

Supporting Information-III

A Seven-step, One-pot Regioselective Synthesis of Biologically Important 3-Aryllawsones: Scope and Applications

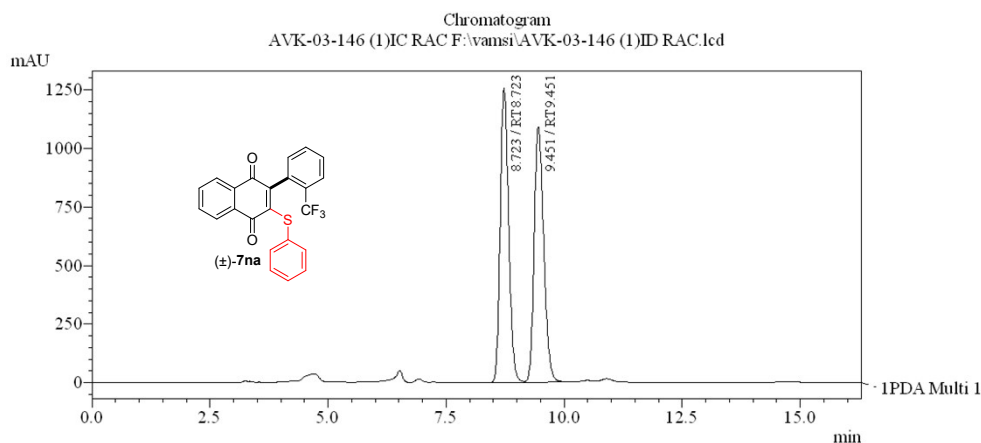
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General Methods: The ^1H NMR and ^{13}C NMR spectra were recorded at 500 and 400 MHz and 125 and 100 MHz, respectively. The chemical shifts are reported in ppm downfield to TMS ($\delta = 0$) for ^1H NMR and relative to the central CDCl_3 resonance ($\delta = 77.0$) for ^{13}C NMR. *In the ^{13}C NMR spectra, the nature of the carbons (C, CH, CH_2 or CH_3) was determined by recording the DEPT-135 experiment, and is given in parentheses.* The coupling constants J are given in Hz. Column chromatography was performed using Acme's silica gel (particle size 0.063-0.200 mm). High-resolution mass spectra were recorded on micromass ESI-TOF MS. IR spectra were recorded on JASCO FT/IR-5300. Mass spectra were recorded on either VG7070H mass spectrometer using EI technique or Shimadzu-LCMS-2010 A mass spectrometer. The X-ray diffraction measurements were carried out at 298 K on an automated Enraf-Nonious MACH 3 diffractometer using graphite monochromated, Mo- $\text{K}\alpha$ ($\lambda = 0.71073 \text{ \AA}$) radiation with CAD4 software or the X-ray intensity data were measured at 298 K on a Bruker SMART APEX CCD area detector system equipped with a graphite monochromator and a Mo- $\text{K}\alpha$ fine-focus sealed tube ($\lambda = 0.71073 \text{ \AA}$). For thin-layer chromatography (TLC), silica gel plates Merck 60 F254 were used and compounds were visualized by irradiation with UV light and/or by treatment with a solution of *p*-anisaldehyde (23 mL), conc. H_2SO_4 (35 mL), acetic acid (10 mL), and ethanol (900 mL) followed by heating.

The enantiomeric excess (*ee*) of the products **7**, **10** were determined by chiral stationary phase HPLC using a Daicel Chiralpak ID or Daicel Chiralpak AD-H column and hexane/2-propanol as the eluent. Retention times and solvent ratios are indicated in the respective entries.

