

Supporting Information

for

Chemoenzymatic Synthesis of Optically Active Alcohols Possessing 1,2,3,4-Tetrahydroquinoline Moiety Employing Lipases or Variants of the Acyltransferase from *Mycobacterium smegmatis*

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Table S1. List of commercial enzyme preparations employed in these studies.

Enzyme and its origin (microorganism/tissue)	Enzyme preparation ^[a] (brand name)	Usage form of enzyme preparation	Enzyme specified activity	Commercial supplier (Cat. No.)
Lipase from <i>Candida antarctica</i> B (CAL-B)	Novozym 435	immobilized on the macroporous acrylic resin [poly (methyl methacrylate-co-butyl methacrylate)]	>10000 U/g or 10 PLU/mg, water content 1.4%	Novozymes A/S (Bagsvaerd, Denmark)
	Novozym 435-STREM	immobilized on a hydrophobic carrier (acrylic resin)	10000 PLU/g	STREM Chemicals, INC. (cat. nr.: 06-3123) in collaboration with Novozymes A/S
	Lipozyme 435	immobilized on Lewatit VP OC 1600	unspecified	Novozymes A/S (Bagsvaerd, Denmark)
	Chirazyme L-2, c.-f., C2, Lyo.	immobilized on the carrier-fixed on (carrier 2)	150 kU	Roche
	Chirazyme L-2, c.-f., C3, Lyo.	immobilized on the carrier-fixed on (carrier 3)	150 kU	Roche
Lipase from <i>Burkholderia cepacia</i> (formerly <i>Pseudomonas cepacia</i>)	Amano PS	native	>23.000 U/g	Amano Pharmaceutical Co., Ltd.
	Amano PS-IM	immobilized on diatomite	500 U/g	Amano Pharmaceutical Co., Ltd.
Lipase from <i>Pseudomonas fluorescens</i>	Amano AK	native	>20.000 U/g	Amano Pharmaceutical Co., Ltd.
Lipase from <i>Thermomyces lanuginosus</i>	Lipozyme TL IM	immobilized on a non-compressible silica gel carrier into an immobilized granulate (a silica granulated)	170 IUN/g	Novozymes A/S (Bagsvaerd, Denmark)
Lipase from <i>Rhizomucor miehei</i>	Lipozyme RM IM	immobilized on macroporous anion-exchange resin	150 IU/g	Novozymes A/S (Bagsvaerds, Denmark)
Lipase from <i>Candida rugosa</i>	Lipase from <i>Candida rugosa</i> Type VII	native	≥700 unit/mg	Sigma-Aldrich (cat. nr.: L1754)
Lipase from wheat germ	Lipase from wheat germ Type I	native	5-15 units/mg	Sigma-Aldrich (cat. nr.: L3001)
Lipase from <i>Rhizopus niveus</i>	Lipase from <i>Rhizopus niveus</i>	native	≥1.5 U/mg	Sigma-Aldrich (cat. nr.: 62310)

[a] All commercial formulations of enzymes studied herein were used without any pretreatment.

Table S2. The results of specific rotation values for the EKR products.







Product of EKR	ee [%]	Measured specific rotation $[\alpha]_D$	Literature specific rotation $[\alpha]_D^{\text{lit.}}$
 (S)-(+)- 2a	98	$[\alpha]_D^{26.0} = +22.75$ (c 1.06, CHCl ₃)	Lack of data
 (R)-(-)- 3a	99	$[\alpha]_D^{28.0} = +4.90$ (c 1.02, CHCl ₃)	Lack of data
 (S)-(+)- 2b	>99	$[\alpha]_D^{28.0} = +19.42$ (c 1.03, CHCl ₃)	Lack of data
 (R)-(-)- 3b	98	$[\alpha]_D^{28.0} = +4.85$ (c 1.03, CHCl ₃)	Lack of data
 (S)-(+)- 2c	>99	$[\alpha]_D^{28.0} = +75.12$ (c 1.02, CHCl ₃)	Lack of data
 (R)-(-)- 3c	94	$[\alpha]_D^{28.0} = +23.90$ (c 1.02, CHCl ₃)	Lack of data

Table S3. Analytical separation conditions of studied compounds by GC column.

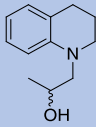
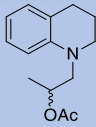
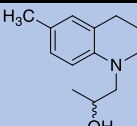
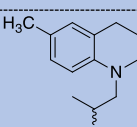
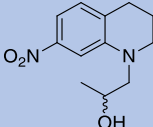
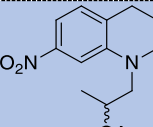
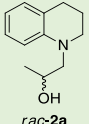
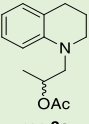
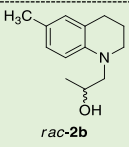
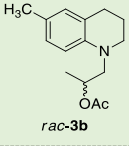
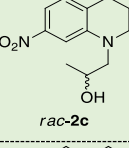
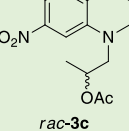
Compound	Temperature program [°C]	Retention time [min]
 $rac-2a$	150–260 (10 °C/min)	6.04
 $rac-3a$		6.86
 $rac-2b$	150–260 (10 °C/min)	6.71
 $rac-3b$		7.61
 $rac-2c$	200–260 (10 °C/min)	7.28
 $rac-3c$		7.50

Table S4. HPLC analytical separation conditions of racemic alcohols and acetates.

Compound	HPLC Column	Mobile Phase	Flow Rate [mL/min] / Pressure [MPa]	Detection [nm] / Temperature [°C]	Retention Time [min]
		<i>n</i> -Hexane/IPA [v/v] ^[a]			
 <i>rac-2a</i>	Chiralcel OJ-H	90:10	0.8 / 3.6	260 / 30	8.495 (<i>S</i>) and 9.120 (<i>R</i>)
 <i>rac-3a</i>	Chiralcel OJ-H	90:10	0.8 / 3.6	260 / 30	7.369 (<i>S</i>) and 7.955 (<i>R</i>)
 <i>rac-2b</i>	Chiralcel OJ-H	97:3	0.8 / 3.4	260 / 30	15.023 (<i>S</i>) and 16.400 (<i>R</i>)
 <i>rac-3b</i>	Chiralcel OJ-H	97:3	0.8 / 3.4	260 / 30	8.831 (<i>S</i>) and 9.866 (<i>R</i>)
 <i>rac-2c</i>	Chiralcel OD-H	98:2	0.8 / 3.5	260 / 30	38.392 (<i>S</i>) and 41.245 (<i>R</i>)
 <i>rac-3c</i>	Chiralcel OD-H	99:1	0.7 / 3.0	260 / 30	23.062 (<i>S</i>) and 24.774 (<i>R</i>)

^[a] IPA states for 2-PrOH (propan-2-ol).

Table S5. Crystal data and structure refinement parameters for (S)-(+)-**2c**

Compound	(S)-(+)- 2c
Formula	C ₁₂ H ₁₆ N ₂ O ₃
$D_{calc.}/\text{g cm}^{-3}$	1.342
μ/mm^{-1}	0.803
Formula Weight	236.27
Size/ mm^3	0.83×0.50×0.17
T/K	293
Crystal System	monoclinic
Flack Parameter	0.03(9)
Space Group	$P2_1$
$a/\text{\AA}$	9.1028(2)
$b/\text{\AA}$	5.18900(10)
$c/\text{\AA}$	12.4899(3)
$\alpha/^\circ$	90
$\beta/^\circ$	97.670(2)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	584.68(2)
Z	2
Z'	1
Wavelength/ \AA	1.54184
Radiation type	Cu K α
$\Theta_{min}/^\circ$	3.571
$\Theta_{max}/^\circ$	67.002
Measured Refl's.	18271
Indep't Refl's	2086
Refl's $I \geq 2\sigma(I)$	1998
R_{int}	0.0673
Parameters	164
Restraints	5
Largest Peak	0.122
Deepest Hole	-0.125
GooF	1.043
wR_2 (all data)	0.0773
wR_2	0.0760
R_1 (all data)	0.0305
R_1	0.0290

Table S6. Atomic Occupancies for carbon atoms that are not fully occupied in (S)-(+)-**2c**.

Atom	Occupancy
C2	0.951(5)
C2A	0.049(5)

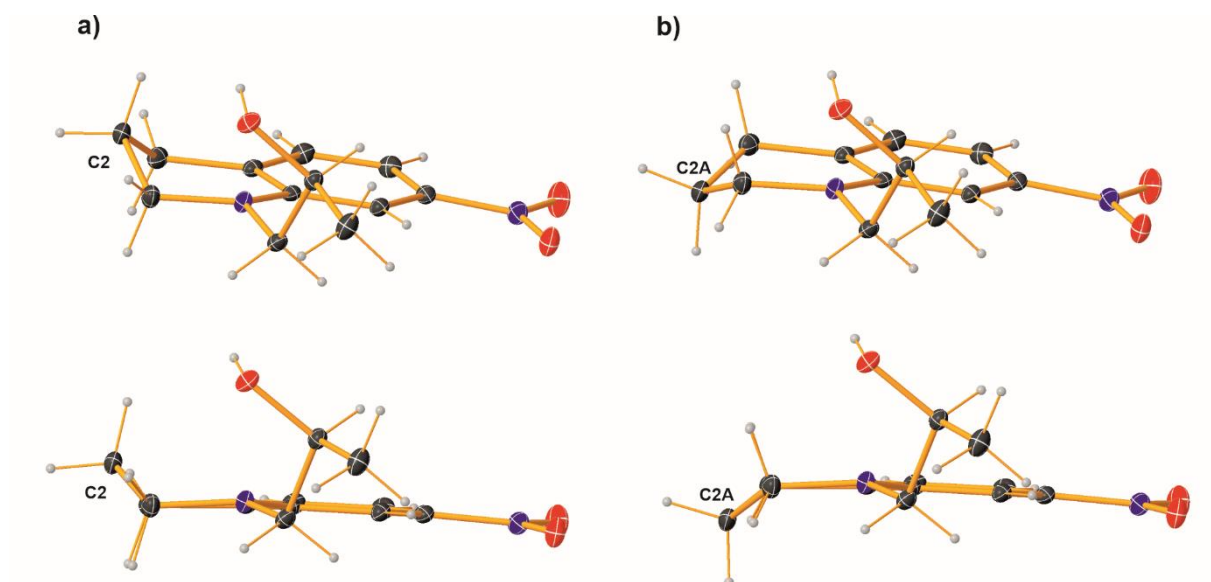


Figure S1. The geometry of two conformations observed for (*S*)-(+)-**2c** molecule in the solid state a) primary (95.1%), b) secondary (4.9%)

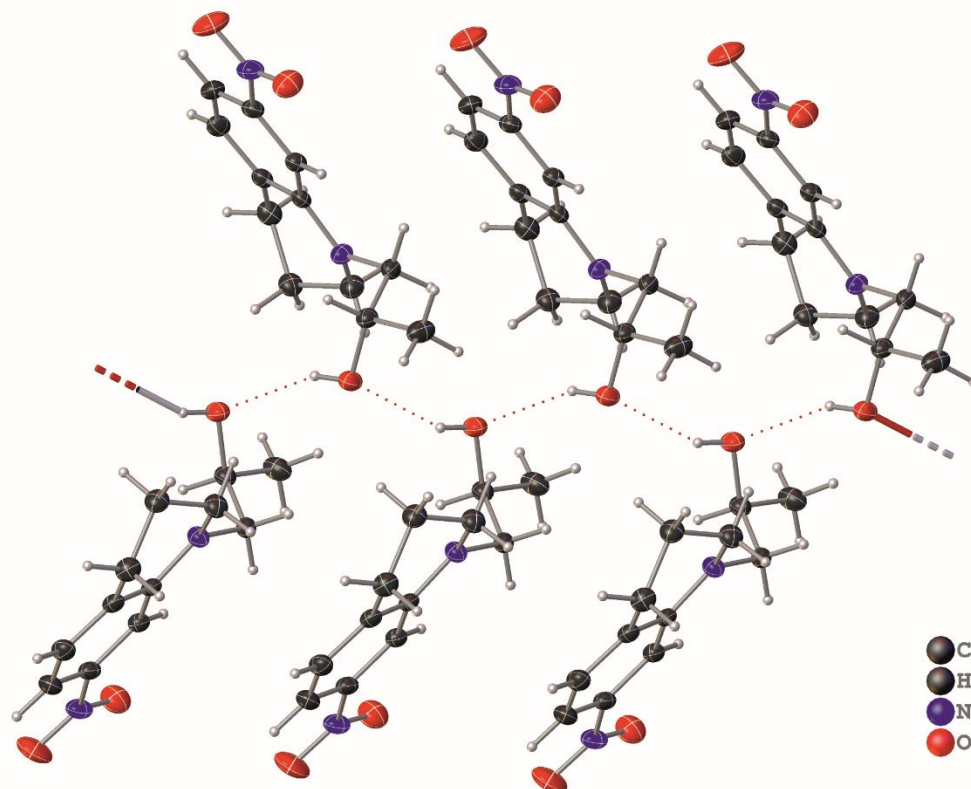


Figure S2. Crystal packing of (*S*)-(+)-**2c** showing H-bond topology.

