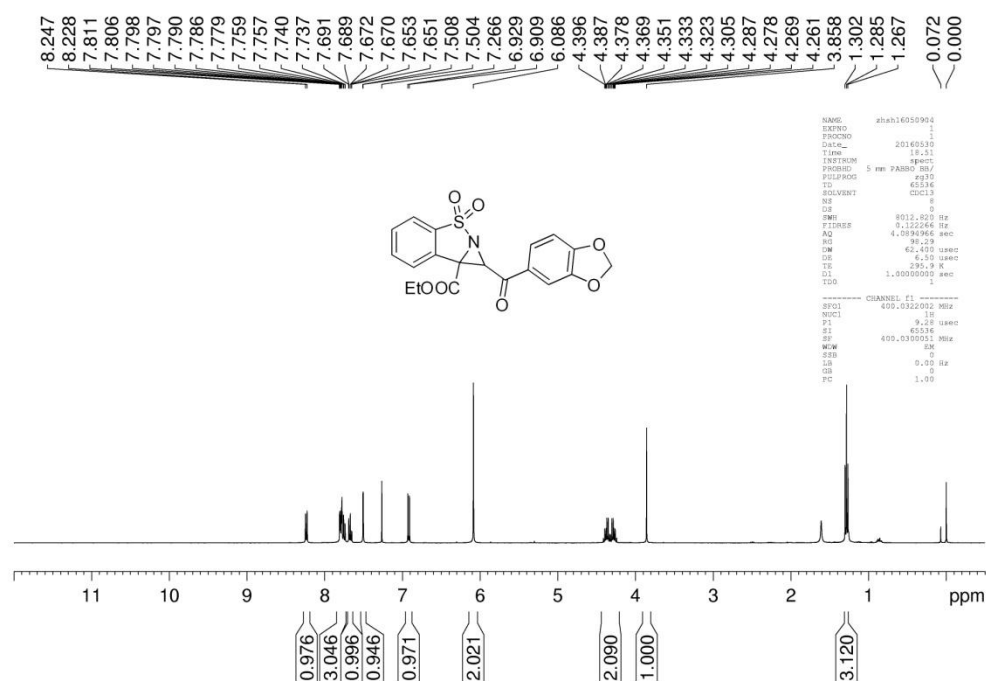
4ao ¹H NMR



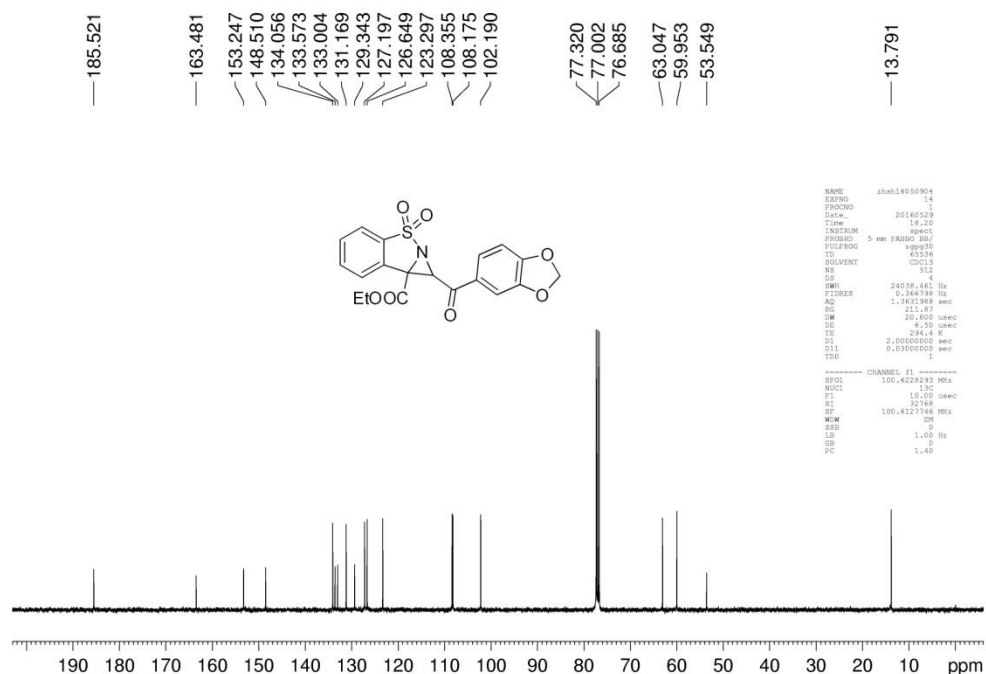
4ao ¹³C NMR



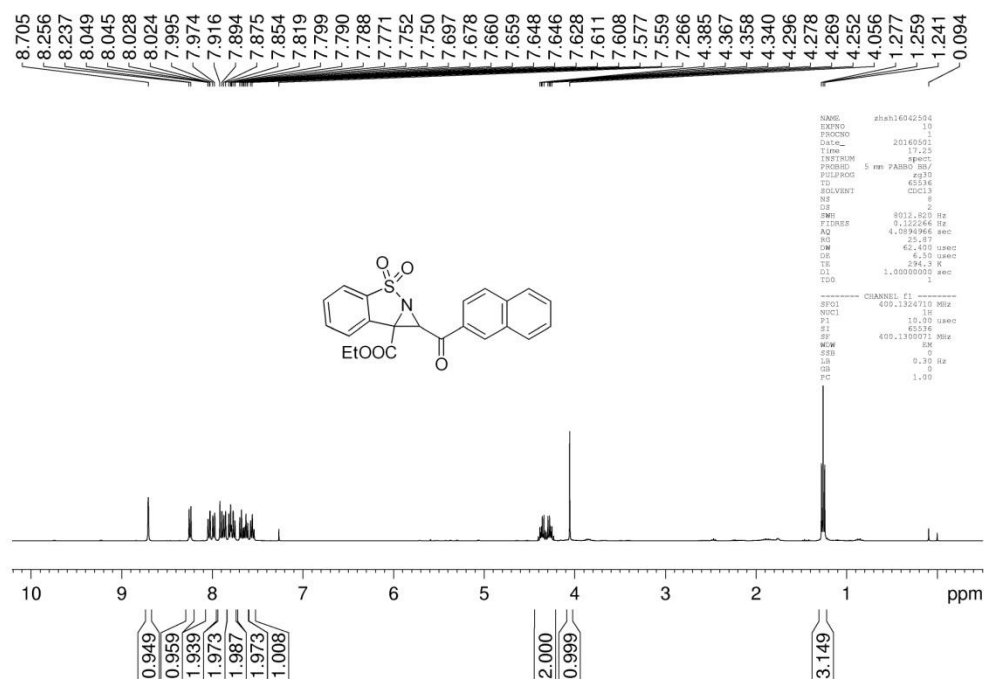
4ap ¹H NMR



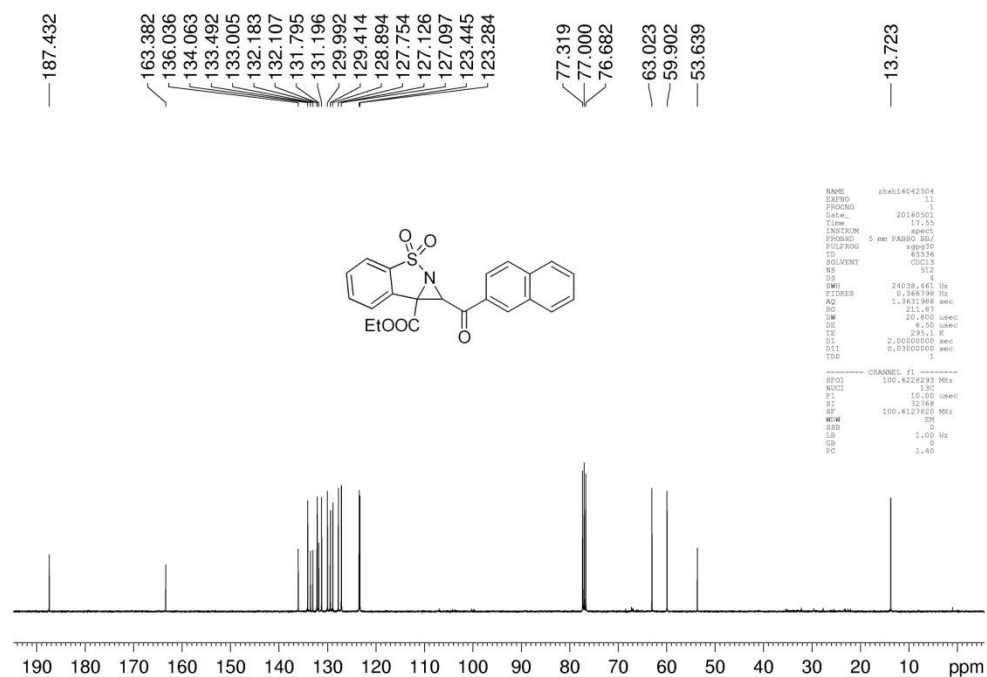
4ap ¹³C NMR



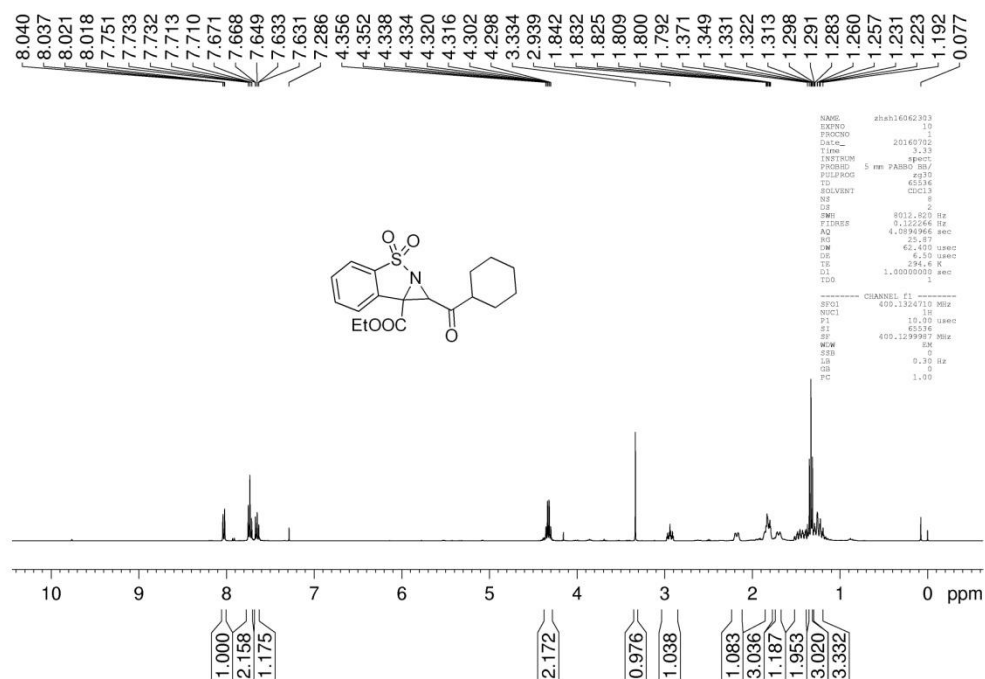
4aq ¹H NMR



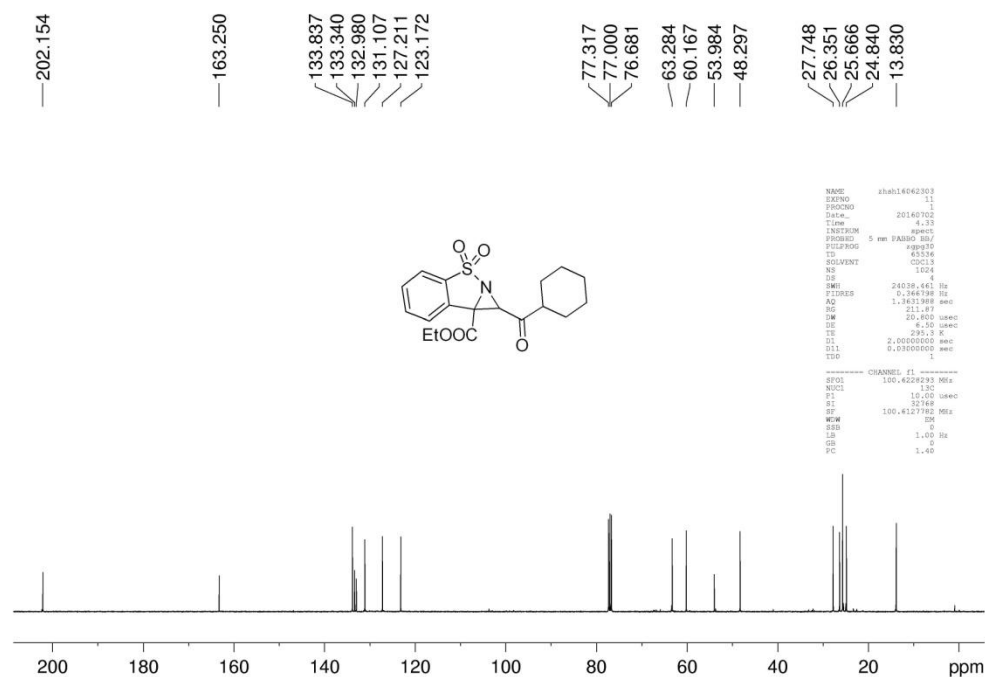
4aq ¹³C NMR



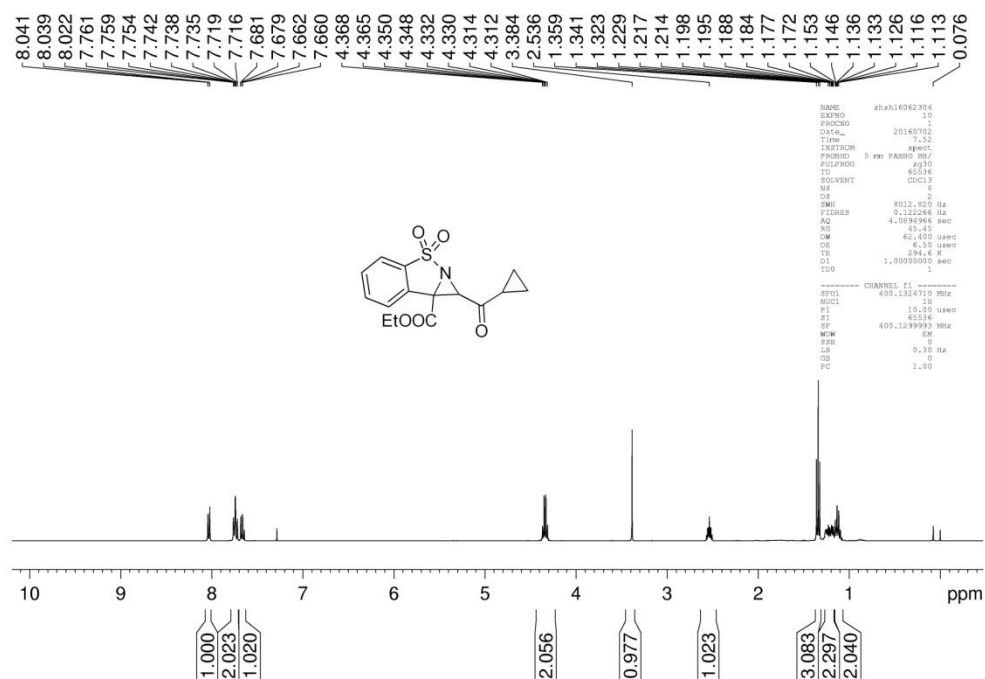
4ar ¹H NMR



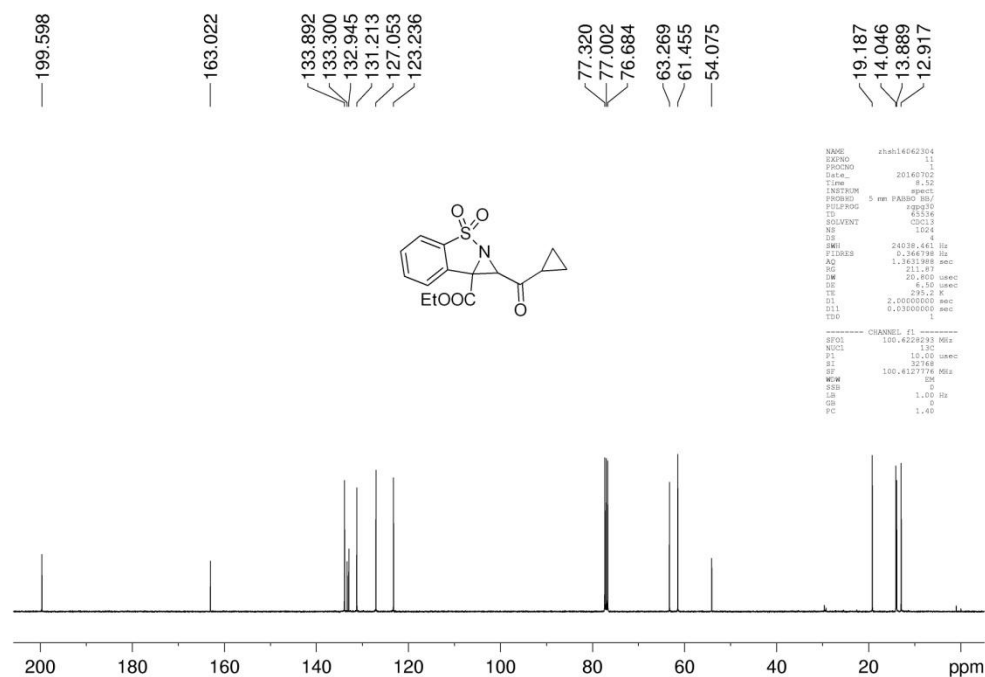
4ar ¹³C NMR



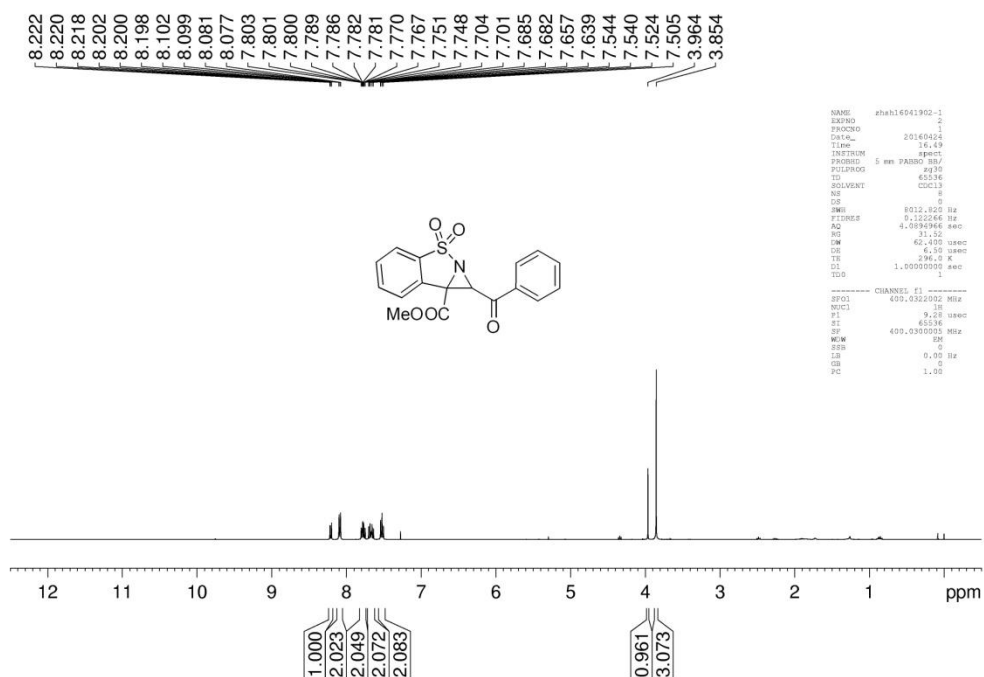
4as ¹H NMR



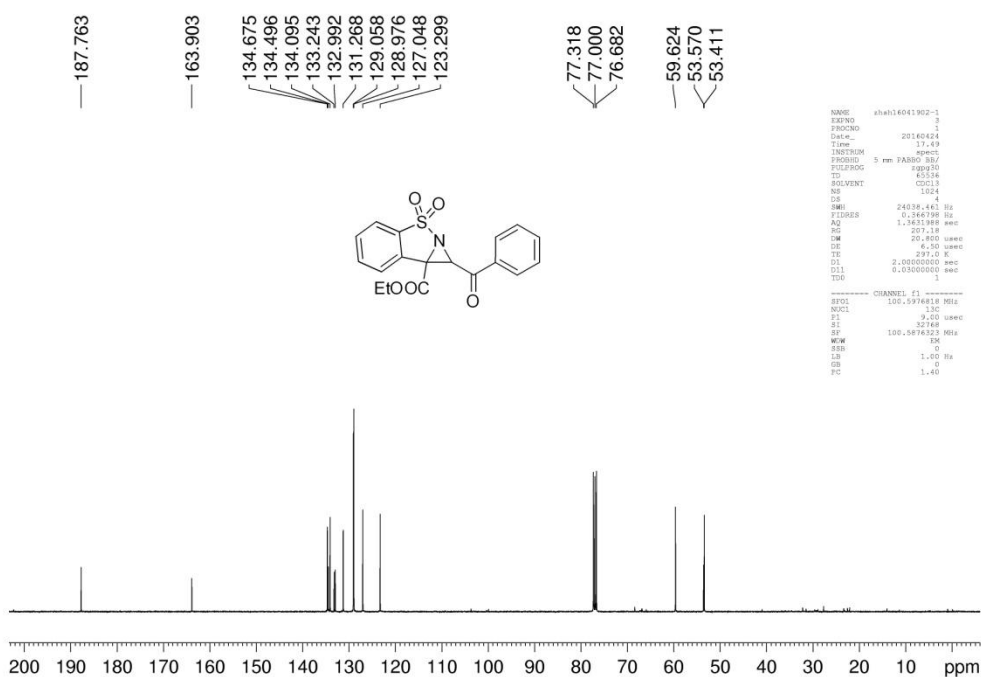
4as ¹³C NMR



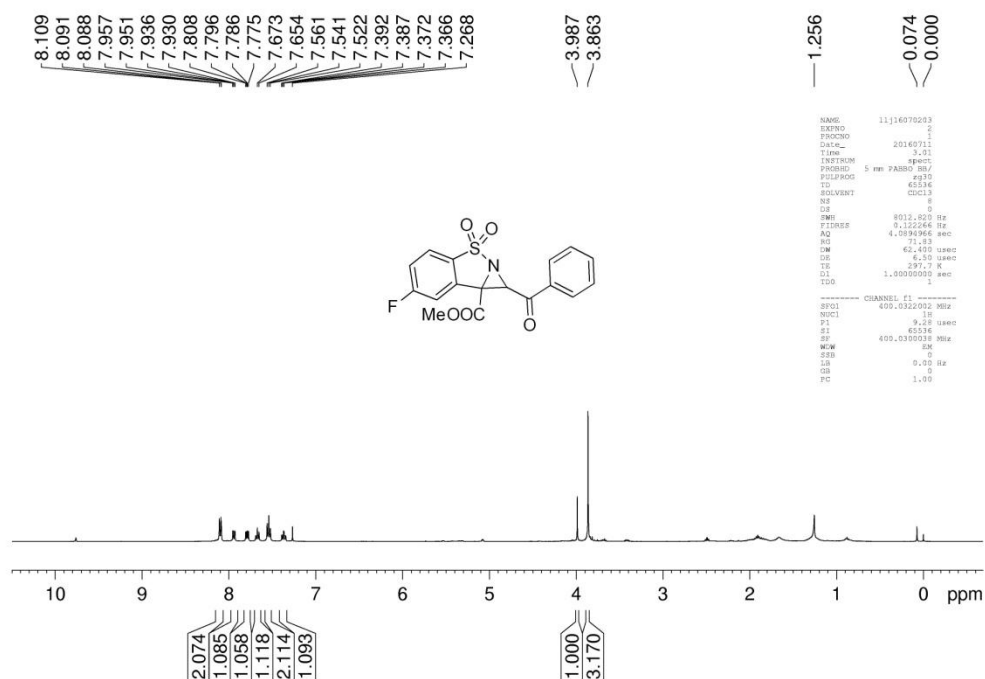
4ba ¹H NMR



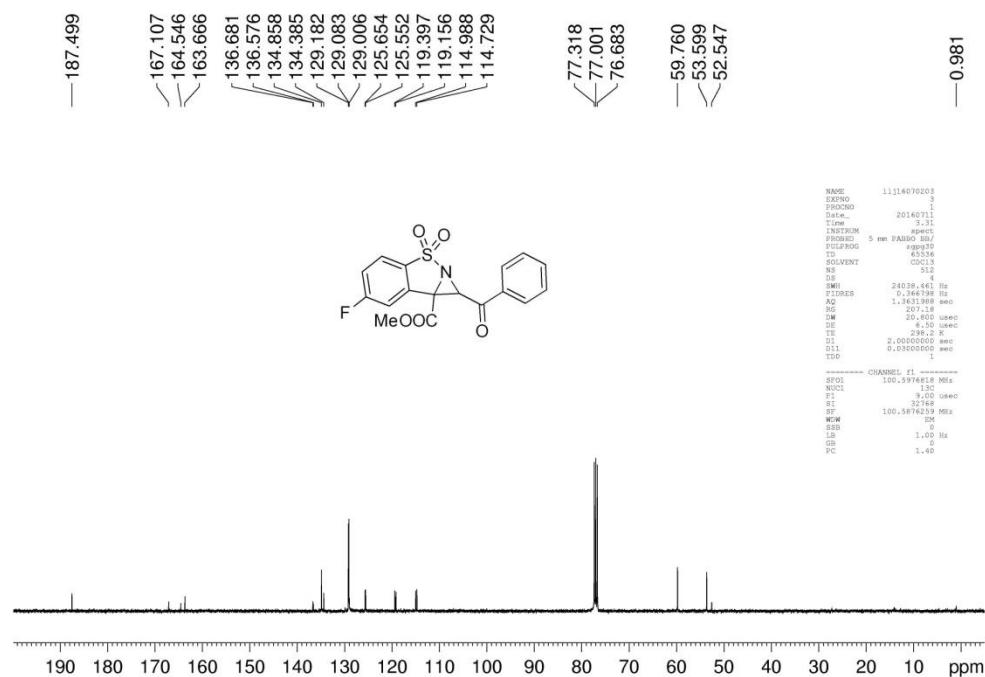
4ba ¹³C NMR



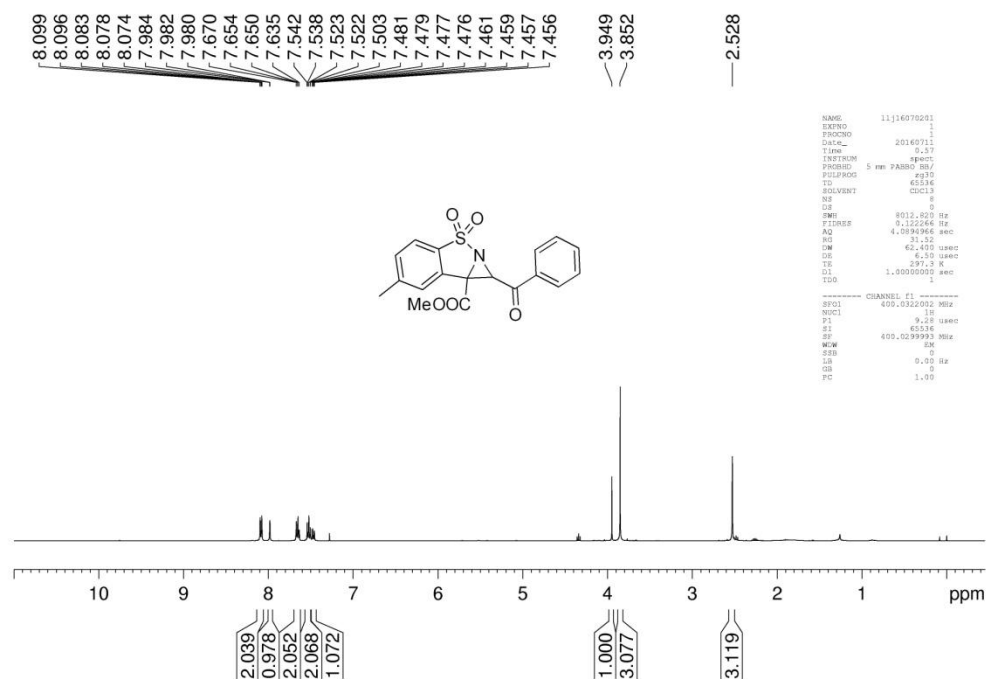
4ca ^1H NMR



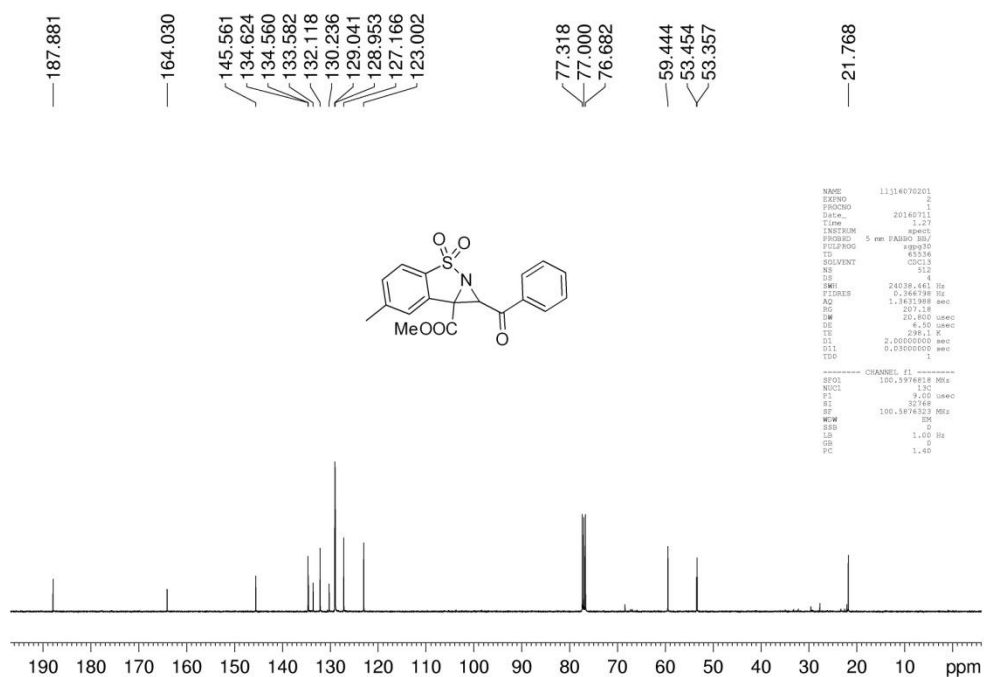
4ca ¹³C NMR



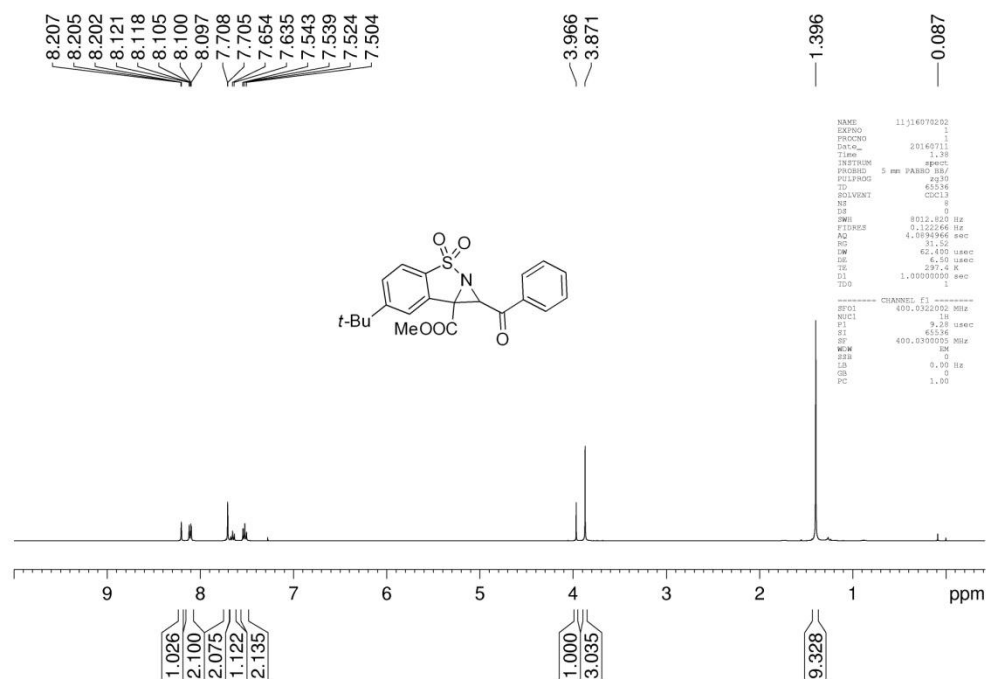
4da ¹H NMR



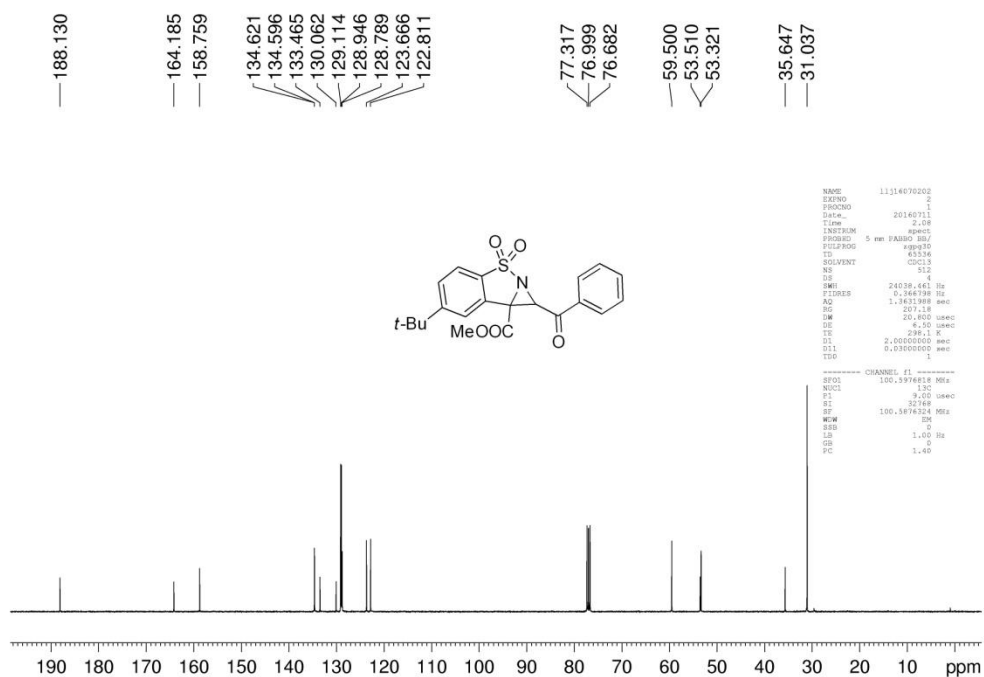
4da ¹³C NMR



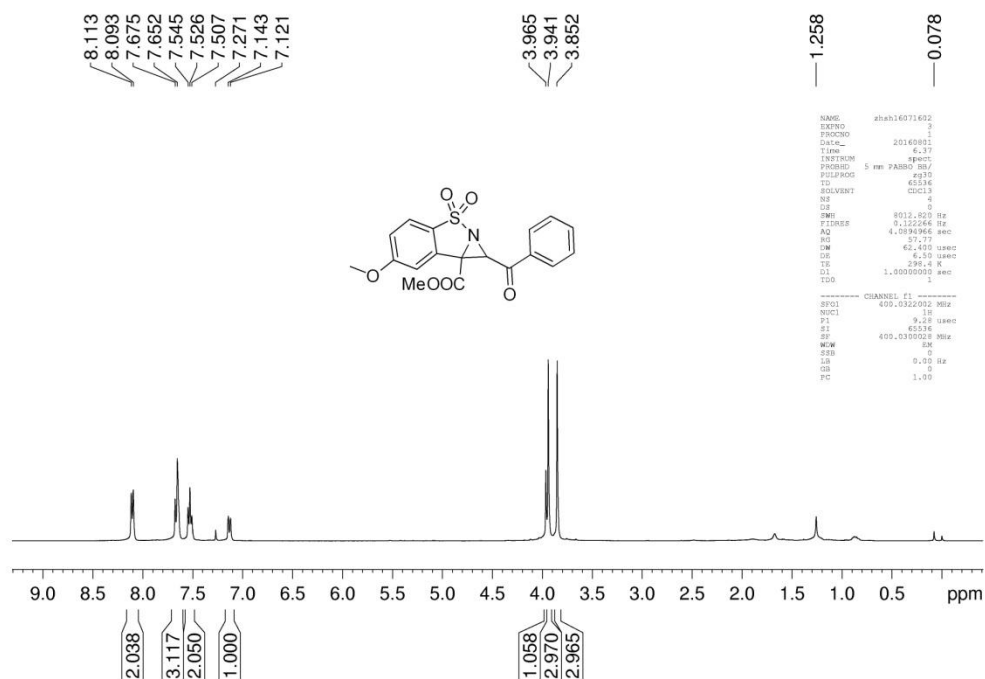
4ea ¹H NMR