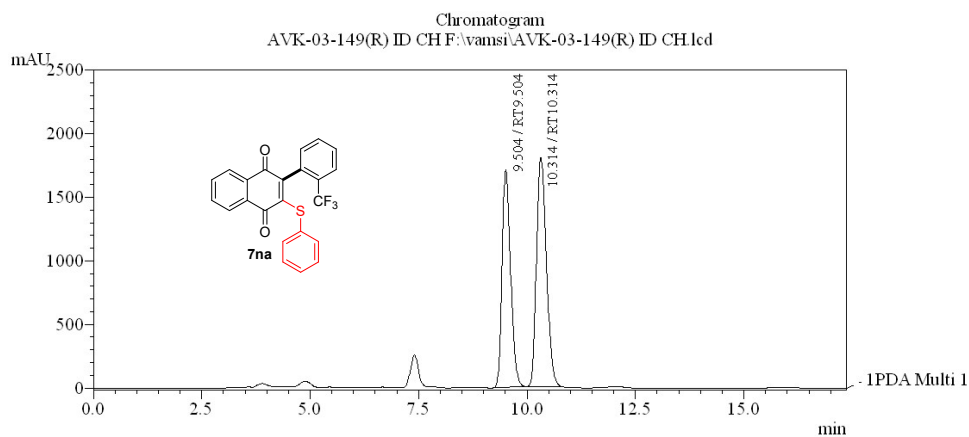
Racemic (\pm)-7na:



Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT8.723	8.723	15450357	1256571	50.123	53.615
2	RT9.451	9.451	15374611	1087115	49.877	46.385
Total			30824968	2343685	100.000	100.000

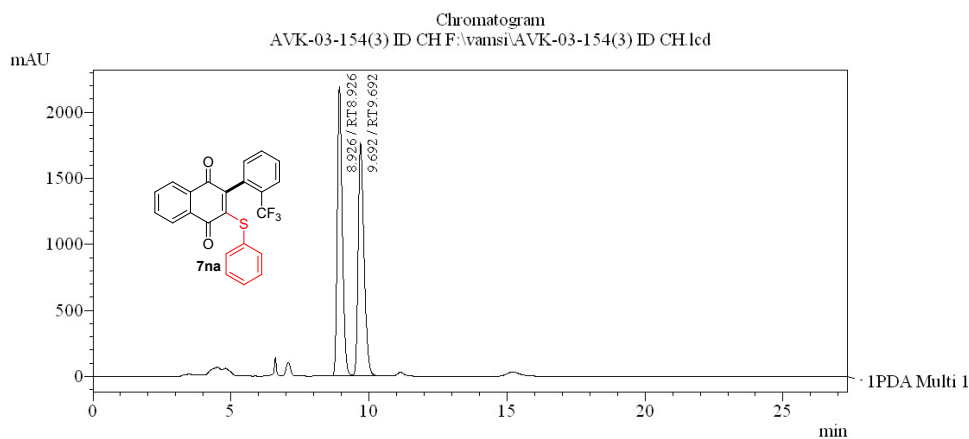
Chiral 7na (10% *ee*) [Table S1, entry 1]:



Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT9.504	9.504	23551743	1710998	45.060	48.673
2	RT10.314	10.314	28715414	1804261	54.940	51.327
Total			52267156	3515258	100.000	100.000

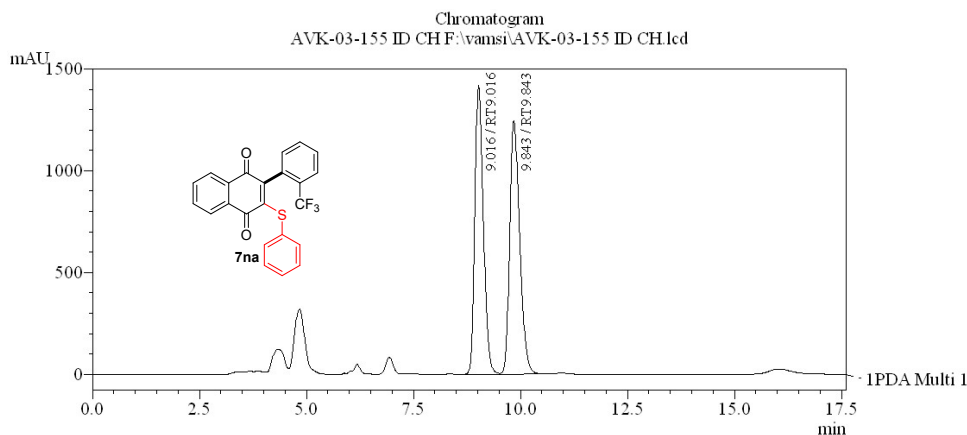
Chiral **7na** (1% *ee*) [Table S1, entry 2]:



Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT8.926	8.926	26982302	2191013	50.435	55.373
2	RT9.692	9.692	26517373	1765792	49.565	44.627
Total			53499675	3956805	100.000	100.000

7na
(1% *ee*)
[Table S1, entry 3]:

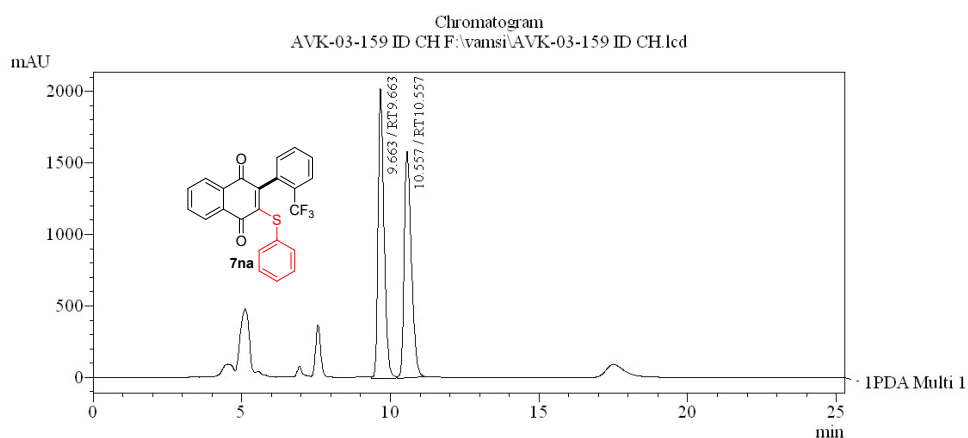


Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

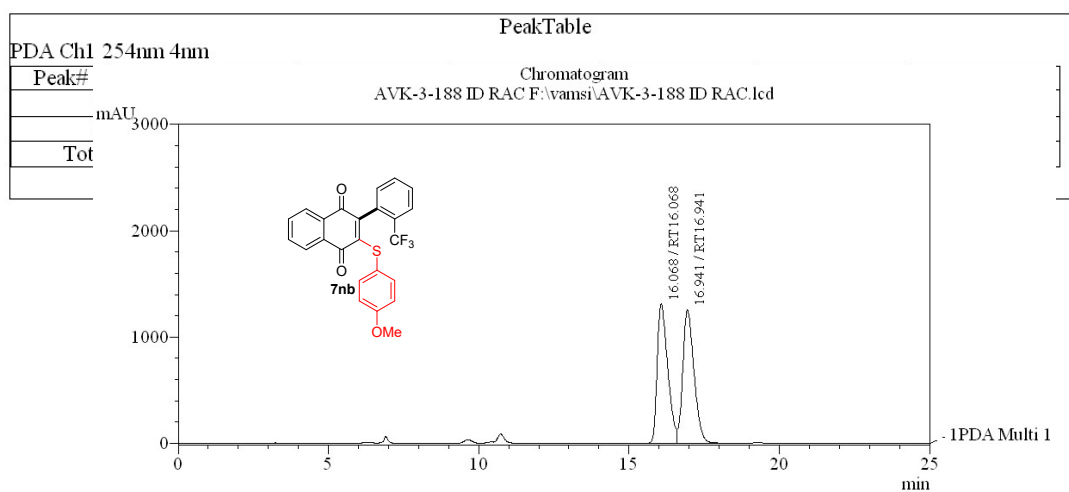
PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT9.016	9.016	19688291	1418094	49.169	53.267
2	RT9.843	9.843	20354121	1244128	50.831	46.733
Total			40042413	2662222	100.000	100.000

Chiral
(1% *ee*)
[Table S1, entry 3]:

Chiral **7na** (2% ee) [Table S1, entry 4]:



Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,



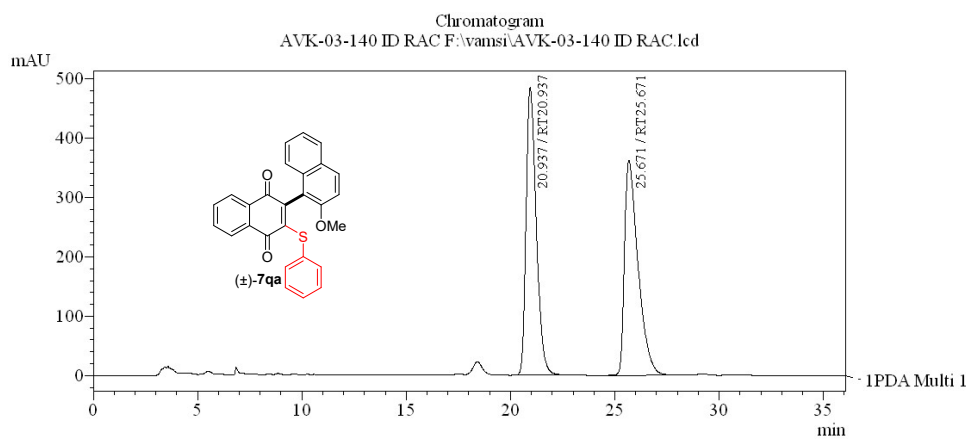
Racemic

Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

(±)-**7nb**:

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT16.068	16.068	31951879	1310647	49.316	51.076
2	RT16.941	16.941	32837559	1255442	50.684	48.924
Total			64789438	2566089	100.000	100.000

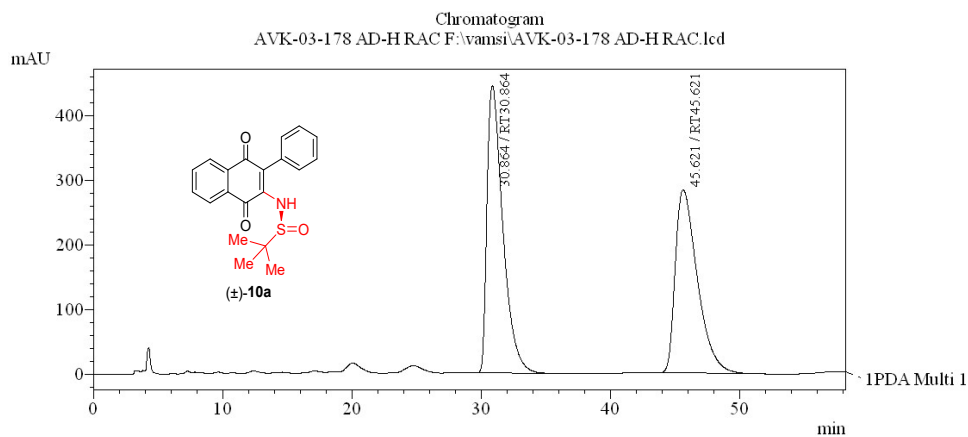
Racemic (\pm)-7qa:



Chiralpak ID, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0 mL/min,

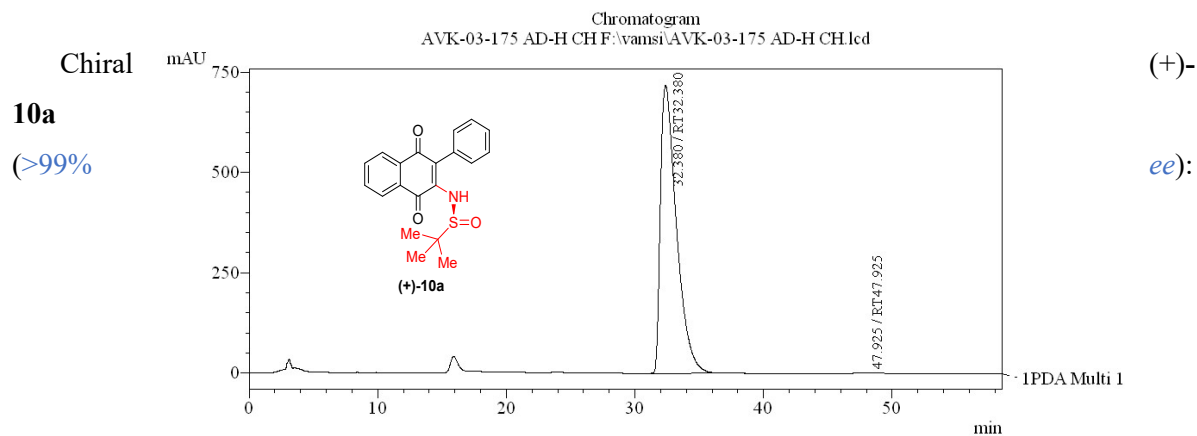
PeakTable						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT20.937	20.937	16446164	485143	50.122	57.242
2	RT25.671	25.671	16366176	362392	49.878	42.758
Total			32812340	847535	100.000	100.000