Table S7. Hydrogen Bond information for (*S*)-(+)-**2c**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	O1 ¹	0.82(3)	2.23(3)	2.9827(16)	154(2)

¹1-x,1/2+y,2-z

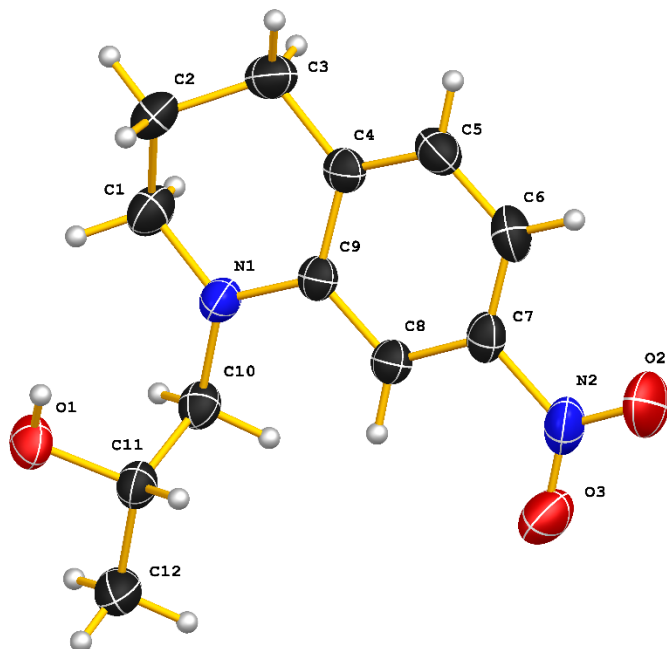


Figure S3. Crystal structure of (*S*)-(+)-**2c** with the atom numbering scheme.

Table S8. Bond Lengths in Å for (*S*)-(+)-**2c**.

Atom	Atom	Length/Å
O1	C11	1.438(2)
O2	N2	1.220(3)
O3	N2	1.216(3)
N1	C1	1.457(2)
N1	C9	1.384(2)
N1	C10	1.454(2)
N2	C7	1.470(3)
C1	C2	1.500(3)
C1	C2A	1.499(12)
C3	C4	1.506(3)
C3	C2	1.512(3)
C3	C2A	1.492(12)
C4	C5	1.381(3)
C4	C9	1.417(3)
C5	C6	1.384(3)
C6	C7	1.374(3)
C7	C8	1.383(3)
C8	C9	1.399(3)
C10	C11	1.518(3)
C11	C12	1.508(3)

Table S9. Bond Angles in ° for (*S*)-(+)-**2c**.

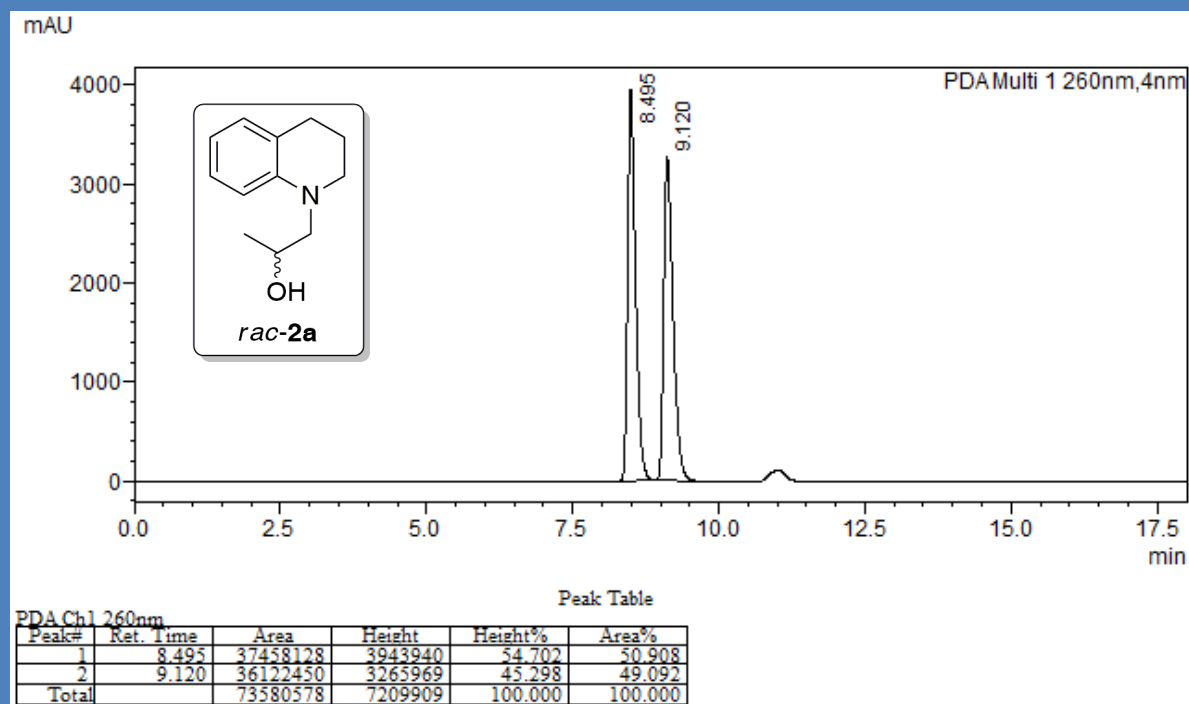
Atom	Atom	Atom	Angle/°
C9	N1	C1	120.14(15)
C9	N1	C10	121.56(15)
C10	N1	C1	115.52(16)
O2	N2	C7	118.3(2)
O3	N2	O2	122.6(2)
O3	N2	C7	119.10(18)
N1	C1	C2	111.82(18)
N1	C1	C2A	118.4(12)
C4	C3	C2	110.55(16)
C2A	C3	C4	115.1(12)
C5	C4	C3	120.37(18)
C5	C4	C9	119.73(18)
C9	C4	C3	119.90(18)
C4	C5	C6	122.38(19)
C7	C6	C5	117.02(19)
C6	C7	N2	118.34(18)
C6	C7	C8	123.15(18)
C8	C7	N2	118.50(19)
C7	C8	C9	119.62(17)
N1	C9	C4	120.62(16)
N1	C9	C8	121.38(16)
C8	C9	C4	117.99(16)
N1	C10	C11	114.01(17)
O1	C11	C10	110.85(15)
O1	C11	C12	106.77(16)
C12	C11	C10	110.98(19)
C1	C2	C3	109.57(19)
C3	C2A	C1	110.8(10)

Table S10. Torsion Angles in ° for (*S*)-(+)-**2c**.

Atom	Atom	Atom	Atom	Angle/°
O2	N2	C7	C6	2.8(3)
O2	N2	C7	C8	-177.9(2)
O3	N2	C7	C6	-176.4(2)
O3	N2	C7	C8	2.9(3)
N1	C1	C2	C3	57.4(2)
N1	C1	C2A	C3	-41(3)
N1	C10	C11	O1	61.1(2)
N1	C10	C11	C12	179.59(17)
N2	C7	C8	C9	-177.57(17)
C1	N1	C9	C4	8.2(3)
C1	N1	C9	C8	-173.15(18)
C1	N1	C10	C11	-103.4(2)
C3	C4	C5	C6	-176.5(2)
C3	C4	C9	N1	-5.1(3)
C3	C4	C9	C8	176.19(18)
C4	C3	C2	C1	-53.5(3)
C4	C3	C2A	C1	42(3)
C4	C5	C6	C7	-0.4(3)
C5	C4	C9	N1	175.21(18)
C5	C4	C9	C8	-3.5(3)
C5	C6	C7	N2	177.20(19)
C5	C6	C7	C8	-2.1(3)
C6	C7	C8	C9	1.7(3)
C7	C8	C9	N1	-177.56(18)
C7	C8	C9	C4	1.1(3)
C9	N1	C1	C2	-34.9(3)
C9	N1	C1	C2A	16.0(16)
C9	N1	C10	C11	95.5(2)
C9	C4	C5	C6	3.2(3)
C10	N1	C1	C2	163.67(18)
C10	N1	C1	C2A	-145.4(15)
C10	N1	C9	C4	168.47(17)
C10	N1	C9	C8	-12.9(3)
C2	C3	C4	C5	-151.9(2)
C2	C3	C4	C9	28.4(3)
C2A	C3	C4	C5	158.0(14)
C2A	C3	C4	C9	-21.7(15)

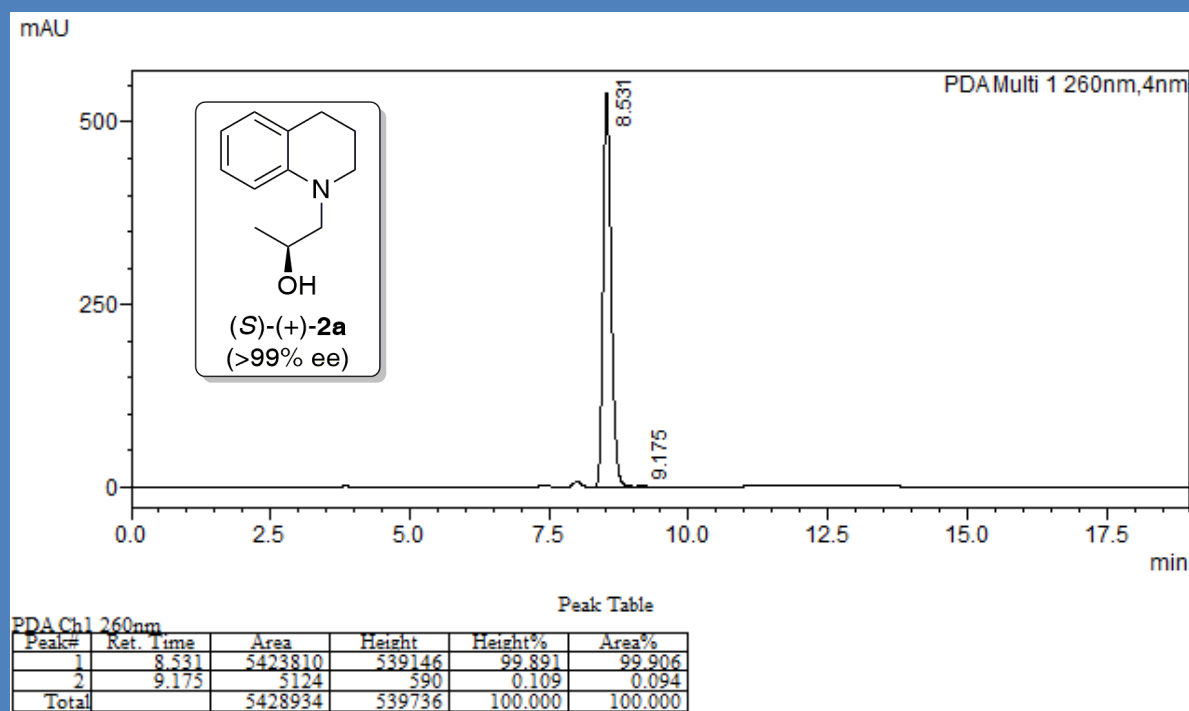
HPLC of *rac*-2a on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); f=0.8 mL/min; λ =260 nm; *p*=3.6 MPa