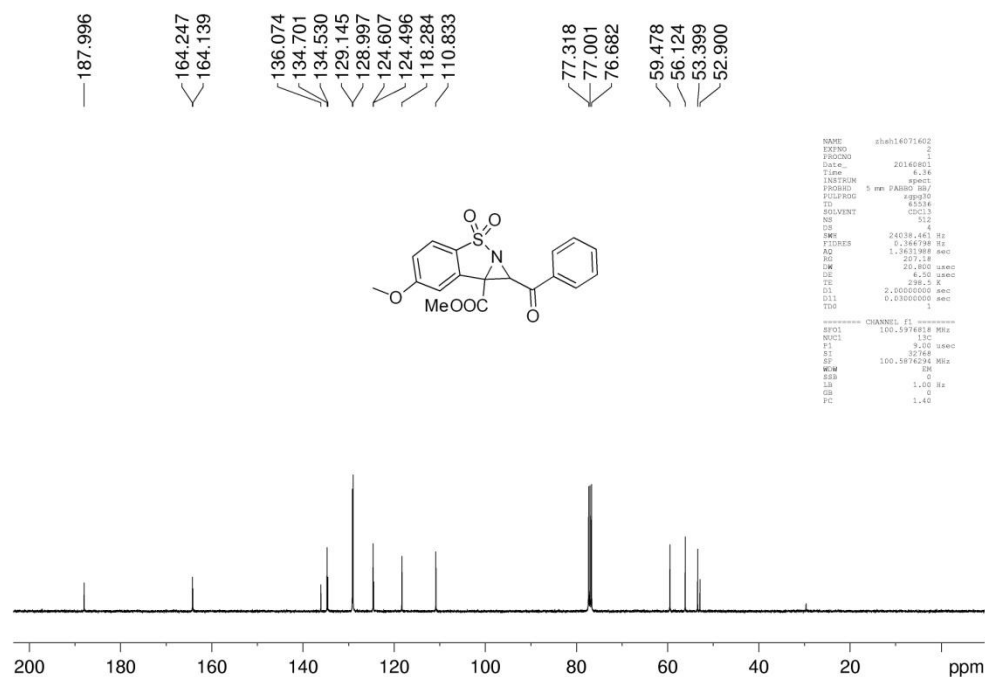
4ea ¹³C NMR



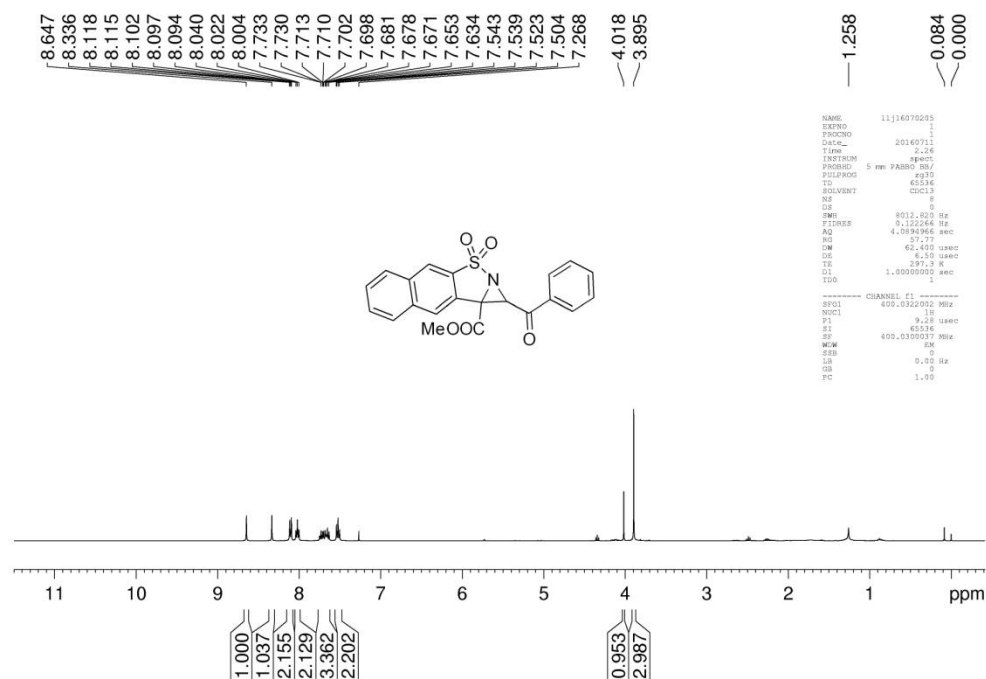
4fa ¹H NMR



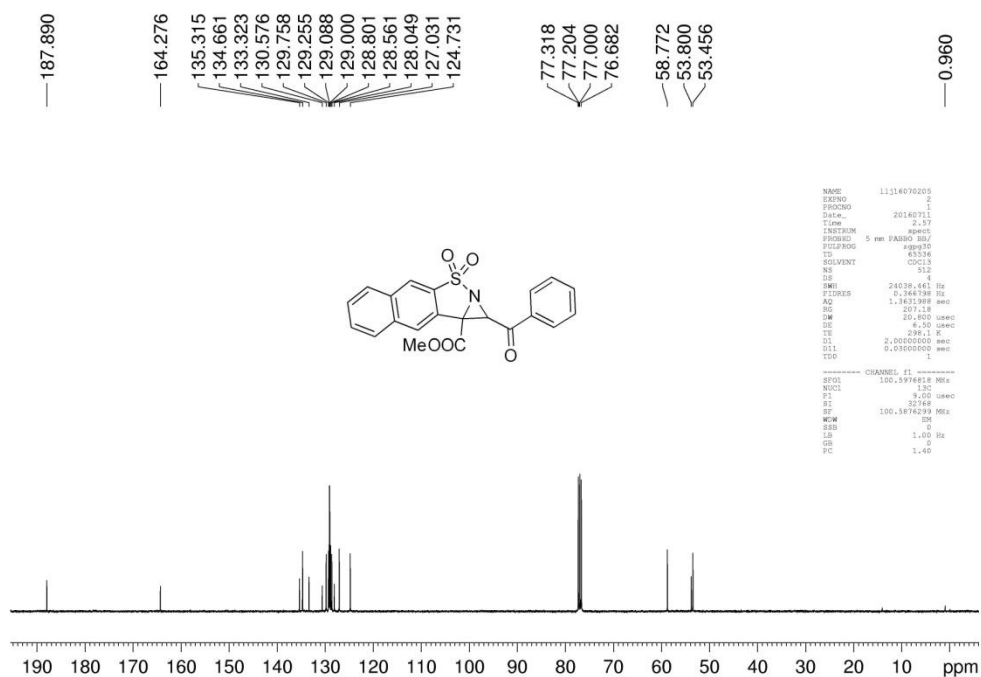
4fa ¹³C NMR



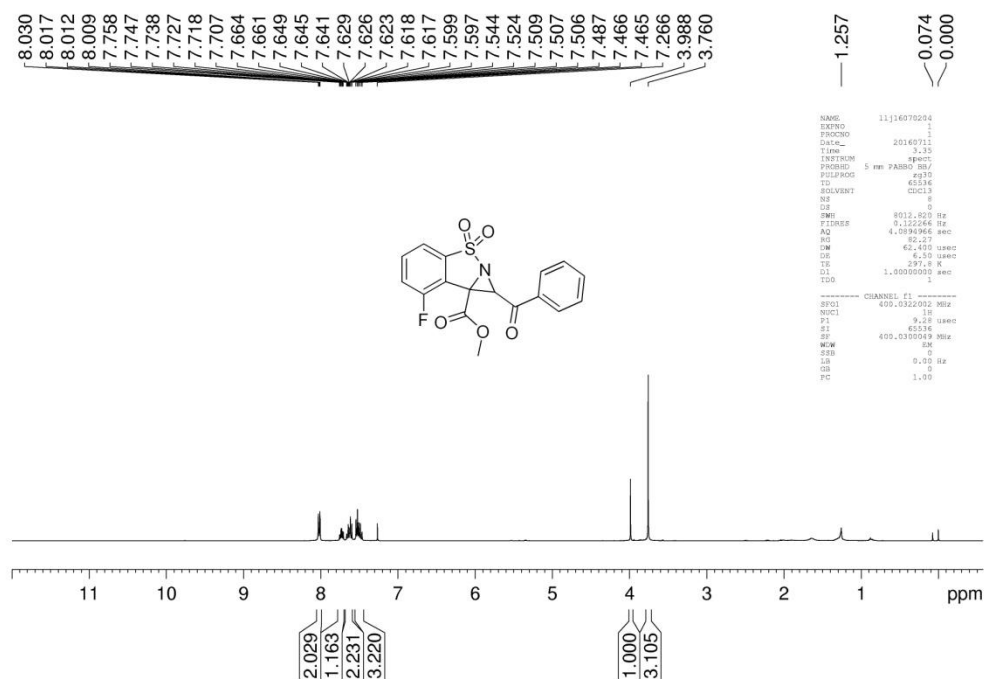
4ga ¹H NMR



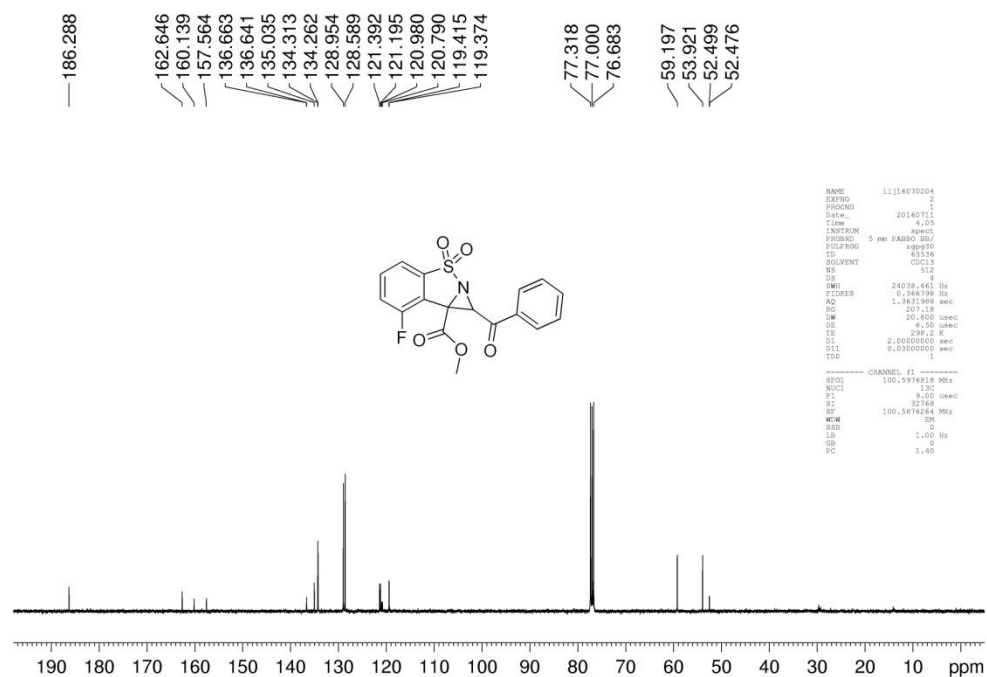
4ga ¹³C NMR



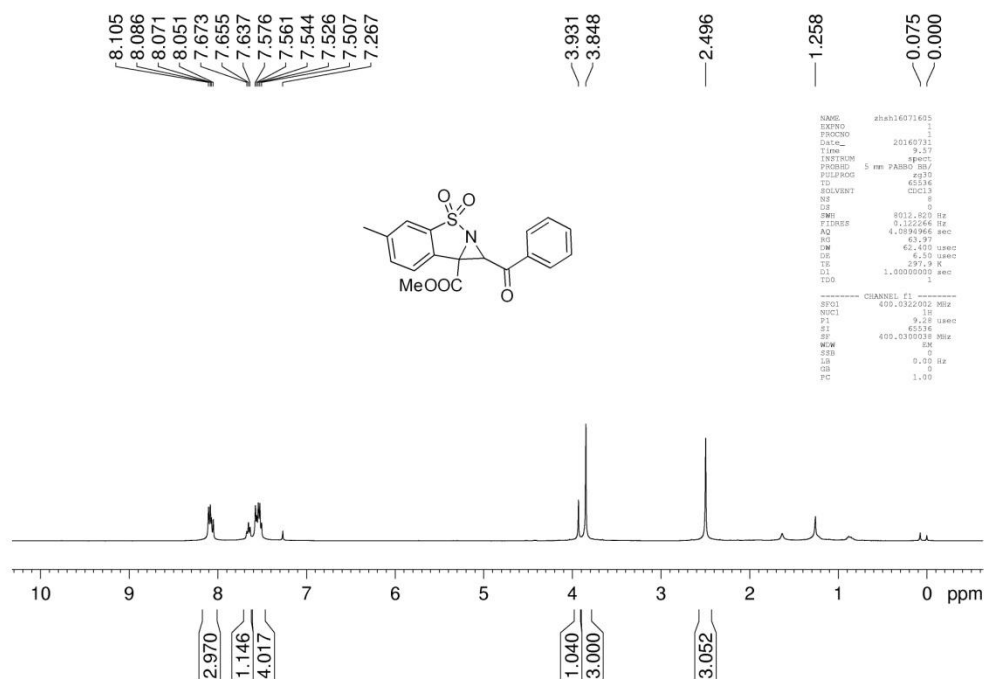
4ha ¹H NMR



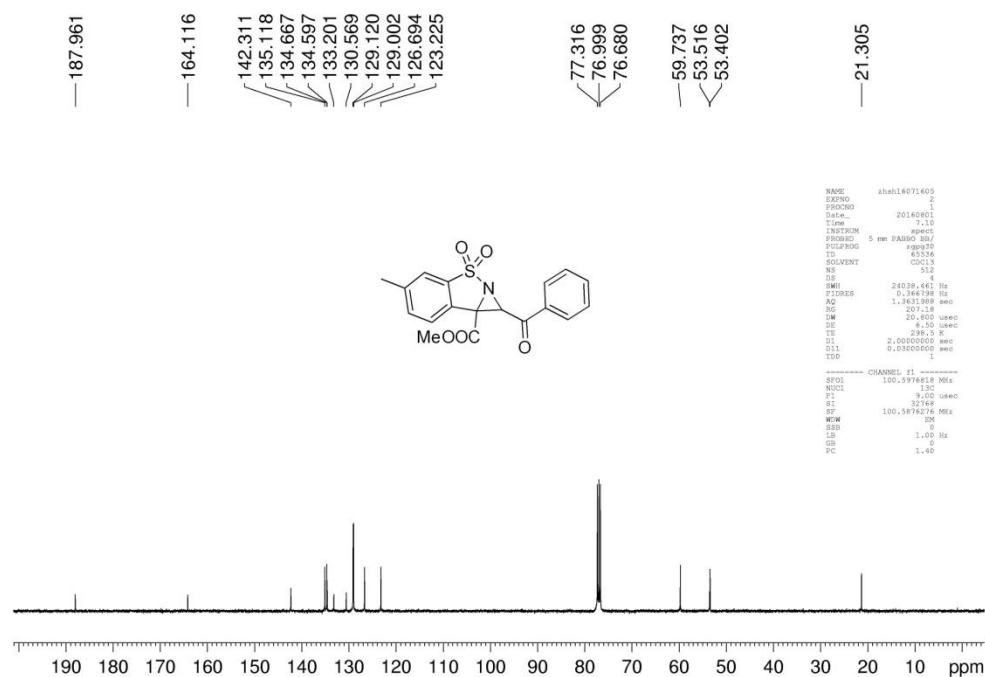
4ha ¹³C NMR



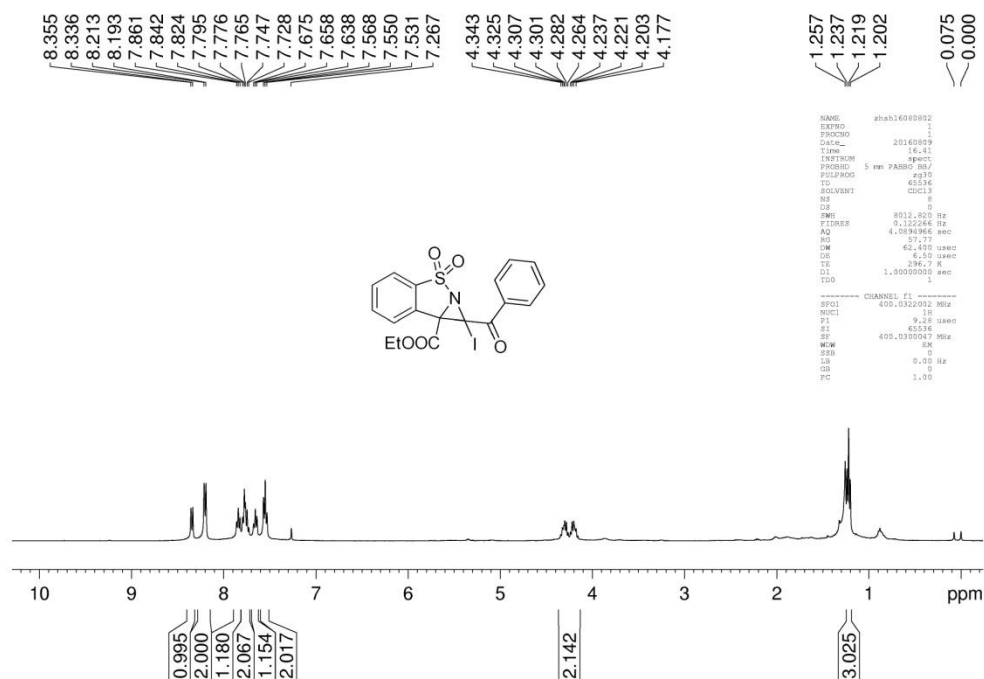
4ia ¹H NMR



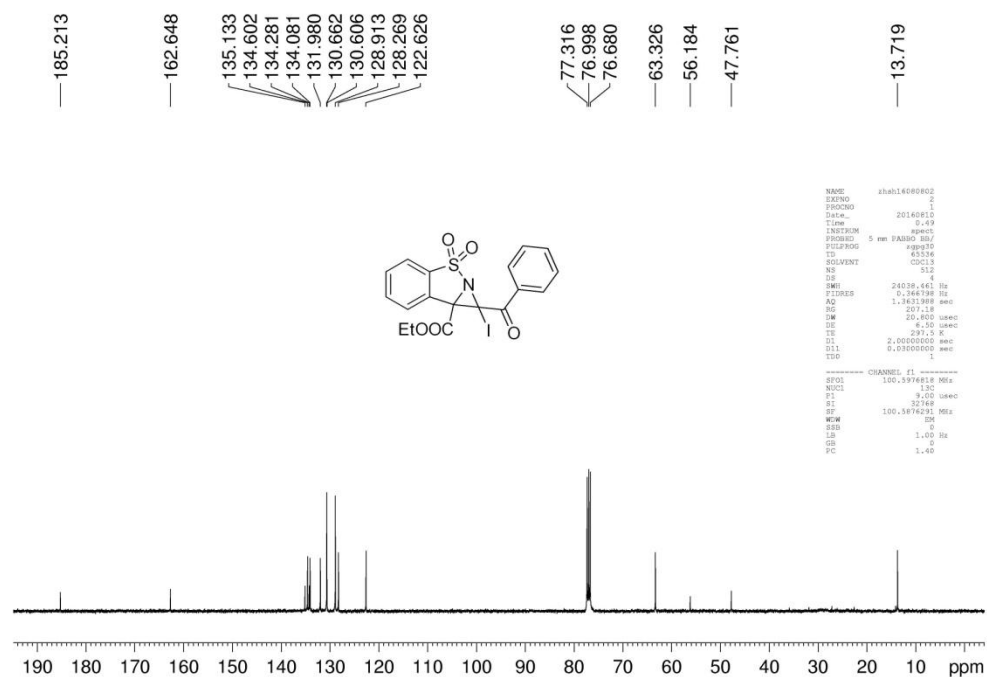
4ia ¹³C NMR



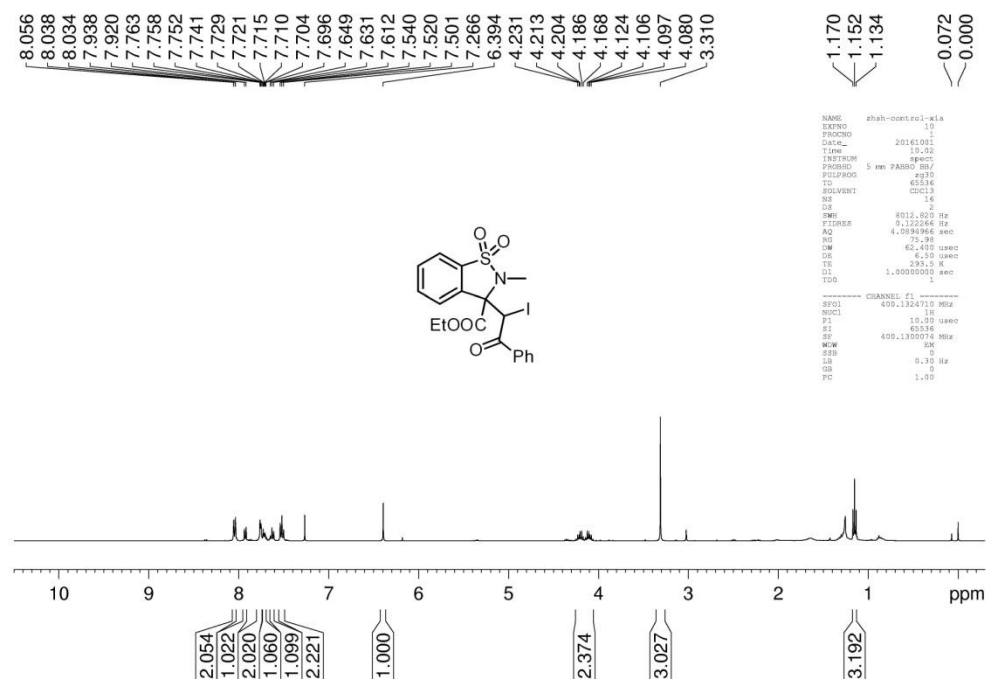
5aa ¹H NMR



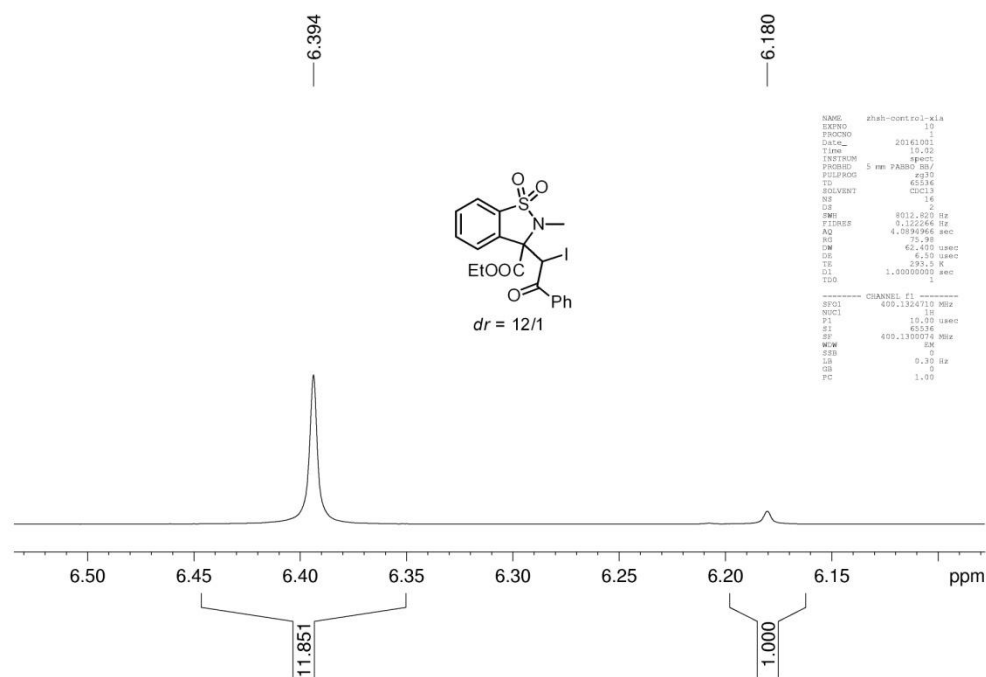
5aa ¹³C NMR



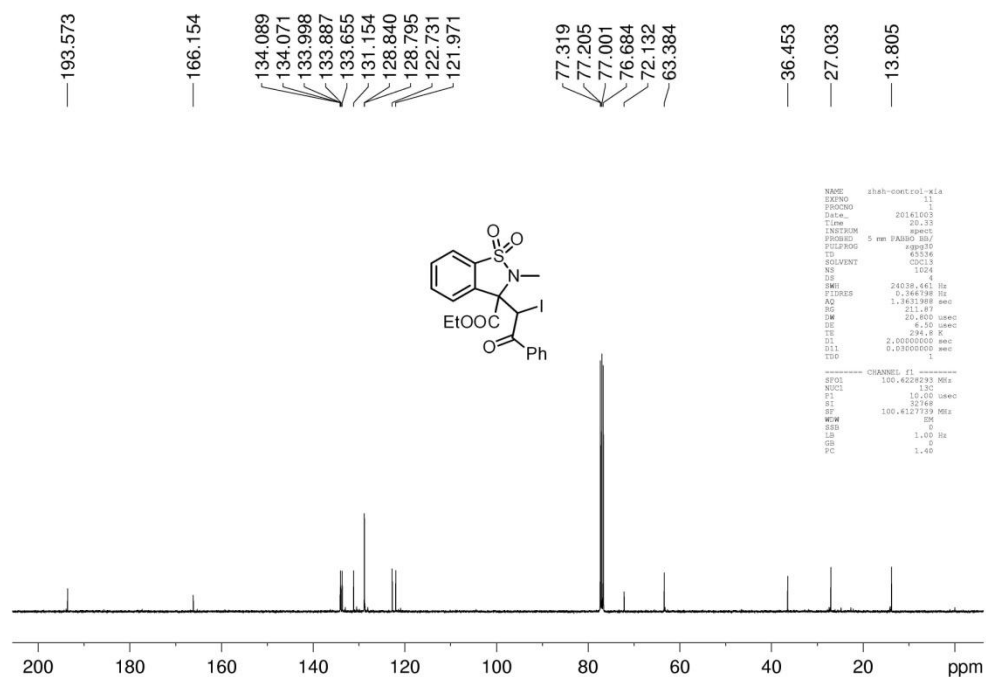
6a ¹H NMR



6a dr-¹H NMR

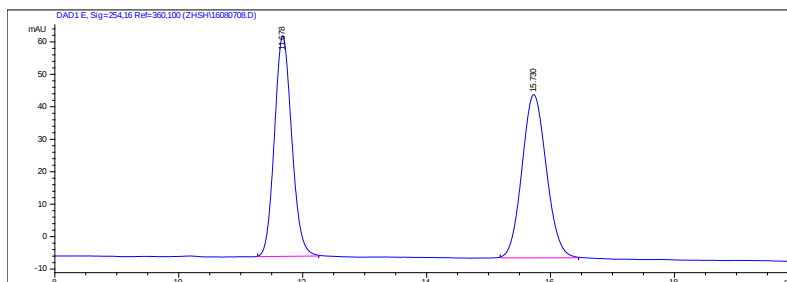


6a ¹³C NMR



Part III HPLC Spectra

3aa racemic sample (Daicel Chiralcel IC, *i*-PrOH/hexanes = 50/50, 1.0 mL/min):

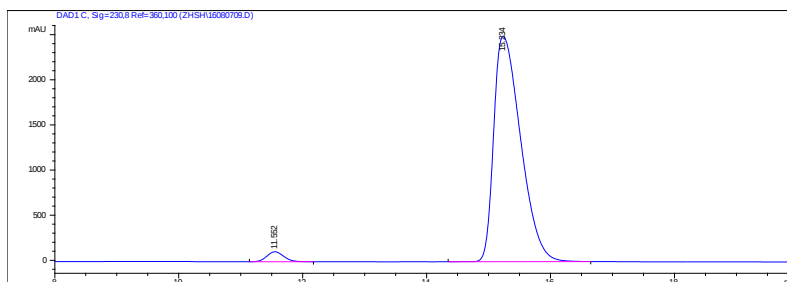


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.678	BB	0.3005	1319.03271	67.92801	49.0157