Racemic (\pm)-**10a**:



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

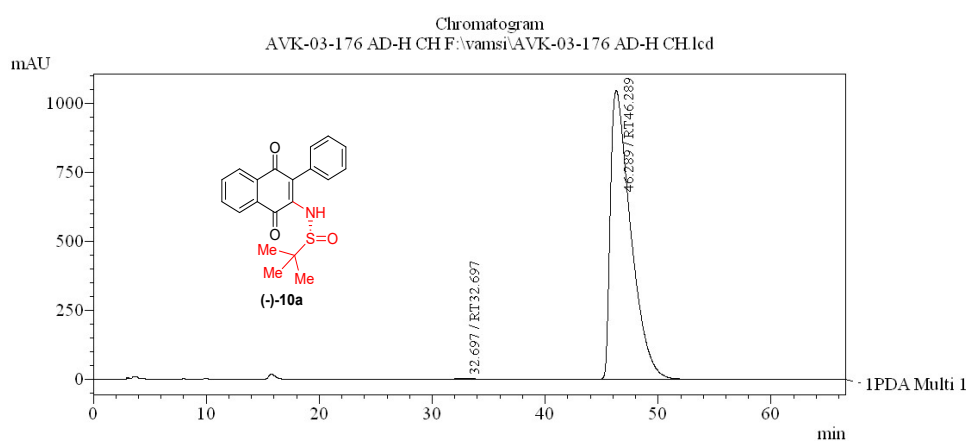
PeakTable						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT30.864	30.864	37868786	445101	52.812	61.043
2	RT45.621	45.621	33835855	284062	47.188	38.957
Total			71704642	729163	100.000	100.000



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

PeakTable						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT32.380	32.380	62181933	717156	99.787	99.768
2	RT47.925	47.925	132891	1665	0.213	0.232
Total			62314824	718820	100.000	100.000

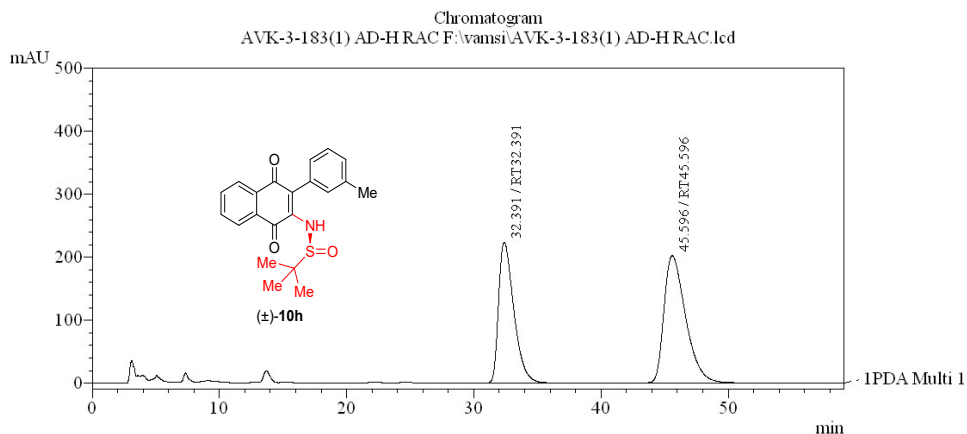
Chiral (-)-**10a** (>99% ee):