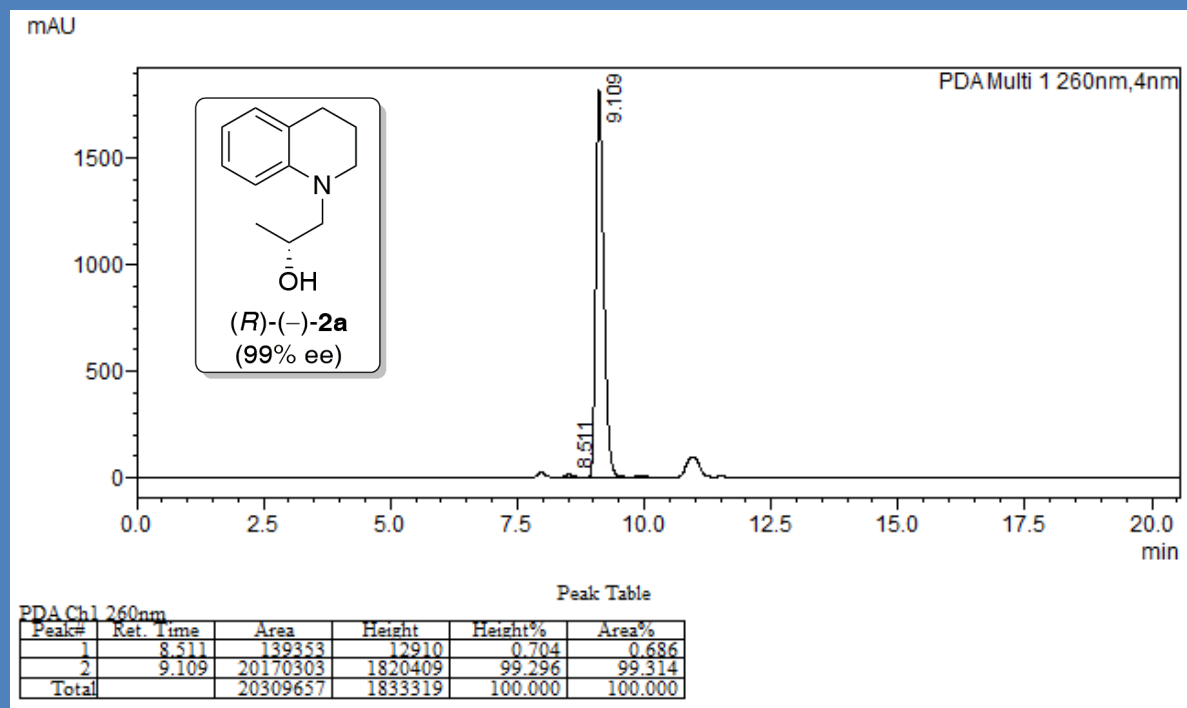
HPLC of (*S*)-(+)-2a after lipase-catalyzed KR of *rac*-2a on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); f=0.8 mL/min; λ =260 nm; *p*=3.6 MPa



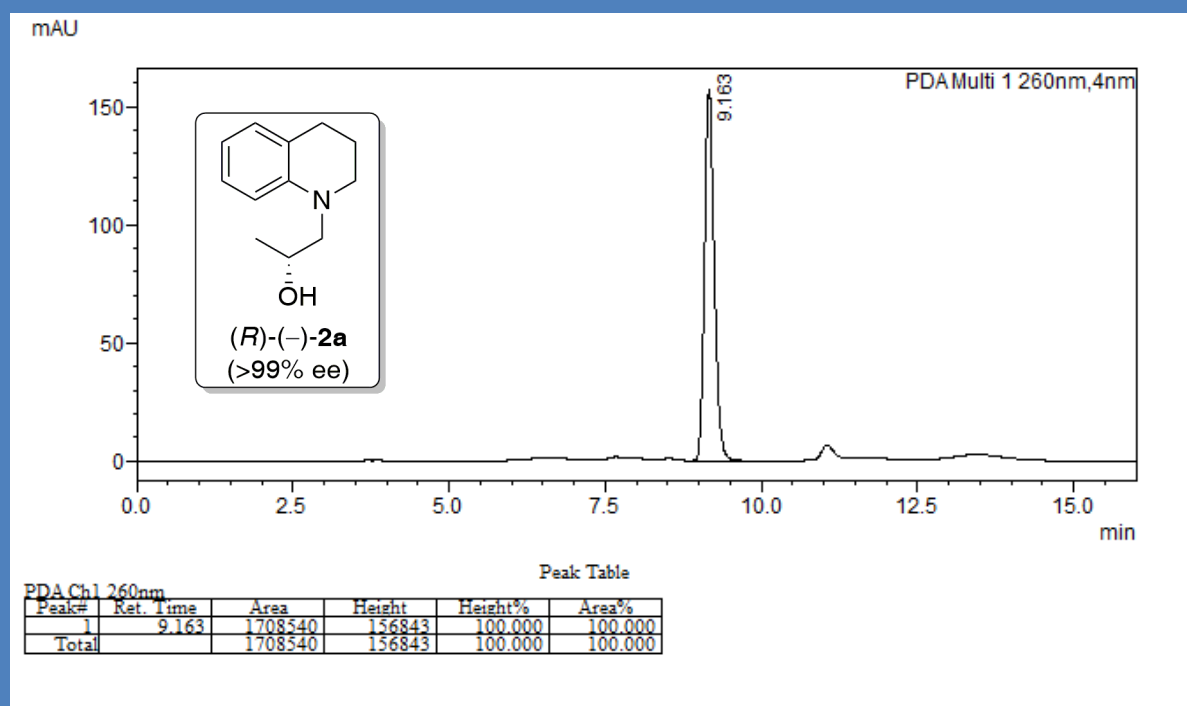
HPLC of (*R*)-(-)-2a after K₂CO₃-catalyzed hydrolysis of (*R*)-(+)-3a on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); f=0.8 mL/min; λ=260 nm; p=3.6 MPa



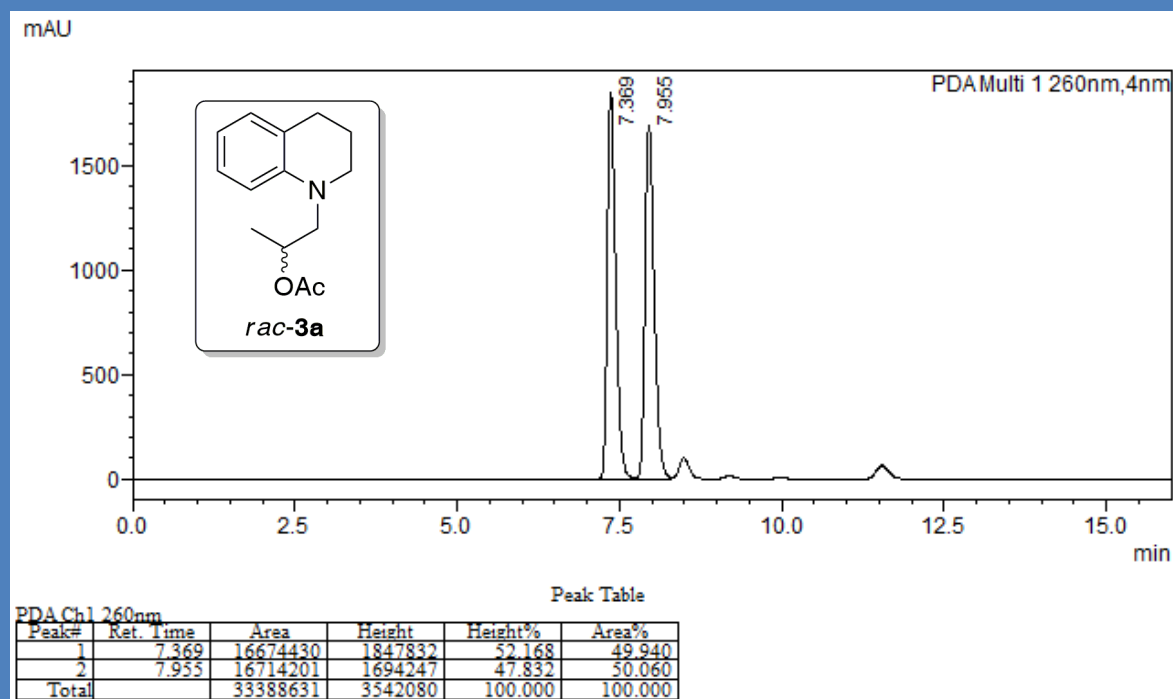
HPLC of (*R*)-(-)-2a obtained using (*R*)-(+)-propylene oxide on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); f=0.8 mL/min; λ=260 nm; p=3.6 MPa



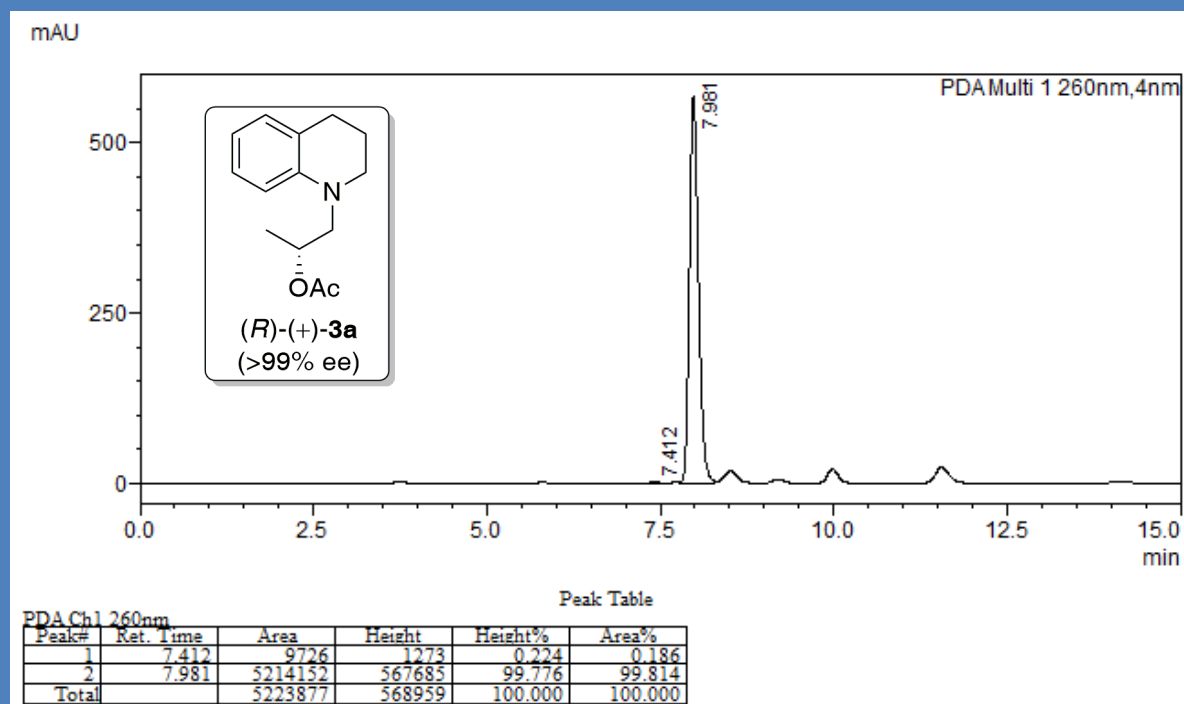
HPLC of *rac*-3a on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.6 MPa



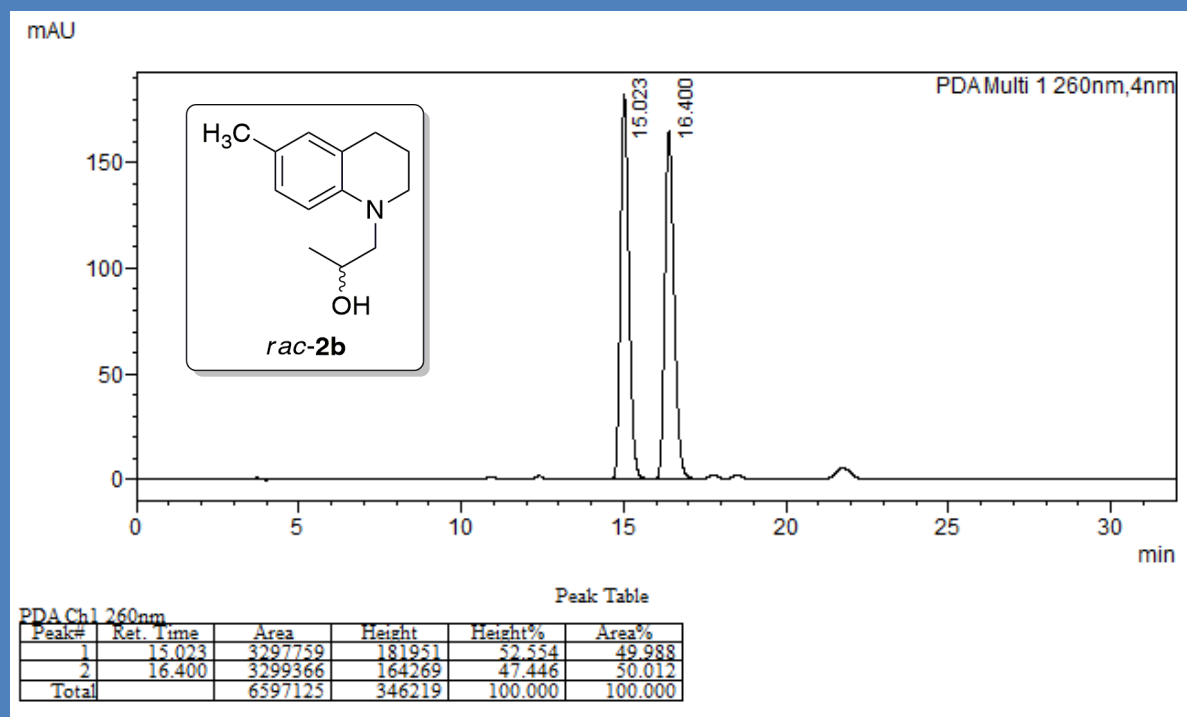
HPLC of (*R*)-(+)-3a after lipase-catalyzed KR of *rac*-2a on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.6 MPa