2	15.730	BB	0.4244	1372.00635	50.27872	50.9843

Totals : 2691.03906 118.20673

3aa (on 0.3 mmol scale):

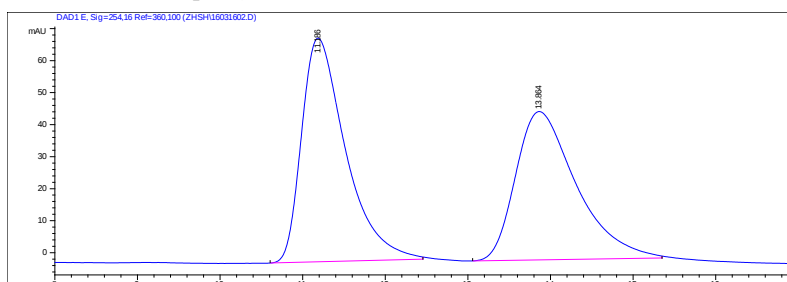


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.552	BB	0.2961	2110.16870	110.86532	2.7231
2	15.234	BB	0.4705	7.53815e4	2494.95557	97.2769

Totals : 7.74917e4 2605.82088

3aa racemic sample (Daicel Chiralcel OD-H, *i*-PrOH/hexanes = 70/30, 0.8 mL/min):

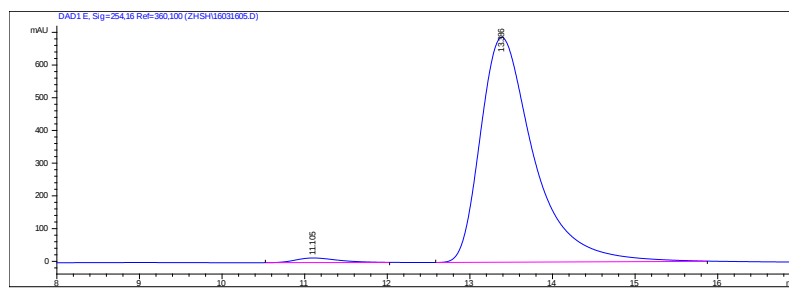


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.186	BB	0.5554	2583.25806	69.86707	52.2336
2	13.864	BB	0.7588	2362.32910	46.33345	47.7664

Totals : 4945.58716 116.20052

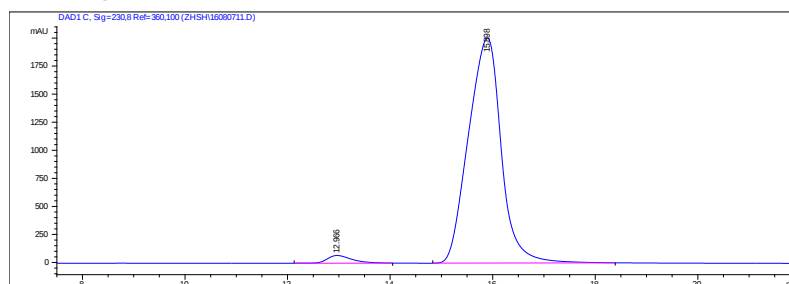
3aa (on 0.1 mmol scale):



Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.105	PB	0.5351	502.47012	14.12321	1.6007
2	13.386	PB	0.6801	3.08885e4	687.59137	98.3993
Totals :				3.13909e4	701.71458	

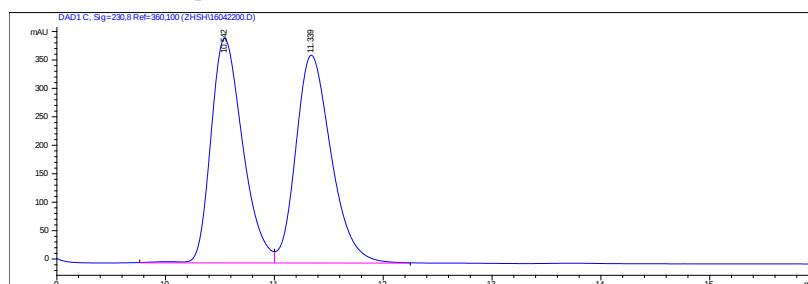
3aa (on gram scale):