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

PeakTable						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT32.697	32.697	244402	3471	0.187	0.331
2	RT46.289	46.289	130575989	1045182	99.813	99.669
Total			130820391	1048653	100.000	100.000

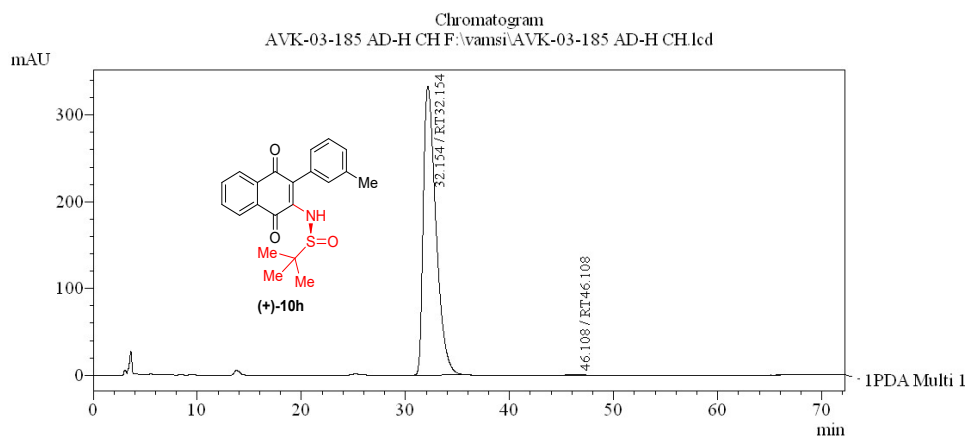
Racemic (\pm)-**10h**:



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT32.391	32.391	18523697	223563	43.845	52.558
2	RT45.596	45.596	23724710	201800	56.155	47.442
Total			42248407	425363	100.000	100.000

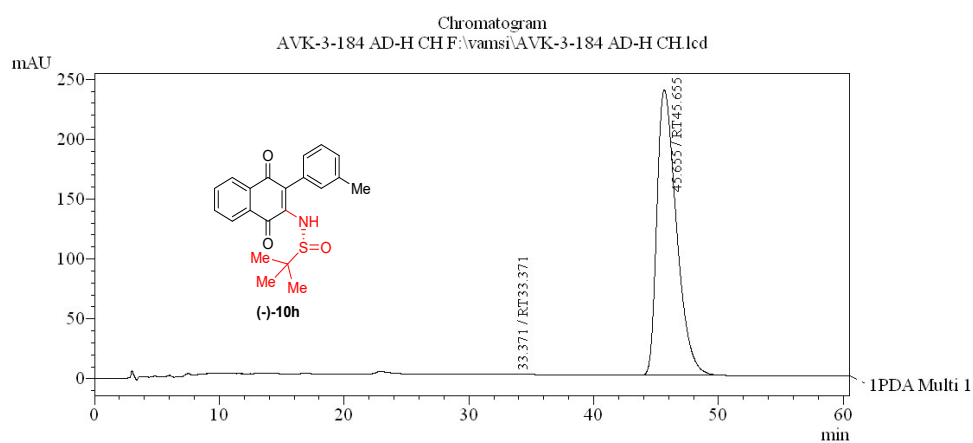
Chiral (+)-10h (>99% ee):



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

PeakTable						
PDA Ch1 254nm 4nm						
Peak#	Name	Ret. Time	Area	Height	Area %	Height %
1	RT32.154	32.154	28067308	332796	99.825	99.857
2	RT46.108	46.108	49334	477	0.175	0.143
Total			28116642	333273	100.000	100.000

Chiral (-)-**10h** (>99% ee):



Chiralpak AD-H, Hexane/*i*-PrOH = 90:10, mL/Min, Flow Rate 1.0

PeakTable							
PDA Ch1 254nm 4nm							
Peak#	Name	Ret. Time	Area	Height	Area %	Height %	
1	RT33.371	33.371	32449	432	0.125	0.181	
2	RT45.655	45.655	25853392	238156	99.875	99.819	
Total			25885840	238588	100.000	100.000	