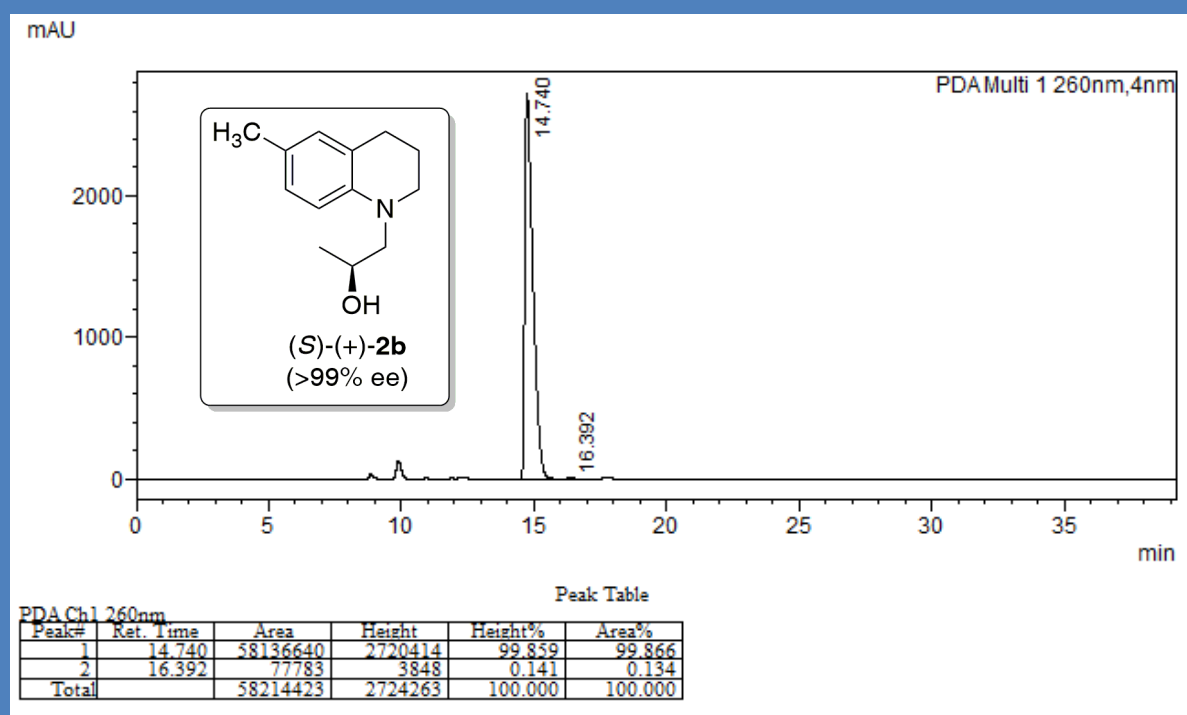
HPLC of *rac*-2b on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.4 MPa



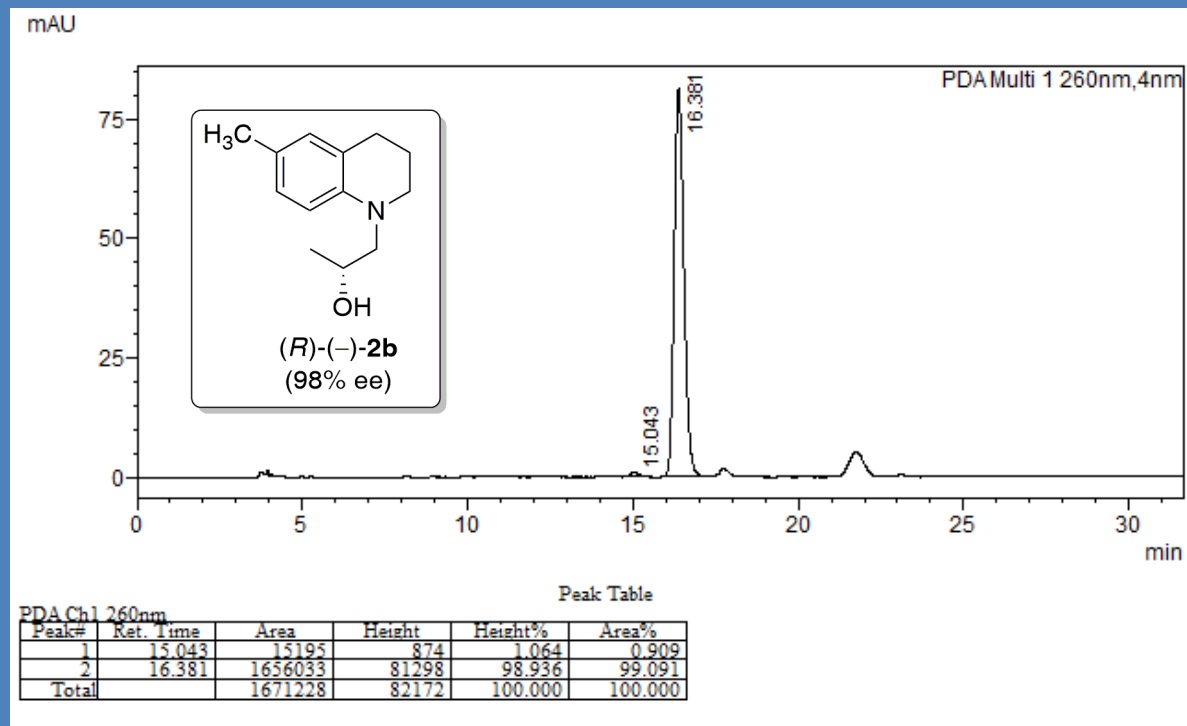
HPLC of (*S*)-(+)-2b after lipase-catalyzed KR of *rac*-2b on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.4 MPa



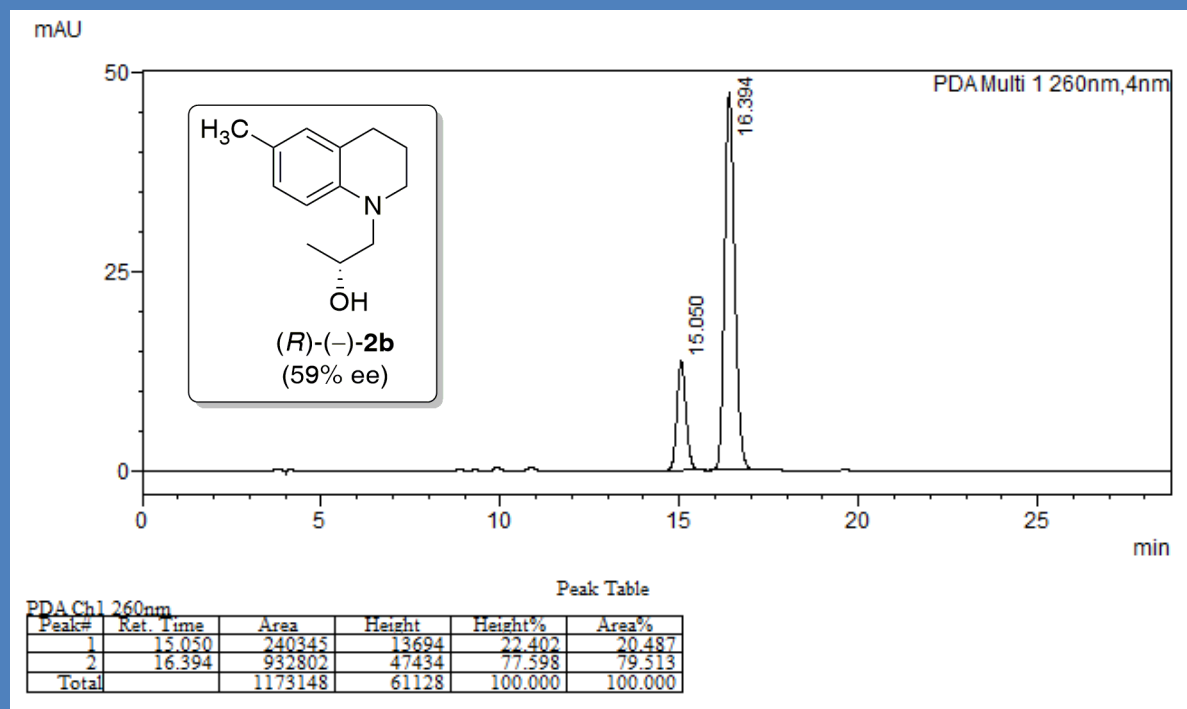
HPLC of (*R*)-(-)-2b after K₂CO₃-catalyzed hydrolysis of (*R*)-(+)-3b on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); f=0.8 mL/min; λ=260 nm; p=3.4 MPa



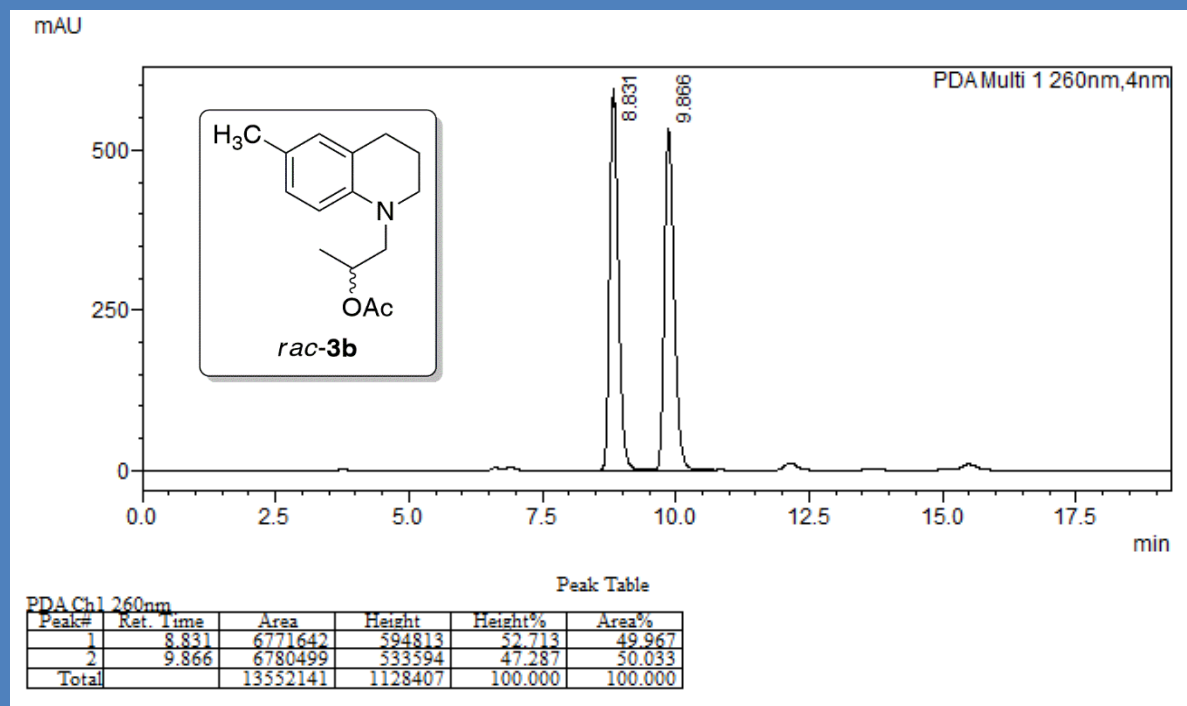
HPLC of (*R*)-(-)-2b obtained using (*R*)-(+)-propylene oxide on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); f=0.8 mL/min; λ=260 nm; p=3.4 MPa