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.966	BB	0.5042	2302.89062	68.84580	2.5215
2	15.898	PB	0.7176	8.90257e4	2006.70703	97.4785
Totals :				9.13286e4	2075.55283	

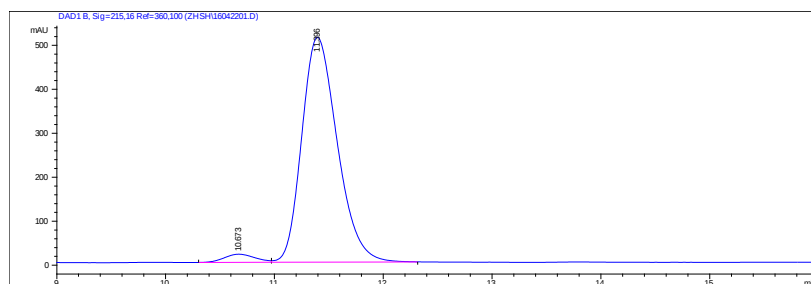
4aa racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.542	EV	0.3143	7990.75830	394.49820	49.2987
2	11.339	VB	0.3485	8218.10938	365.24197	50.7013
Totals :				1.62089e4	759.74017	

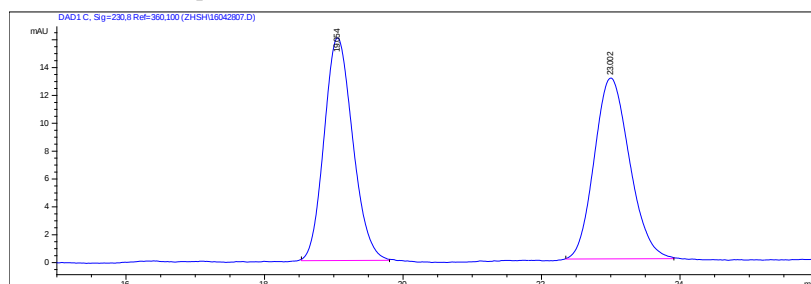
4aa:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.673	PV	0.3042	363.02664	18.55670	3.0382
2	11.396	VB	0.3522	1.15856e4	511.63019	96.9618
Totals :				1.19486e4	530.18689	

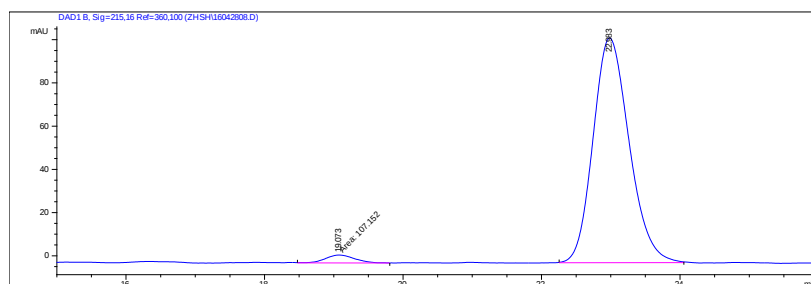
4ab racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.054	BB	0.4380	460.31653	15.98137	50.0044
2	23.002	BB	0.5477	460.23624	12.97994	49.9956
Totals :				920.55276	28.96131	

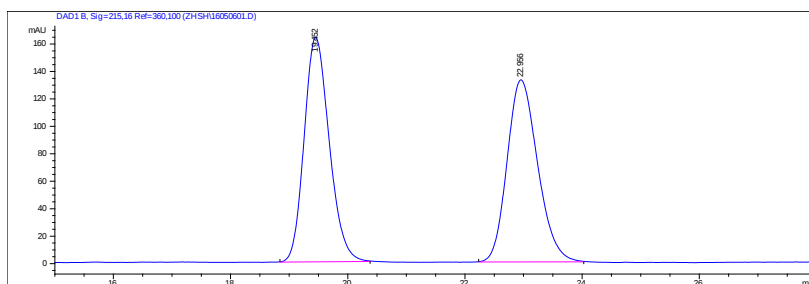
4ab:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.073	MM	0.4908	107.15194	3.63835	2.7682
2	22.983	BB	0.5600	3763.69849	104.04972	97.2318
Totals :				3870.85043	107.68807	

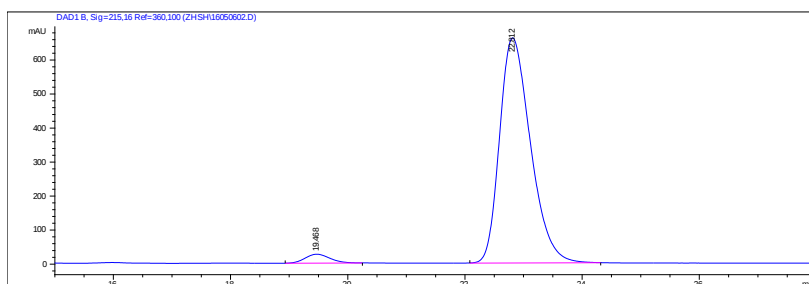
4ac racemic sample:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.452	BB	0.4590	4867.99707	163.64984	50.3108
2	22.956	BB	0.5566	4807.84619	132.72308	49.6892
Totals :				9675.84326	296.37292	

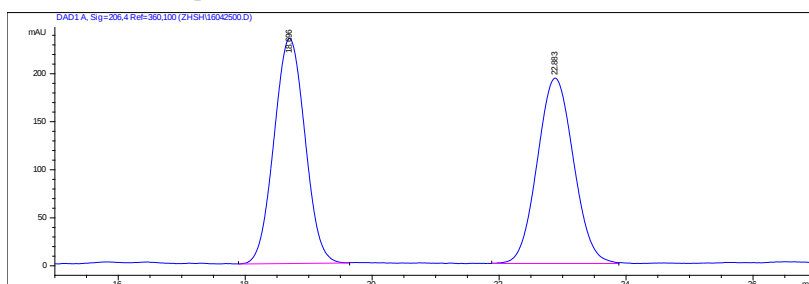
4ac:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.468	BB	0.4485	767.78699	26.15087	3.0686
2	22.812	BB	0.5695	2.42529e4	661.88525	96.9314
Totals :				2.50206e4	688.03612	

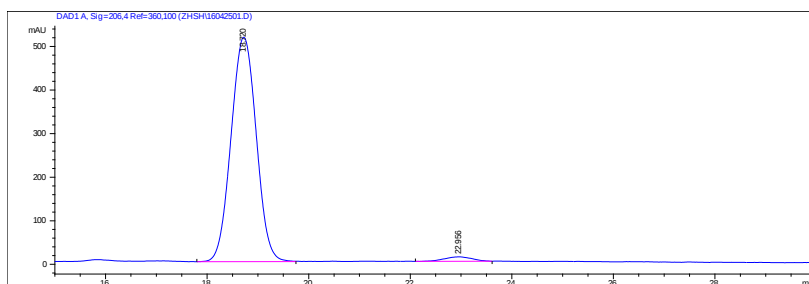
4ad racemic sample:



Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.696	VB	0.5372	7933.76660	234.18597	50.9251
2	22.883	PV	0.6123	7645.52881	192.92894	49.0749
Totals :				1.55793e4	427.11491	

4ad:

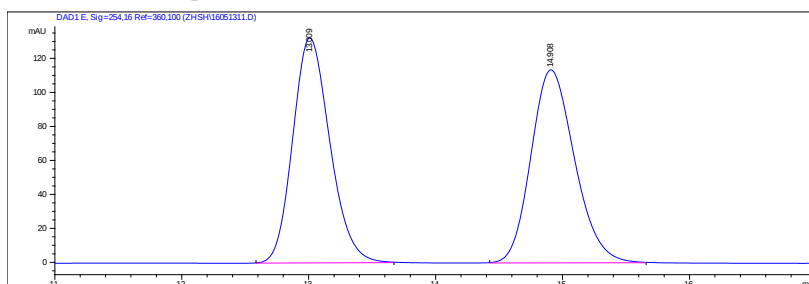


Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.720	VB	0.5422	1.77502e4	514.94617	97.8824
2	22.956	BV	0.4488	384.00562	10.25730	2.1176