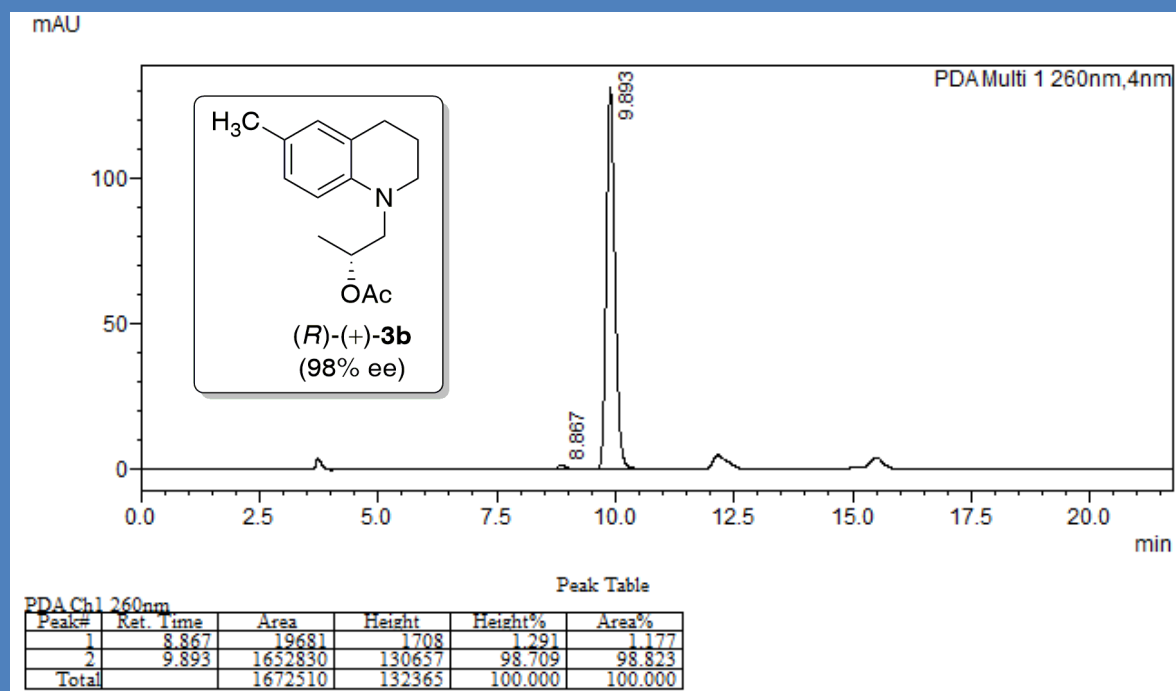
HPLC of *rac*-3b on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.4 MPa



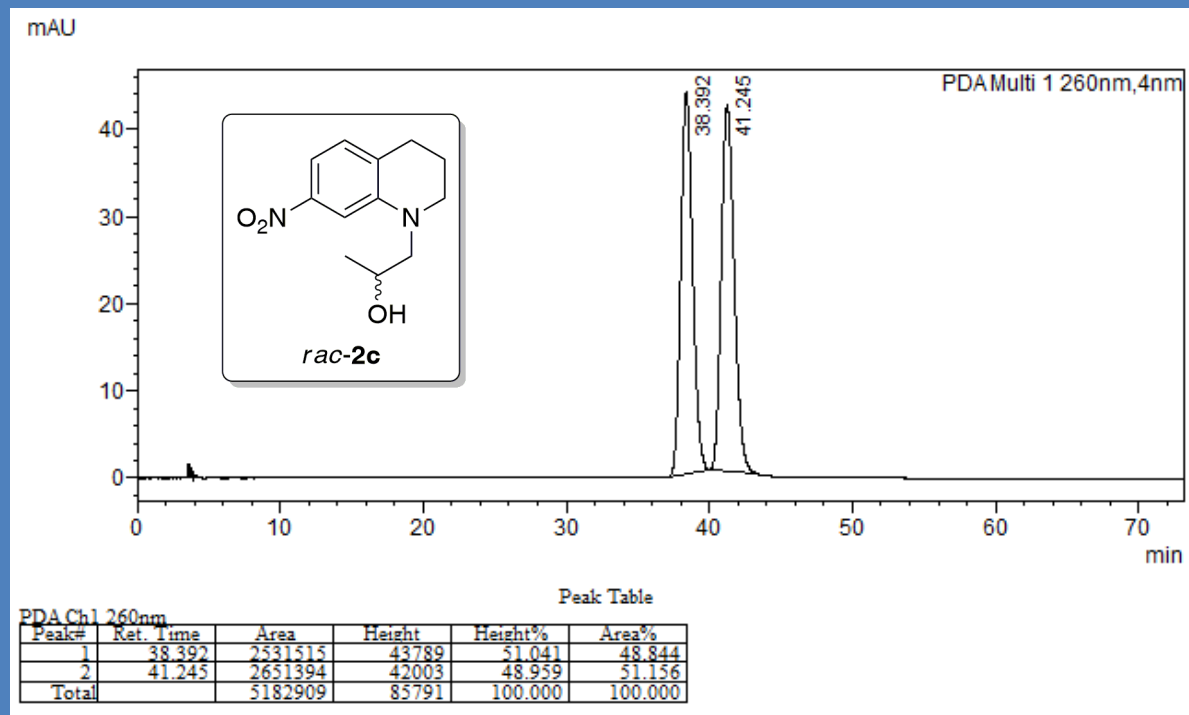
HPLC of (*R*)-(+)-3b after lipase-catalyzed KR of *rac*-2b on Chiralcel OJ-H at 30 °C

Conditions: *n*-hexane-2-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.4 MPa



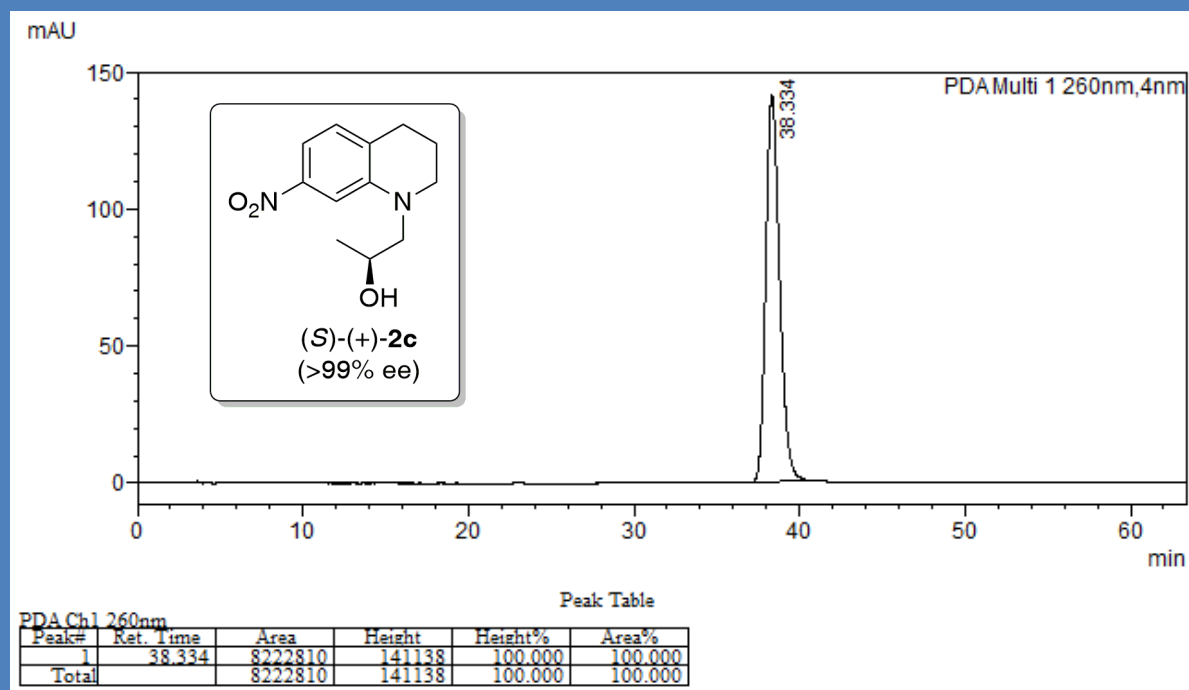
HPLC of *rac*-2c on Chiralcel OD-H at 30 °C

Conditions: *n*-hexane-2-PrOH (98:2, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.5 MPa



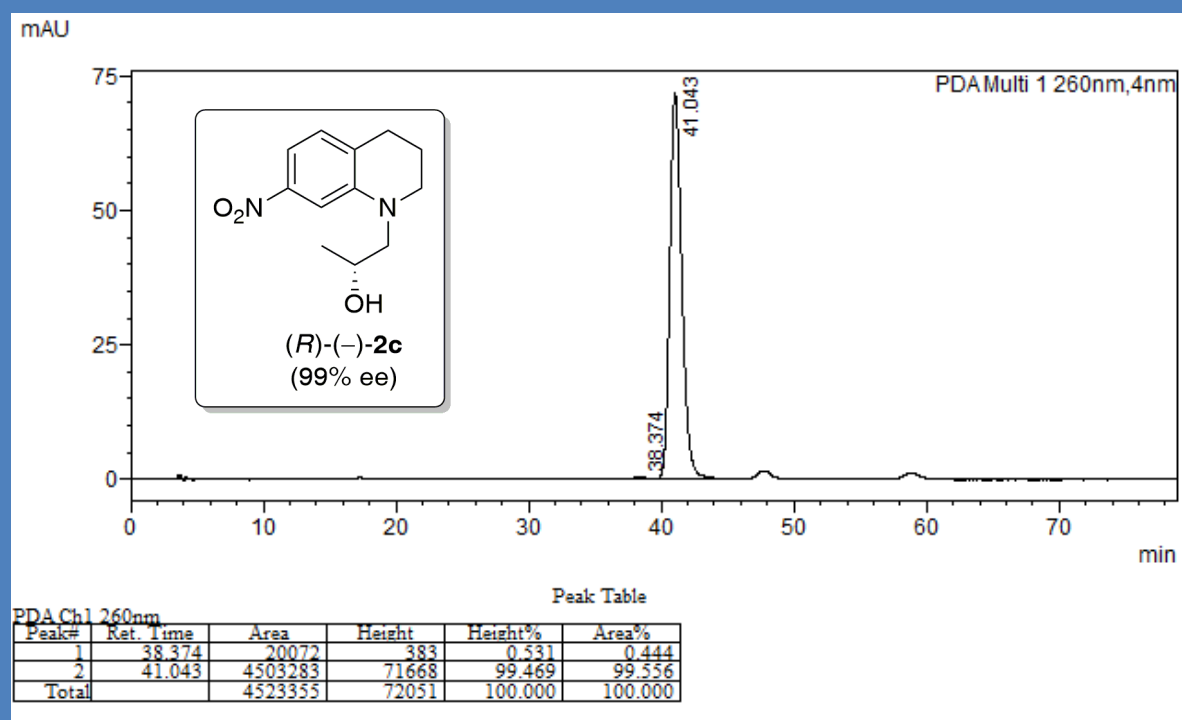
HPLC of (*S*)-(+)-2c after lipase-catalyzed KR of *rac*-2c on Chiralcel OD-H at 30 °C

Conditions: *n*-hexane-2-PrOH (98:2, v/v); *f*=0.8 mL/min; λ =260 nm; *p*=3.5 MPa



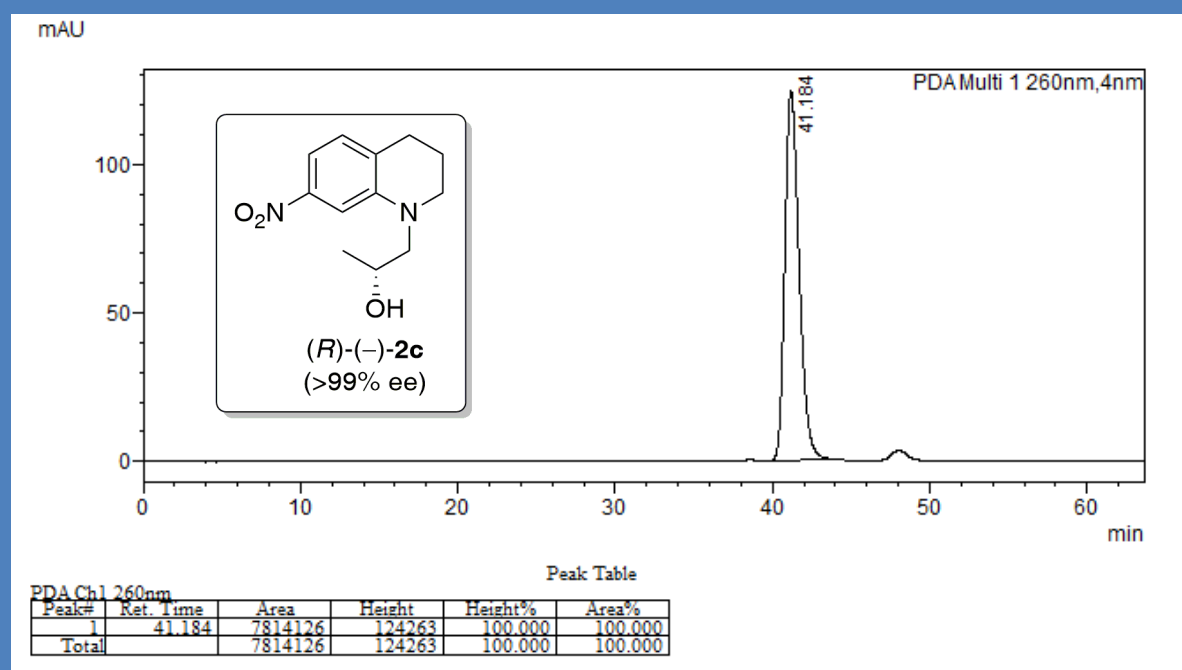
HPLC of (*R*)-(-)-2c after K₂CO₃-catalyzed hydrolysis of (*R*)-(+)-3c on Chiralcel OD-H at 30 °C

Conditions: *n*-hexane-2-PrOH (98:2, v/v); f=0.8 mL/min; λ=260 nm; p=3.5 MPa



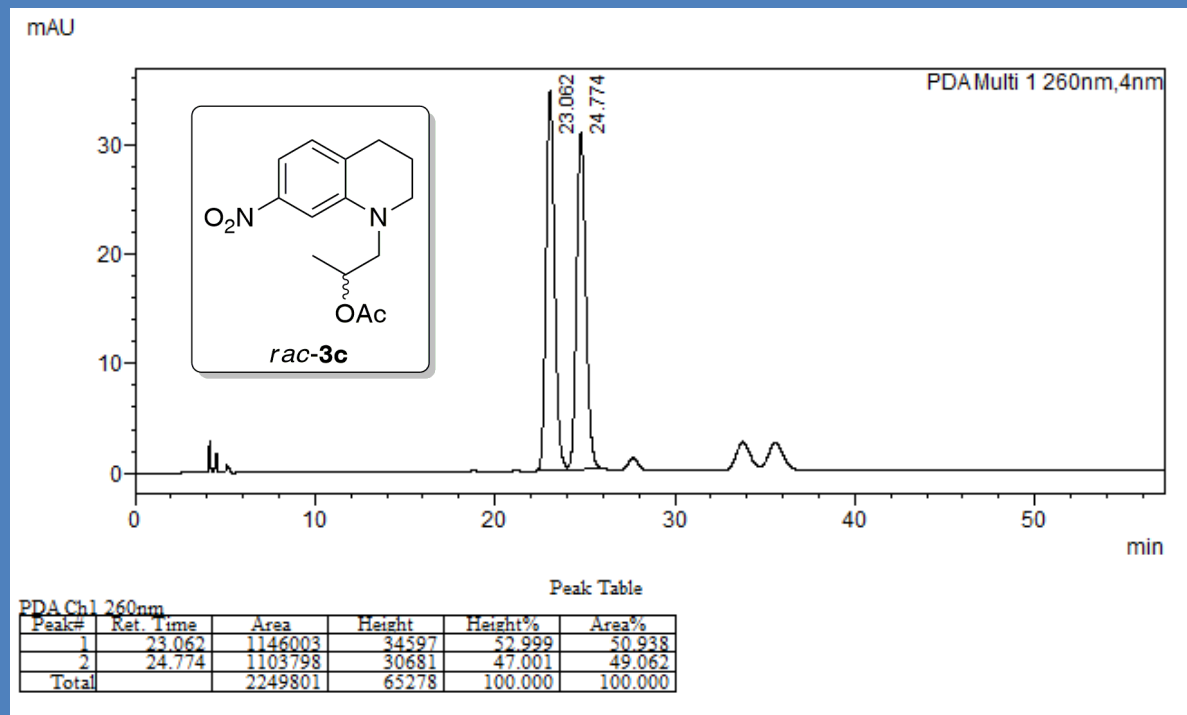
HPLC of (*R*)-(-)-2c obtained using (*R*)-(+)-propylene oxide on Chiralcel OD-H at 30 °C

Conditions: *n*-hexane-2-PrOH (98:2, v/v); f=0.8 mL/min; λ=260 nm; p=3.5 MPa



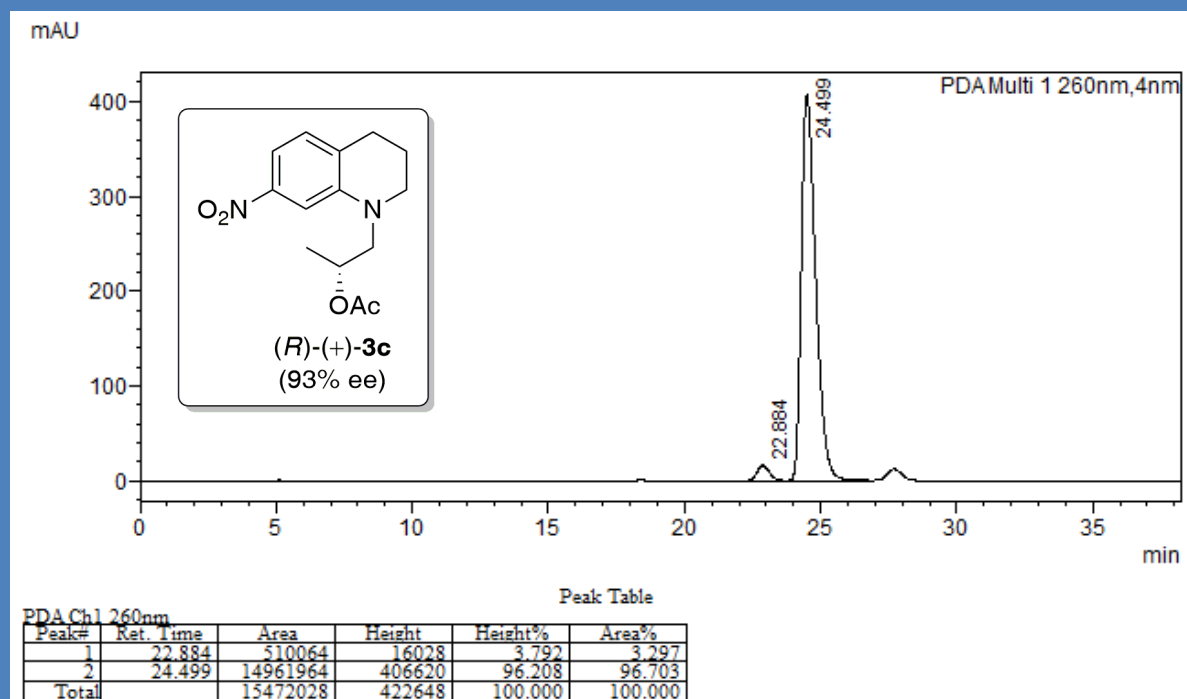
HPLC of *rac*-3c on Chiralcel OD-H at 30 °C

Conditions: *n*-hexane-2-PrOH (99:1, v/v); *f*=0.7 mL/min; λ =260 nm; *p*=3.0 MPa

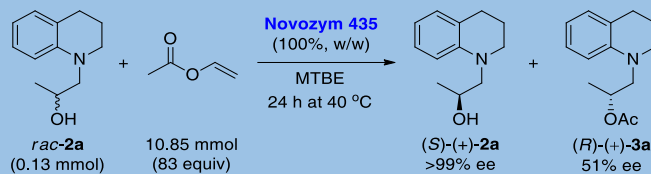


HPLC of (*R*)-(+)-3c after lipase-catalyzed KR of *rac*-2c on Chiralcel OD-H at 30 °C

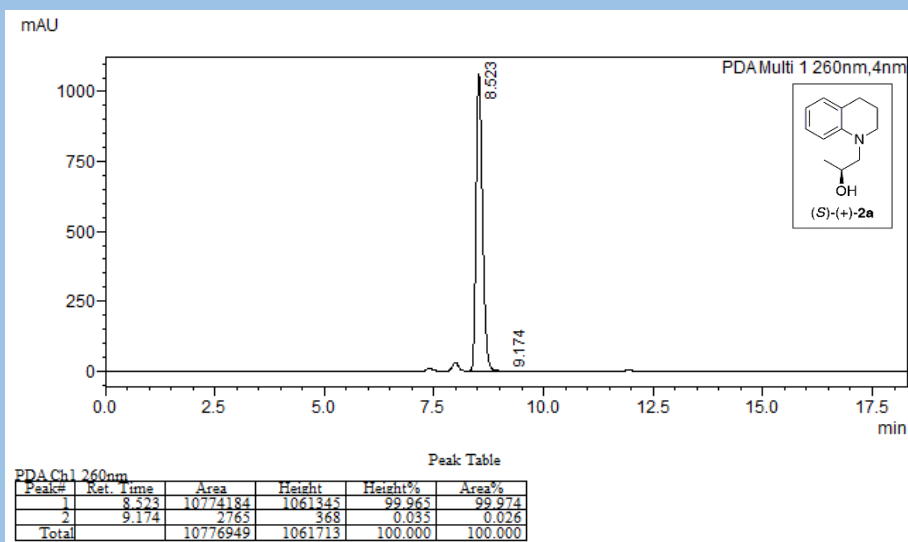
Conditions: *n*-hexane-2-PrOH (99:1, v/v); *f*=0.7 mL/min; λ =260 nm; *p*=3.0 MPa



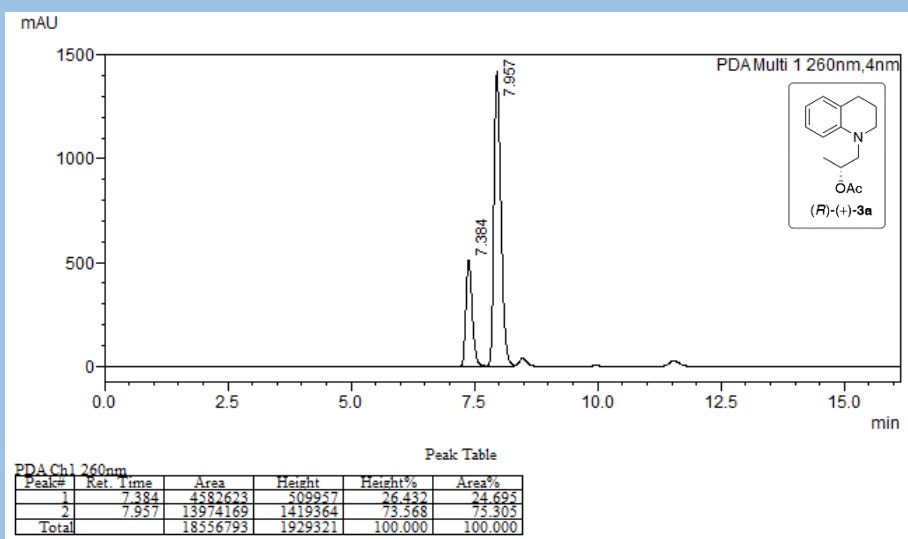
HPLC analysis for the subsequent biocatalytic reaction:



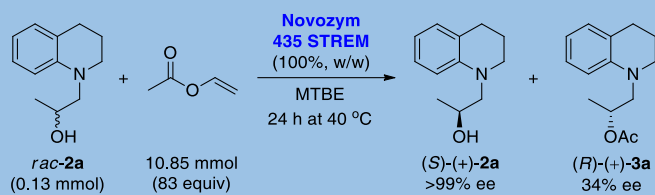
HPLC conditions [for (*S*)-**2a**]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



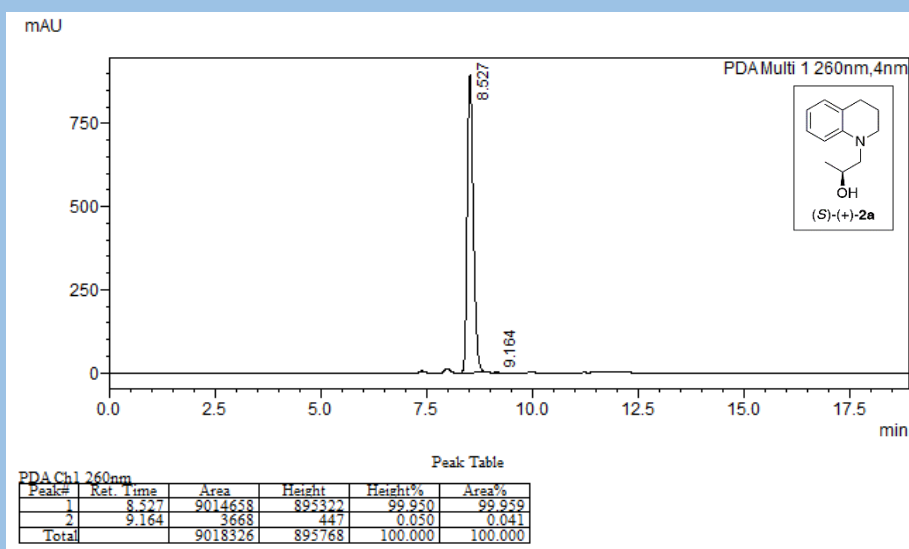
HPLC conditions [for (*R*)-**3a**]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