Totals : 1.81342e4 525.20347

4ae racemic sample:

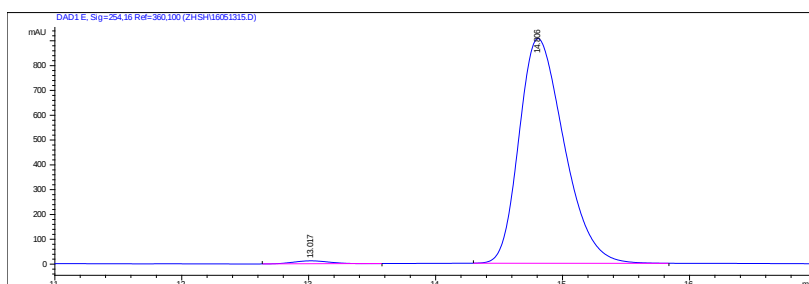


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.009	BB	0.3132	2693.72119	132.47191	49.8126
2	14.908	BB	0.3708	2713.98730	113.58038	50.1874

Totals : 5407.70850 246.05228

4ae:

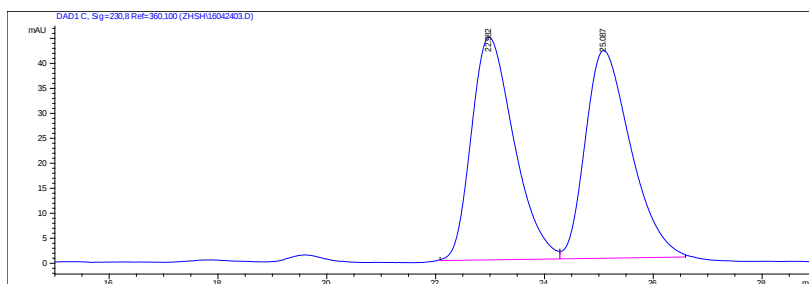


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.017	FP	0.3044	229.82318	11.84152	1.0196
2	14.806	BB	0.3814	2.23115e4	905.82330	98.9804

Totals : 2.25413e4 917.66482

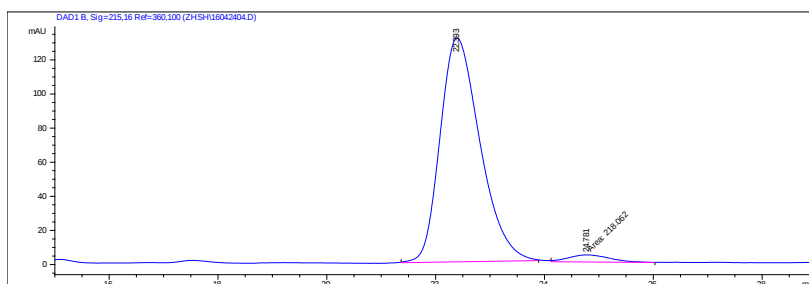
4af racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.982	BY	0.8048	2423.52075	44.53879	50.0682
2	25.087	VB	0.8625	2416.91797	41.56031	49.9318
Totals :				4840.43872	86.09910	

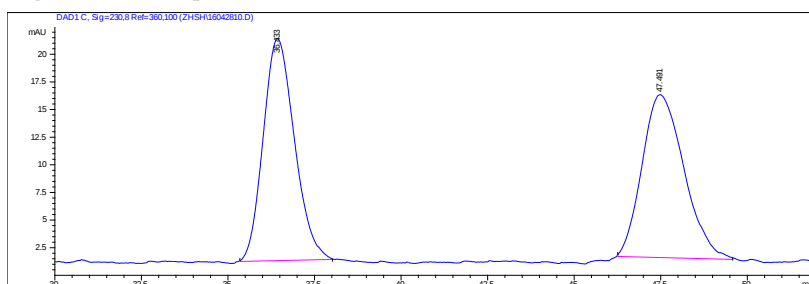
4af:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.393	BB	0.7769	6694.48340	131.29002	96.8454
2	24.781	MM	0.8802	218.06192	4.12903	3.1546
Totals :				6912.54532	135.41905	

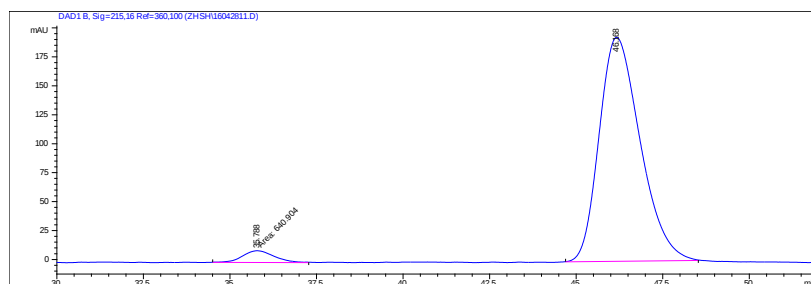
4ag racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.433	BB	0.8454	1259.44263	20.09070	50.4083
2	47.491	BB	1.0073	1239.04089	14.73135	49.5917
Totals :				2498.48352	34.82205	

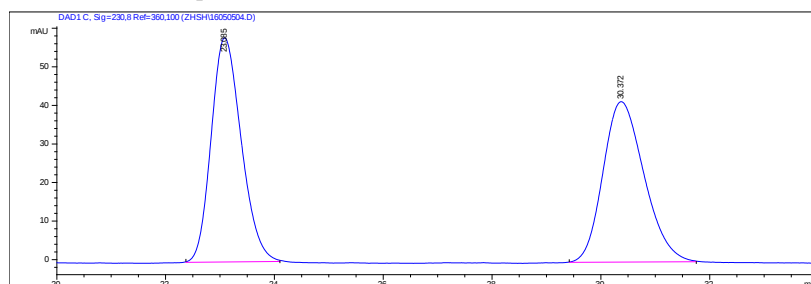
4ag:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.788	MM	1.0530	640.90442	10.14370	3.8704
2	46.168	BB	1.2460	1.59181e4	193.45474	96.1296
Totals :				1.65590e4	203.59844	

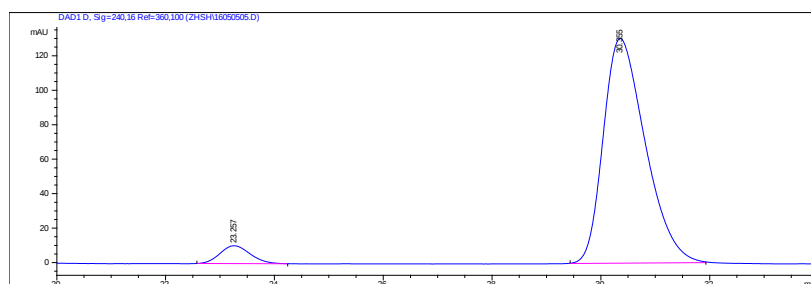
4ah racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.085	BB	0.5897	2229.92578	58.11414	50.5224
2	30.372	BB	0.7883	2183.81104	41.60661	49.4776
Totals :				4413.73682	99.72075	

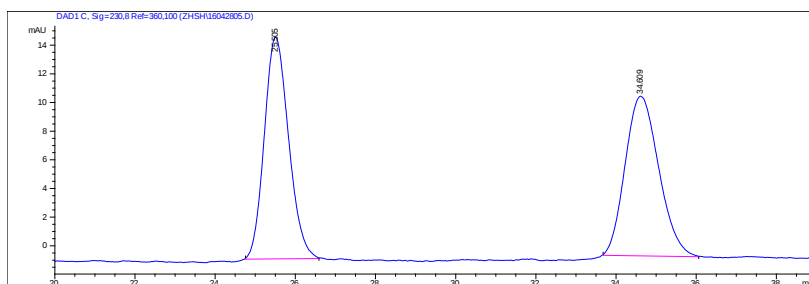
4ah:



Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.257	BB	0.5839	399.92569	10.36980	5.4197
2	30.355	BB	0.8249	6979.22705	130.30948	94.5803
Totals :				7379.15274	140.67928	

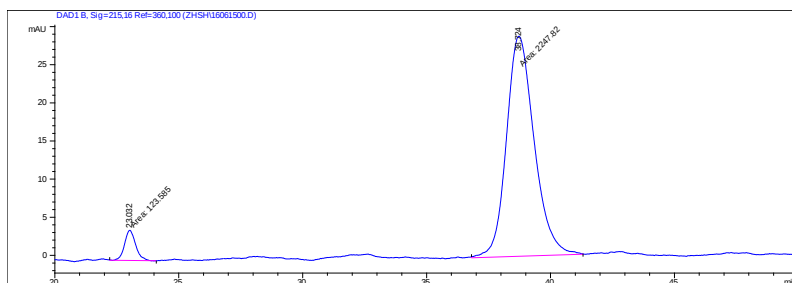
4ai racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.505	BB	0.6297	651.87250	15.46592	50.0707
2	34.609	BB	0.7545	650.03210	11.14399	49.9293
Totals :				1301.90460	26.60991	

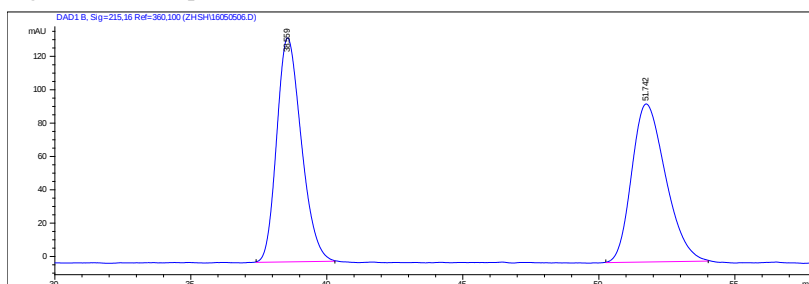
4ai:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.032	MM	0.5204	123.58527	3.95805	5.2115
2	38.724	MM	1.2984	2247.82275	28.85351	94.7885
Totals :				2371.40802	32.81156	

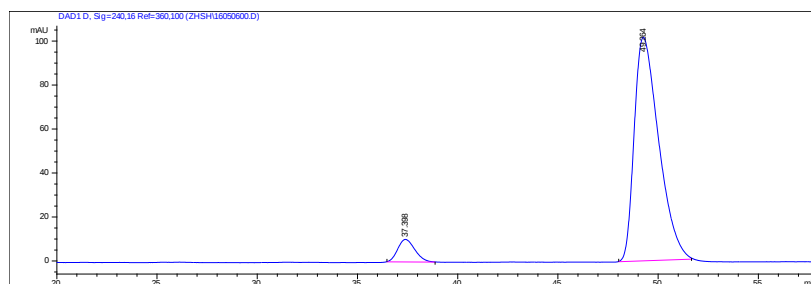
4aj racemic sample:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	38.559	BB	0.9391	8439.01465	134.30240	50.6392
2	51.742	BB	1.2882	8225.97852	94.81699	49.3608
Totals :				1.66650e4	229.11938	

4aj:

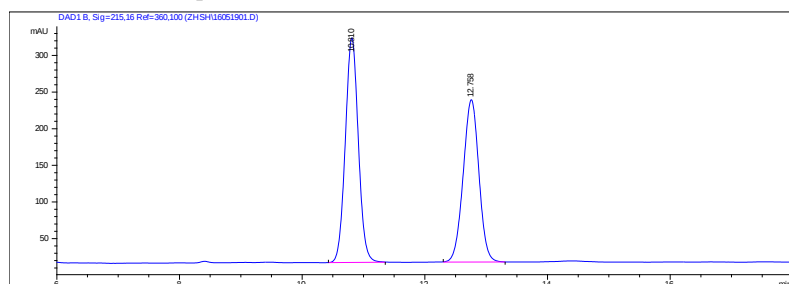


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.398	BB	0.7348	609.58392	10.23647	6.5832
2	49.264	BB	1.2545	8650.13379	101.67929	93.4168

Totals : 9259.71771 111.91576

4ak racemic sample:

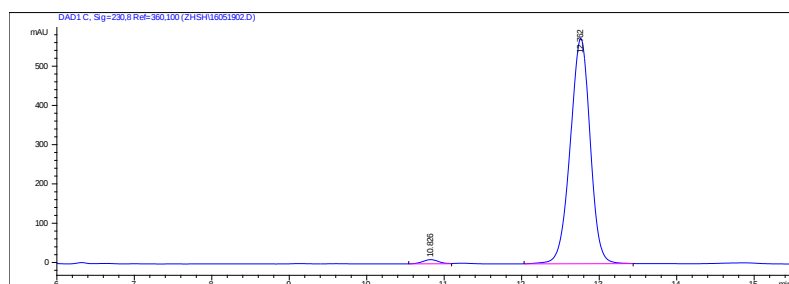


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.810	BB	0.2280	4519.51025	306.47971	53.3753
2	12.758	BB	0.2759	3947.91040	221.50003	46.6247

Totals : 8467.42065 527.97974

4ak:

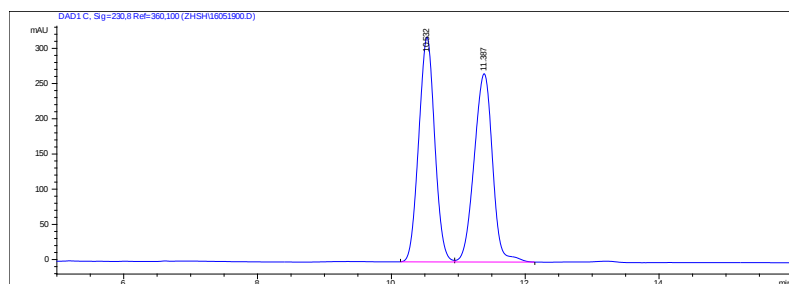


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.826	BV	0.2171	151.18208	10.68184	1.4549
2	12.762	BB	0.2763	1.02398e4	573.57507	98.5451

Totals : 1.03910e4 584.25692

4al racemic sample:

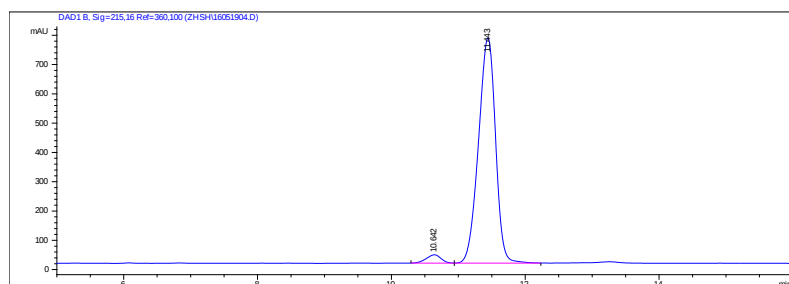


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.532	BV	0.2594	5289.65381	319.11893	50.9010
2	11.387	VB	0.3026	5102.38379	267.45865	49.0990

Totals : 1.03920e4 586.57758

4al:

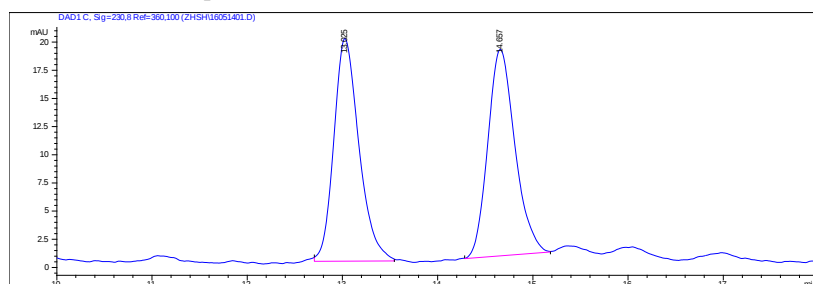


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.642	BV	0.2351	435.18842	28.35088	3.1037
2	11.443	VB	0.2741	1.35863e4	768.99725	96.8963