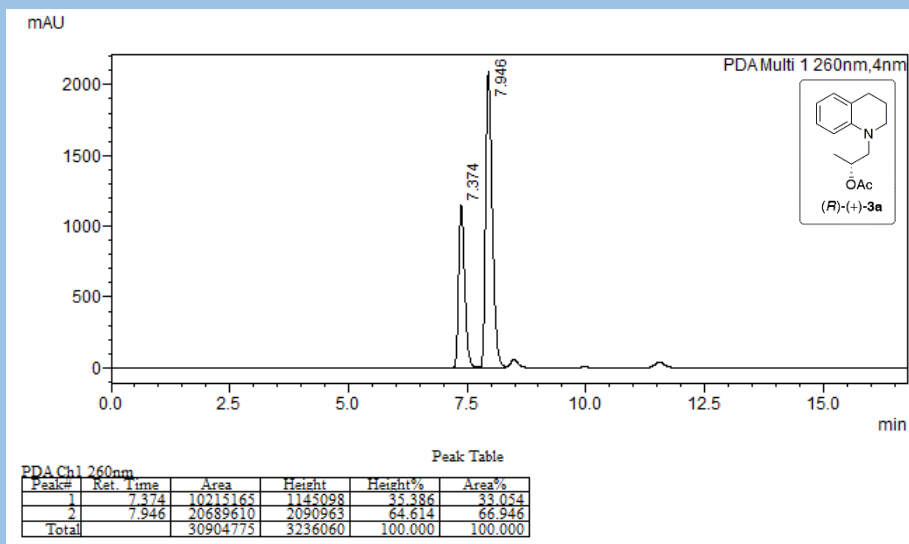
HPLC analysis for the subsequent biocatalytic reaction:



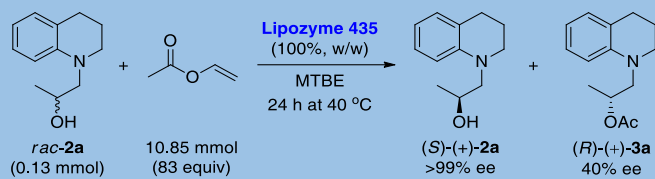
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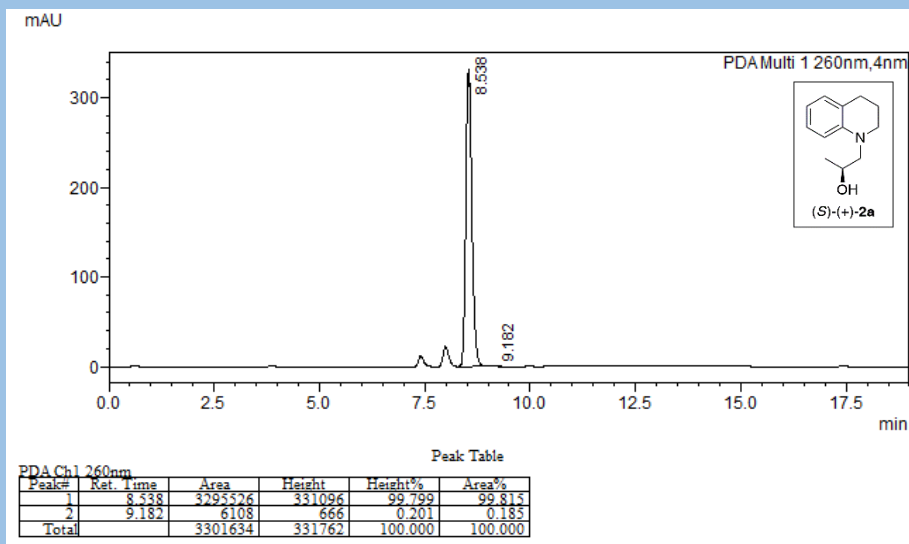
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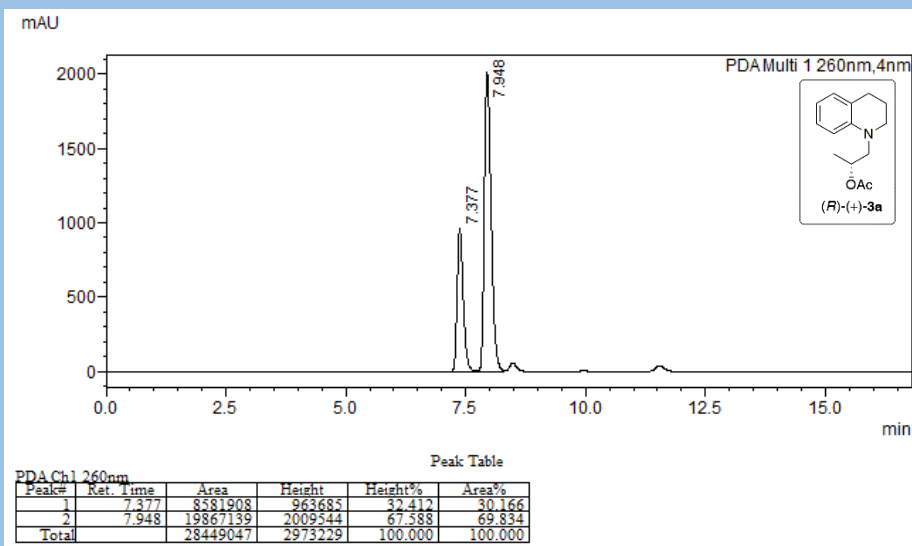
HPLC analysis for the subsequent biocatalytic reaction:



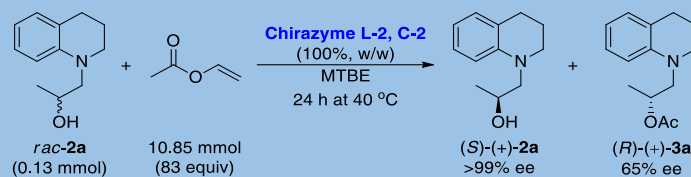
HPLC conditions [for (*S*)-**2a**]: *n*-hexane-*i*-PrOH (90:10, v/v); f=0.8 mL/min; λ=260 nm; Chiralcel OJ-H



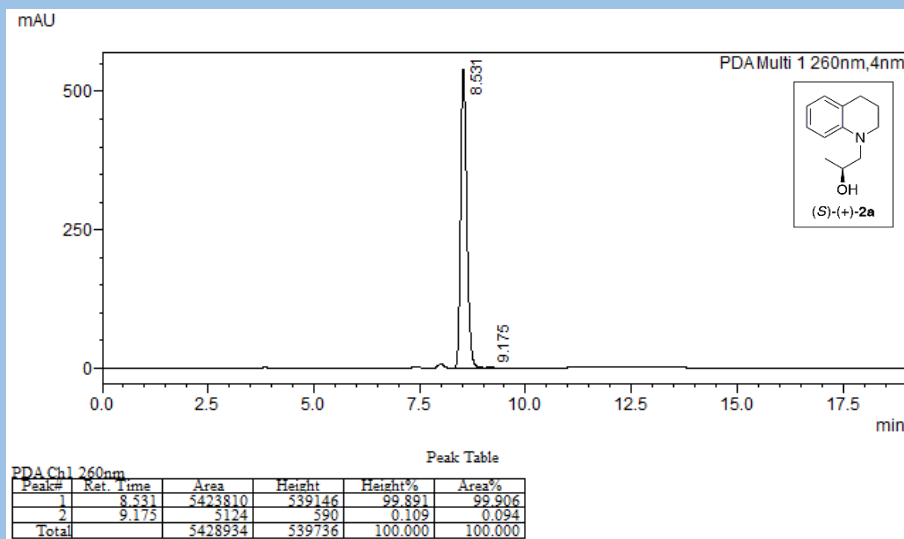
HPLC conditions [for (*R*)-**3a**]: *n*-hexane-*i*-PrOH (90:10, v/v); f=0.8 mL/min; λ=260 nm; Chiralcel OJ-H



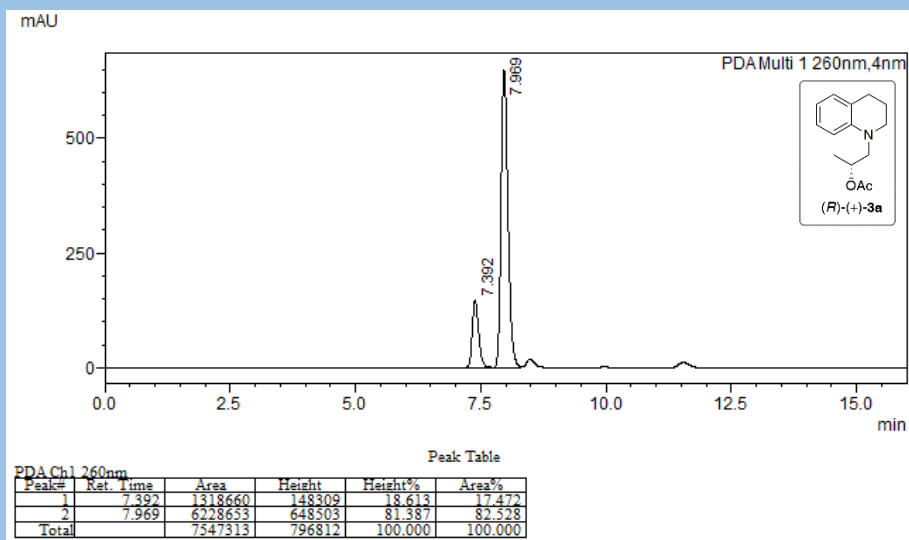
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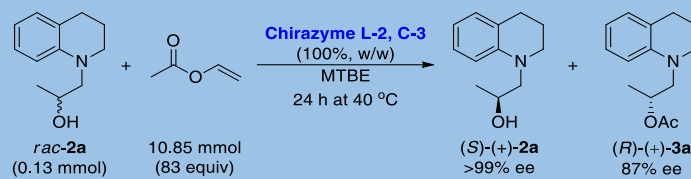
HPLC conditions [for (*S*)-2a]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



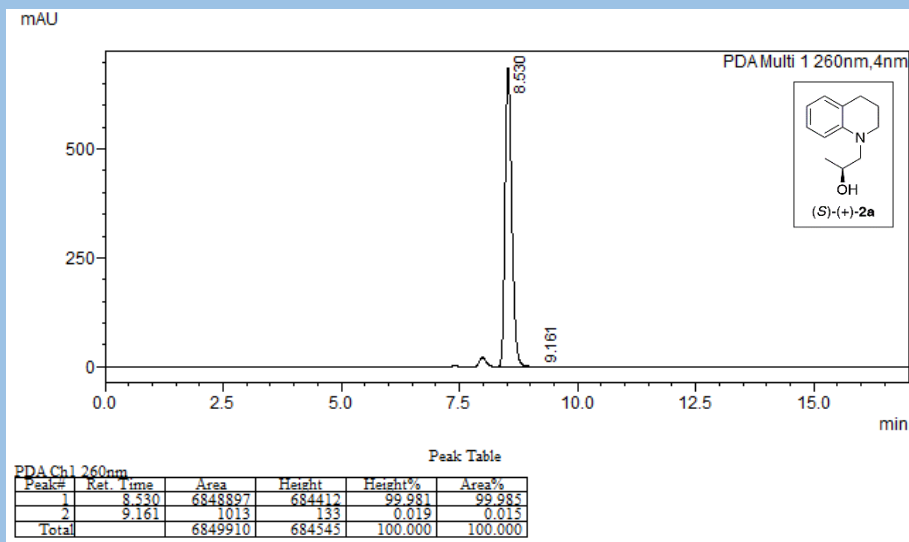
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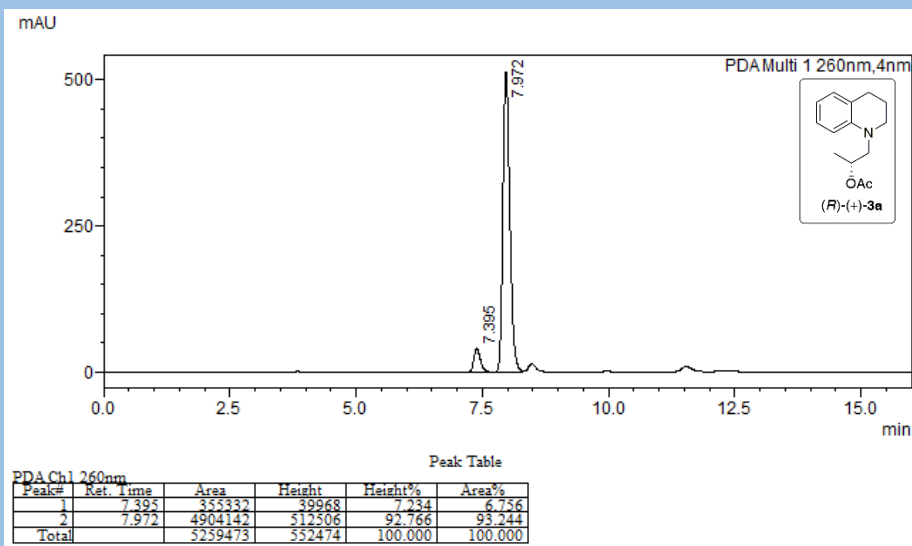
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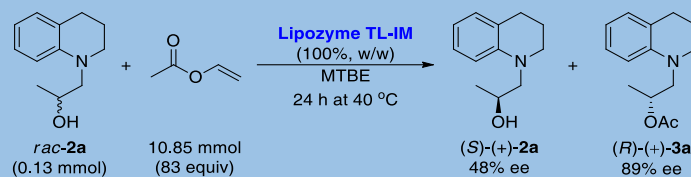
HPLC conditions [for (*S*)-**2a**]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