Totals : 1.40215e4 797.34813

4am racemic sample:

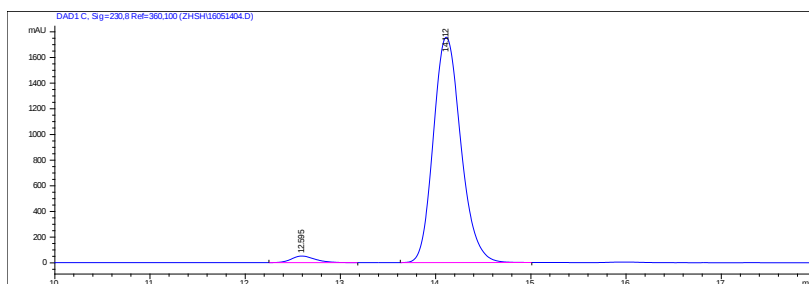


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.025	BB	0.2802	362.74036	19.75455	49.9772
2	14.657	BB	0.3092	363.07126	18.32005	50.0228

Totals : 725.81161 38.07459

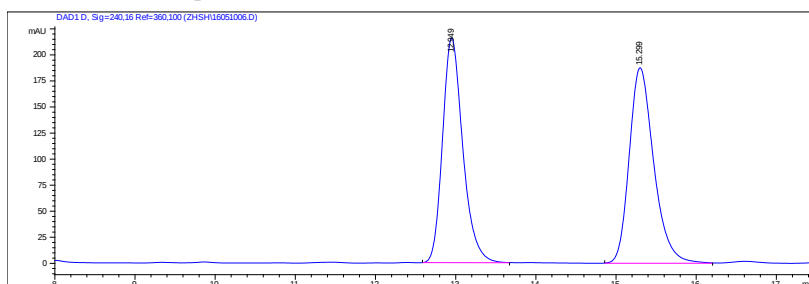
4am:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.595	BB	0.2634	898.85608	51.56773	2.4893
2	14.112	BB	0.3100	3.52102e4	1755.76294	97.5107
Totals :				3.61090e4	1807.33067	

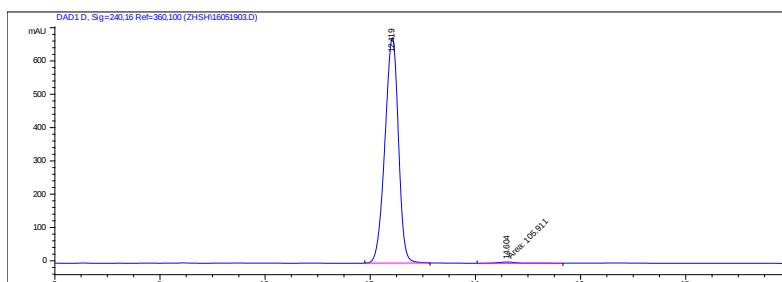
4an racemic sample:



Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.949	BB	0.2690	3789.88843	215.73515	48.7406
2	15.299	BB	0.3259	3985.73633	187.59306	51.2594
Totals :				7775.62476	403.32822	

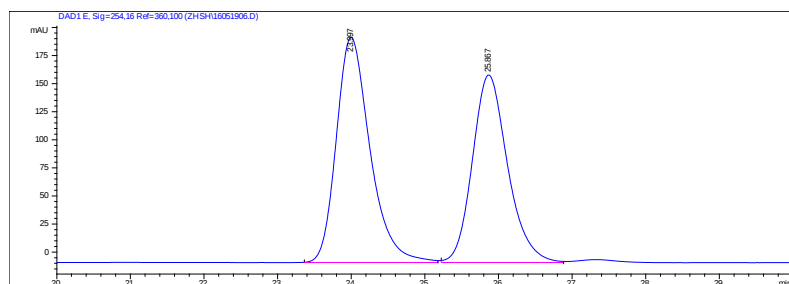
4an:



Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.419	BB	0.2763	1.20759e4	676.39886	99.1306
2	14.604	MM	0.4644	105.91131	3.80140	0.8694
Totals :				1.21818e4	680.20027	

4ao racemic sample:

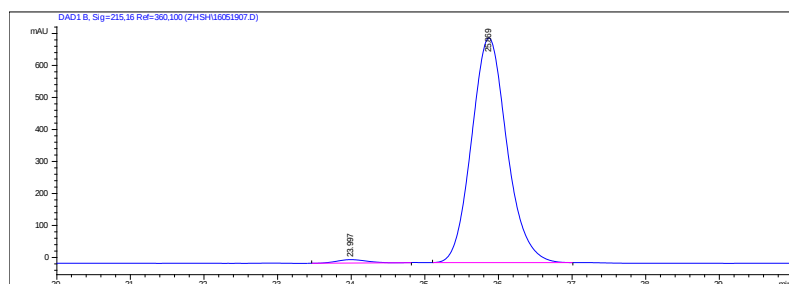


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.997	BB	0.4831	6378.72803	200.52765	53.4820
2	25.867	BB	0.5077	5548.13184	166.95270	46.5180

Totals : 1.19269e4 367.48035

4ao:

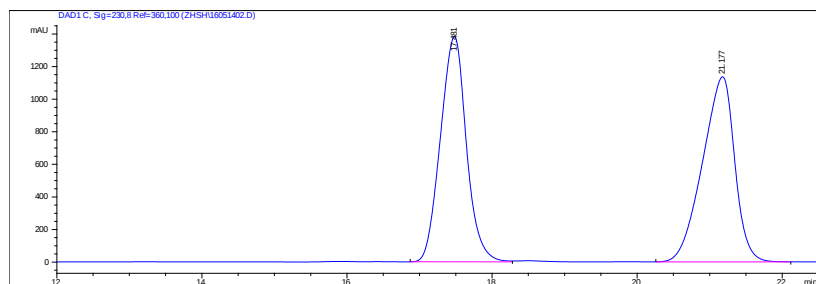


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.997	FB	0.4160	302.67822	10.69959	1.2765
2	25.869	FB	0.5130	2.34092e4	702.07922	98.7235

Totals : 2.37118e4 712.77881

4ap racemic sample:

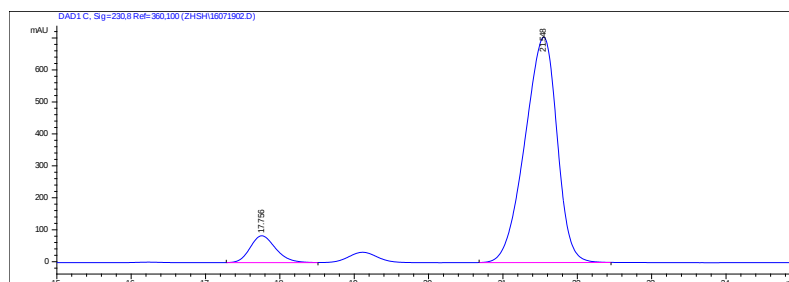


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.481	PV	0.3822	3.43969e4	1382.87341	49.5683
2	21.177	FB	0.4675	3.49961e4	1135.67834	50.4317

Totals : 6.93930e4 2518.55176

4ap:

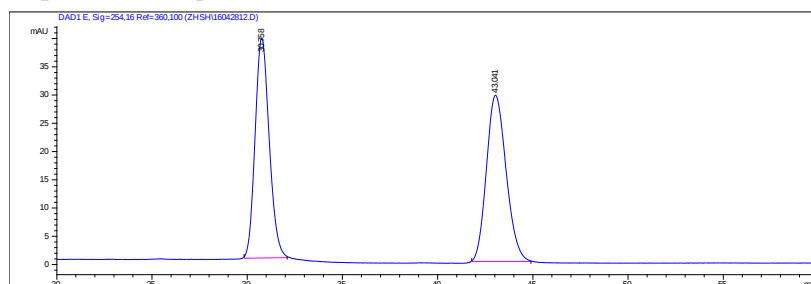


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.756	BB	0.3704	2018.57349	83.97311	8.6967
2	21.548	BB	0.4668	2.11923e4	704.80145	91.3033

Totals : 2.32109e4 788.77456

4aq racemic sample:

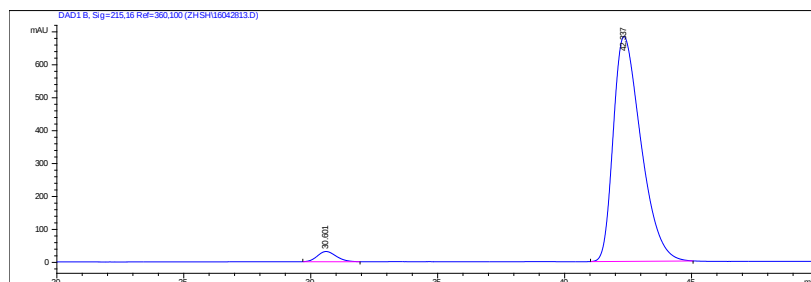


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.758	BB	0.7723	2003.86938	38.94310	48.6175
2	43.041	BB	1.0360	2117.83740	29.41324	51.3825

Totals : 4121.70679 68.35634

4aq:

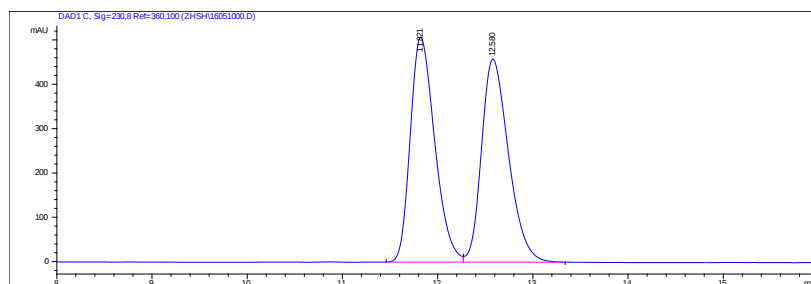


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.601	BB	0.7682	1603.09436	31.05709	2.9980
2	42.337	BB	1.1520	5.18682e4	682.98193	97.0020

Totals : 5.34713e4 714.03902

4ar racemic sample:

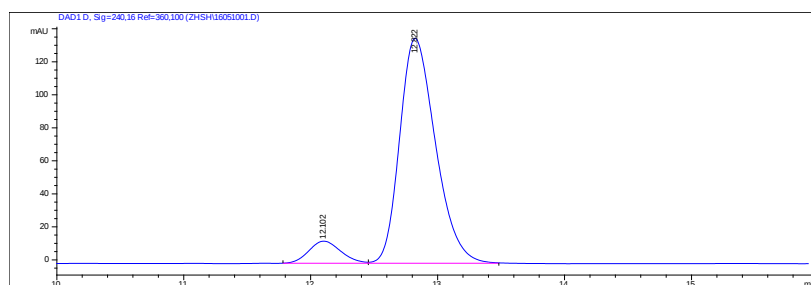


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.821	BV	0.2764	9063.54785	507.31653	50.0831
2	12.580	VB	0.3040	9033.45801	458.25583	49.9169

Totals : 1.80970e4 965.57236

4ar:

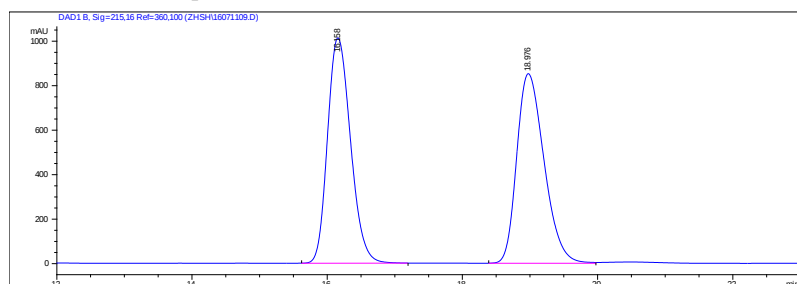


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.102	BV	0.2684	235.27562	13.42796	8.0969
2	12.822	VB	0.3046	2670.48633	136.30681	91.9031

Totals : 2905.76195 149.73477

4as racemic sample:

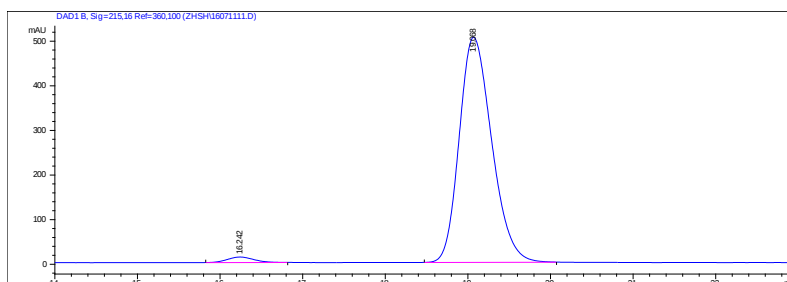


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.158	BB	0.3696	2.39215e4	1012.65424	50.0059
2	18.976	BB	0.4375	2.39158e4	851.94861	49.9941

Totals : 4.78373e4 1864.60284

4as:

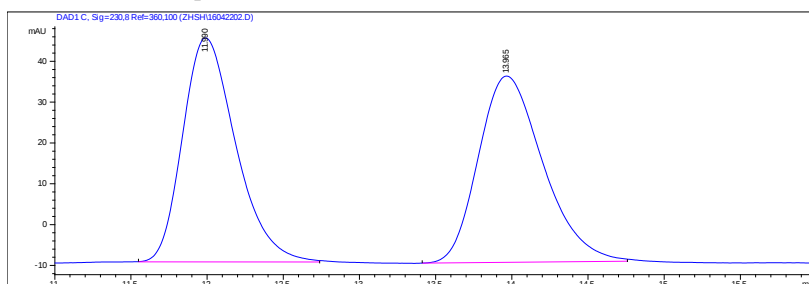


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.242	BB	0.3427	275.87546	12.34710	1.9625
2	19.068	BB	0.4226	1.37811e4	504.62921	98.0375

Totals : 1.40570e4 516.97631

4ba racemic sample:

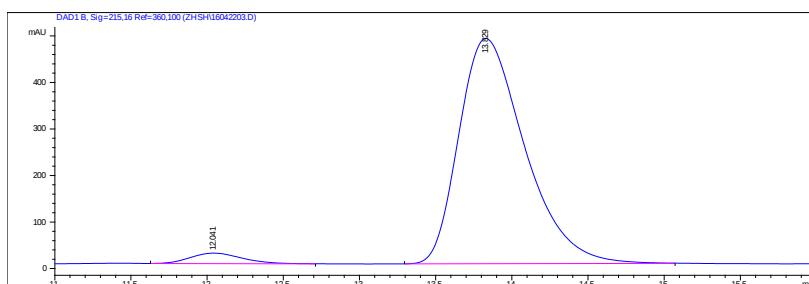


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.990	BB	0.3751	1331.90857	54.88838	49.7782
2	13.965	PB	0.4575	1343.77551	45.63787	50.2218

Totals : 2675.68408 100.02625

4ba:

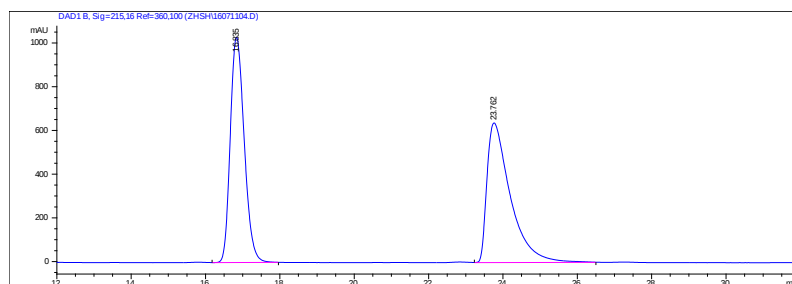


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.041	PB	0.3710	530.94897	22.52116	3.5233
2	13.829	BB	0.4604	1.45389e4	484.09253	96.4767

Totals : 1.50698e4 506.61369

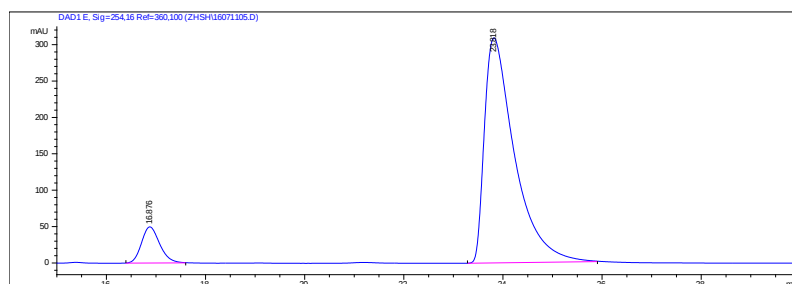
4ca racemic sample:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.835	VB	0.4120	2.68506e4	1030.36902	49.0879
2	23.762	VB	0.6469	2.78484e4	638.43127	50.9121
Totals :				5.46991e4	1668.80029	

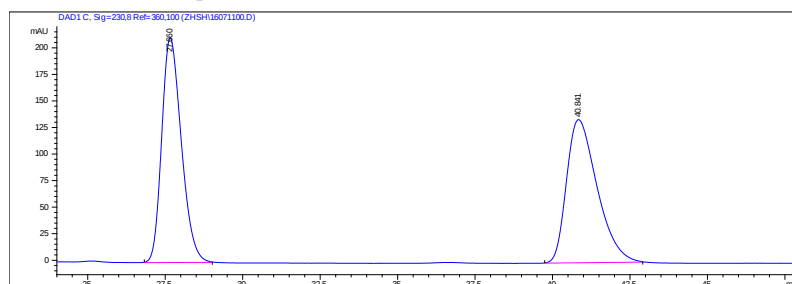
4ca:



Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.876	BB	0.3941	1270.76123	49.72636	8.8653
2	23.818	FB	0.6310	1.30633e4	309.12503	91.1347
Totals :				1.43341e4	358.85139	

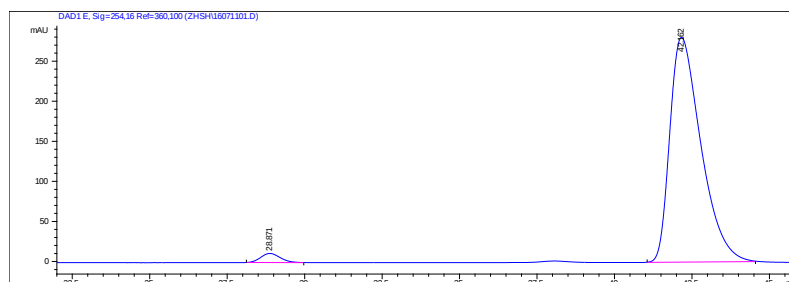
4da racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.660	BB	0.6807	9289.19922	211.39606	50.1369
2	40.841	BB	1.0118	9238.47363	134.76149	49.8631
Totals :				1.85277e4	346.15755	

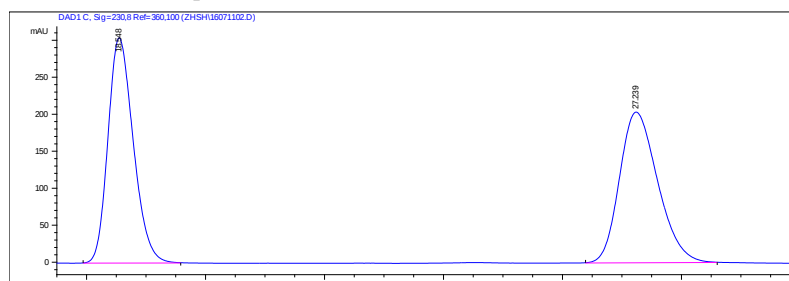
4da:



Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.871	BB	0.6345	496.78516	11.35306	2.4758
2	42.162	BB	1.0639	1.95690e4	280.52173	97.5242
Totals :				2.00658e4	291.87479	

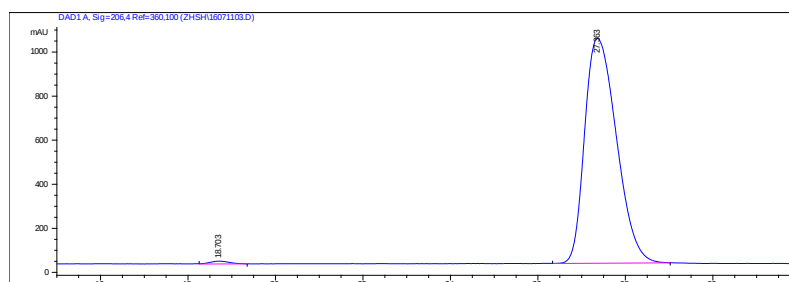
4ea racemic sample:



Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.548	BB	0.4573	9006.34863	304.27567	49.7389
2	27.239	BB	0.6955	9100.91211	203.58954	50.2611
Totals :				1.81073e4	507.86520	

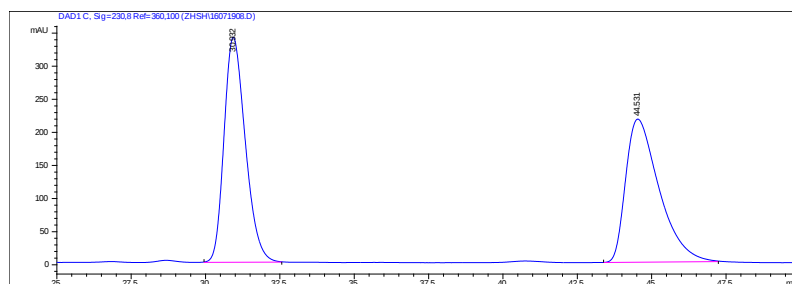
4ea:



Signal 1: DAD1 A, Sig=206,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.703	VV	0.3764	401.33414	12.77868	0.7716
2	27.363	VB	0.7243	5.16152e4	1020.11646	99.2284
Totals :				5.20166e4	1032.89514	

4fa racemic sample:

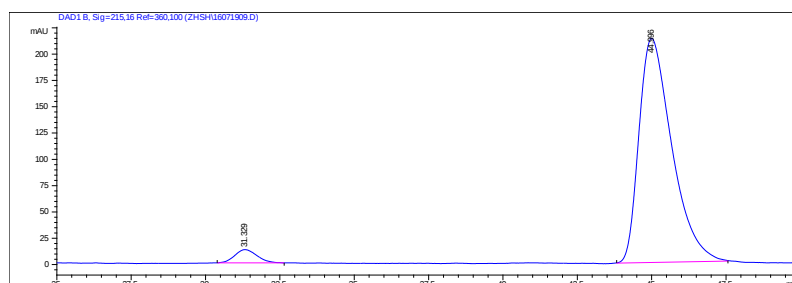


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.932	BB	0.7754	1.69430e4	339.99905	50.0822
2	44.531	BB	1.1729	1.68874e4	216.28754	49.9178

Totals : 3.38305e4 556.28659

4fa:

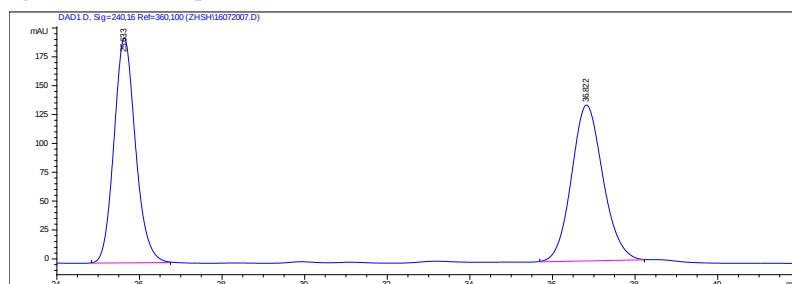


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.329	BP	0.6484	653.50531	12.57323	3.8430
2	44.996	BB	1.1255	1.63515e4	213.03342	96.1570

Totals : 1.70050e4 225.60665

4ga racemic sample:

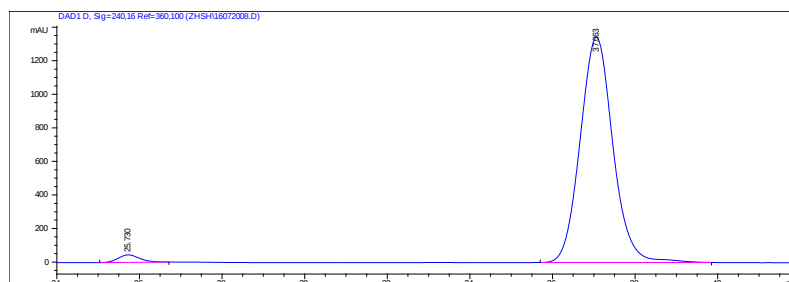


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.633	BB	0.5534	7040.64844	194.90221	49.6385
2	36.822	BB	0.8153	7143.20215	135.01361	50.3615

Totals : 1.41839e4 329.91582

4ga:

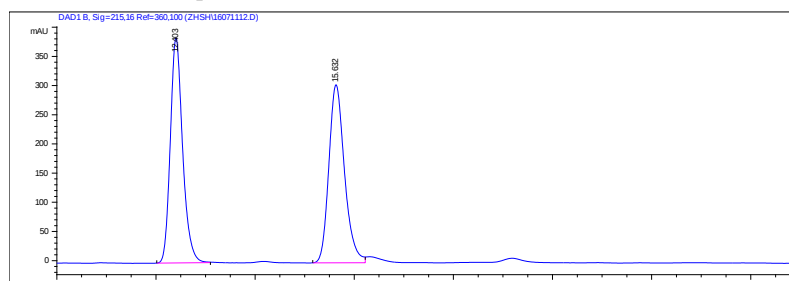


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.730	BB	0.5530	1617.87512	44.83289	2.1415
2	37.063	BB	0.8464	7.39293e4	1342.64563	97.8585

Totals : 7.55472e4 1387.47852

4ha racemic sample:

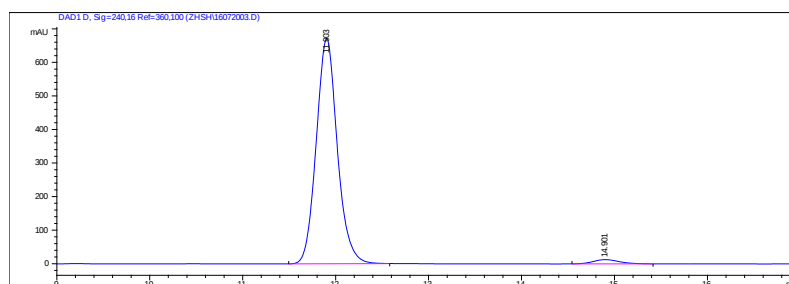


Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.403	BB	0.2630	6643.98682	385.62540	49.8201
2	15.632	BV	0.3339	6691.97705	305.13486	50.1799

Totals : 1.33360e4 690.76025

4ha:

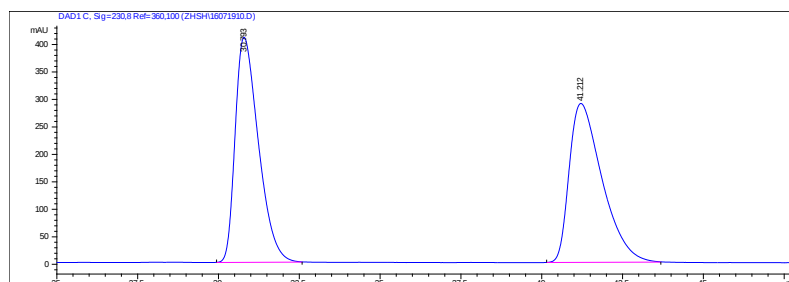


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.903	BB	0.2397	1.05720e4	671.49268	97.6560
2	14.901	BB	0.3027	253.75790	12.83521	2.3440

Totals : 1.08258e4 684.32789

4ia racemic sample:

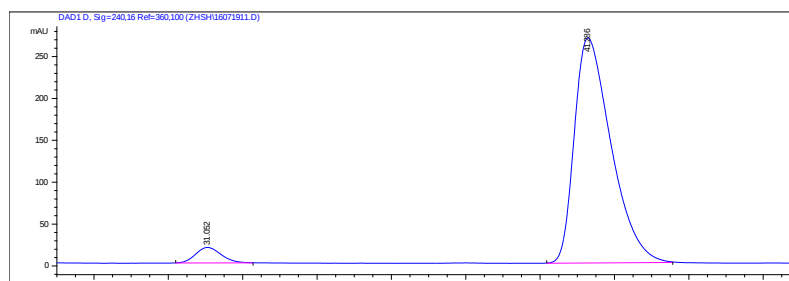


Signal 3: DAD1 C, Sig=230,8 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	30.793	BB	0.7675	2.04887e4	409.65741	50.0222
2	41.212	BB	1.0715	2.04704e4	289.32278	49.9778

Totals : 4.09591e4 698.98019

4ia:

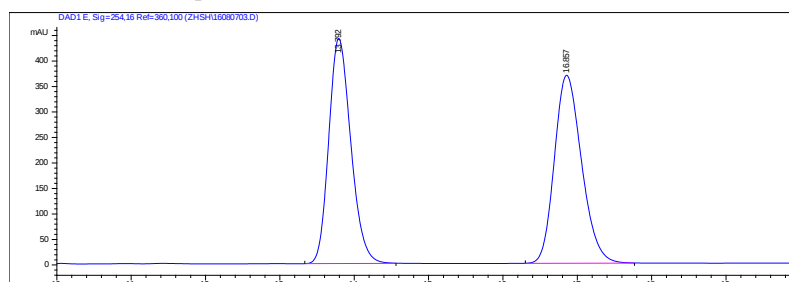


Signal 4: DAD1 D, Sig=240,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.052	BB	0.7353	882.60175	18.47546	4.5709
2	41.286	BB	1.0480	1.84267e4	268.70621	95.4291

Totals : 1.93093e4 287.18166

5aa racemic sample:

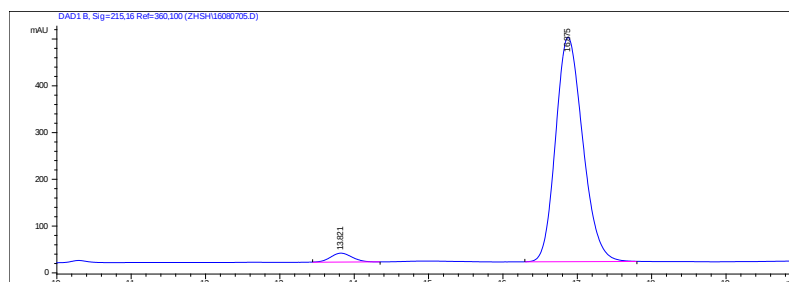


Signal 5: DAD1 E, Sig=254,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.792	BB	0.3208	9110.84082	441.40192	49.2848
2	16.857	BB	0.3946	9375.25879	368.77094	50.7152

Totals : 1.84861e4 810.17285

5aa:



Signal 2: DAD1 B, Sig=215,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.821	BP	0.3106	382.41626	19.01917	3.0470
2	16.875	BB	0.3959	1.21681e4	479.75284	96.9530
Totals :				1.25506e4	498.77201	