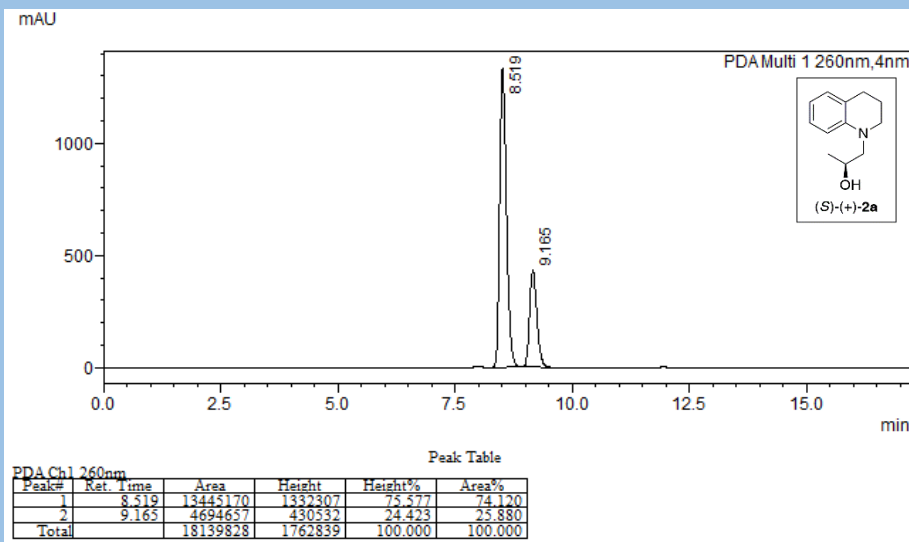
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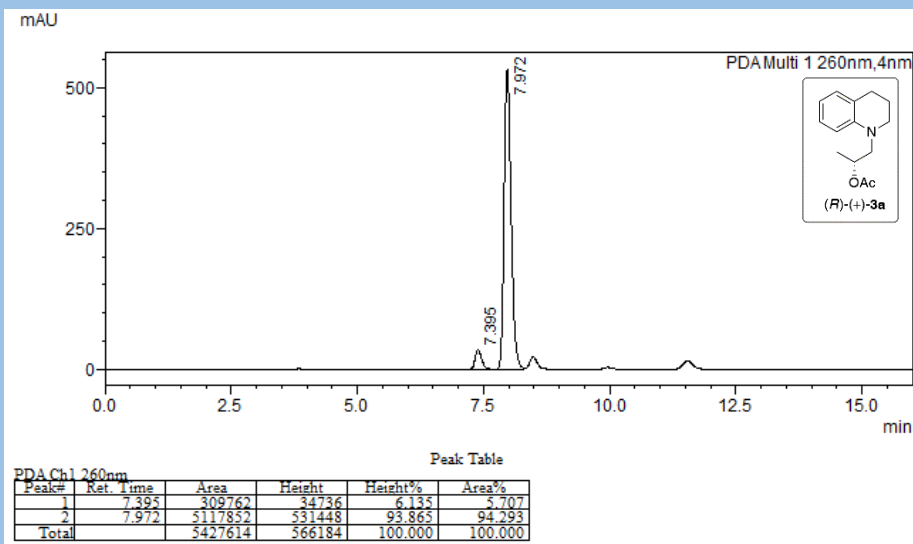
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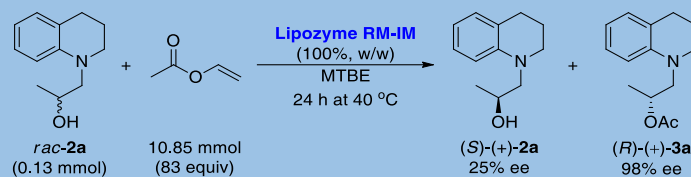
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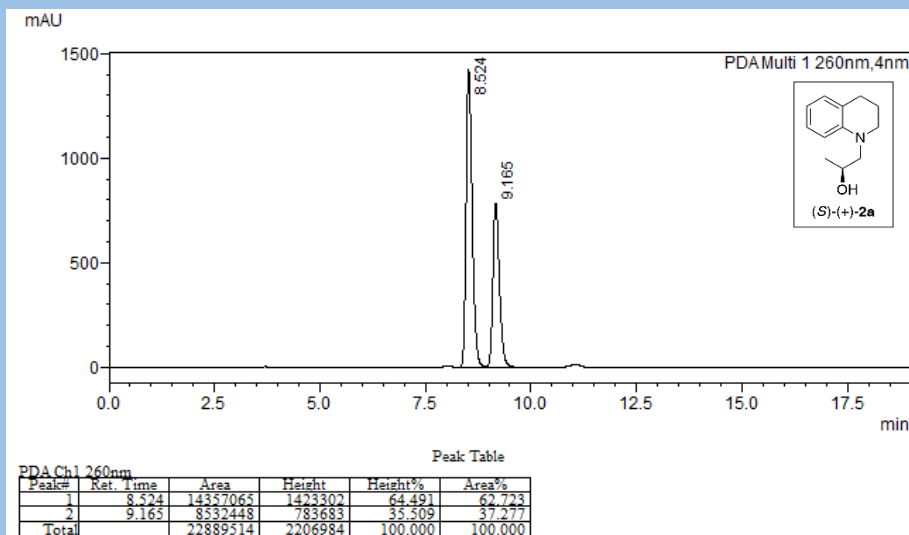
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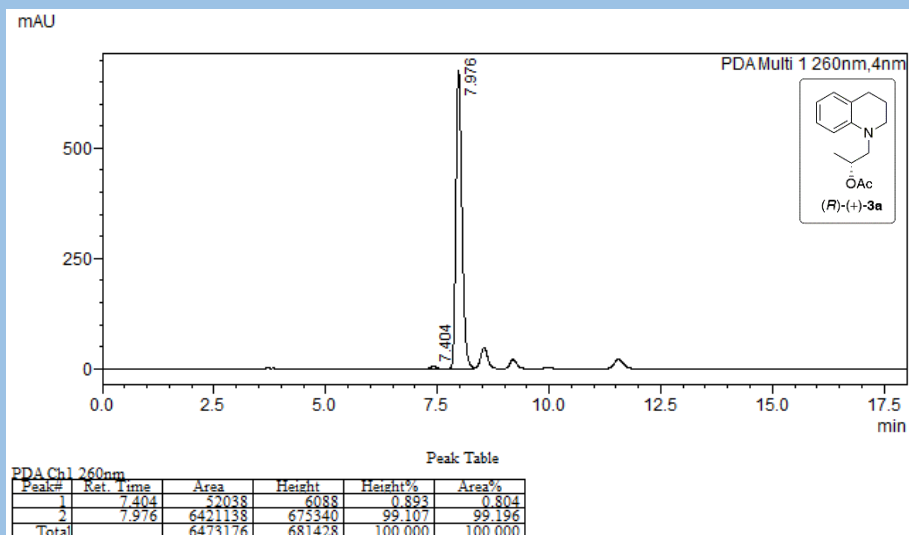
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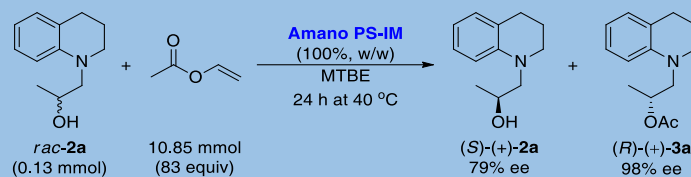
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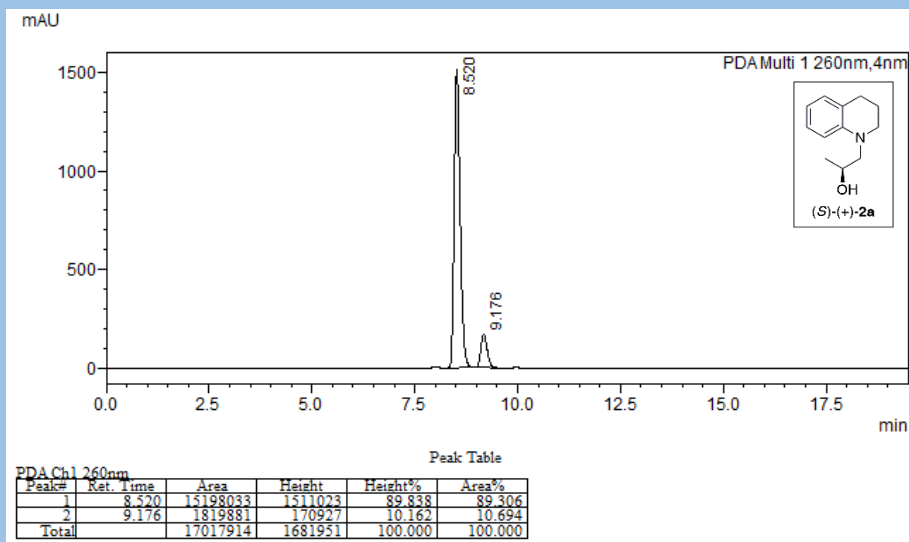
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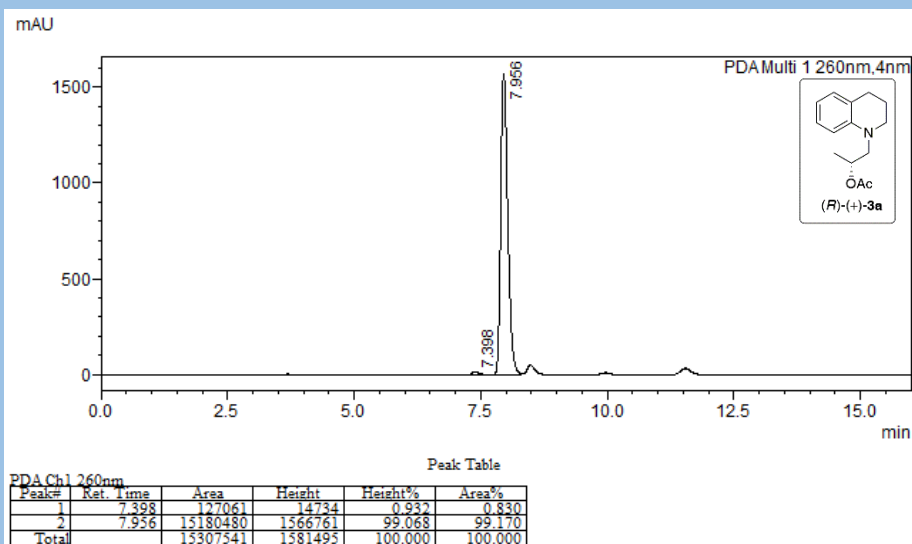
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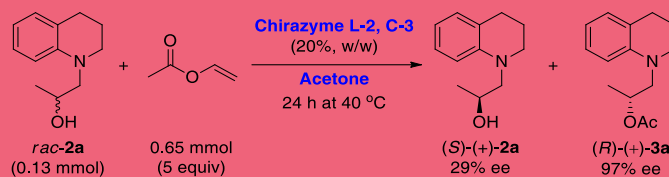
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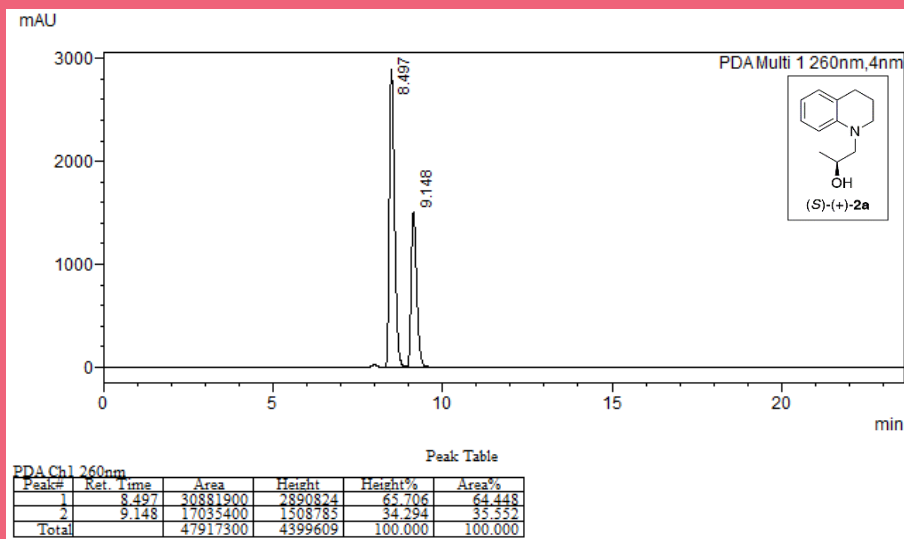
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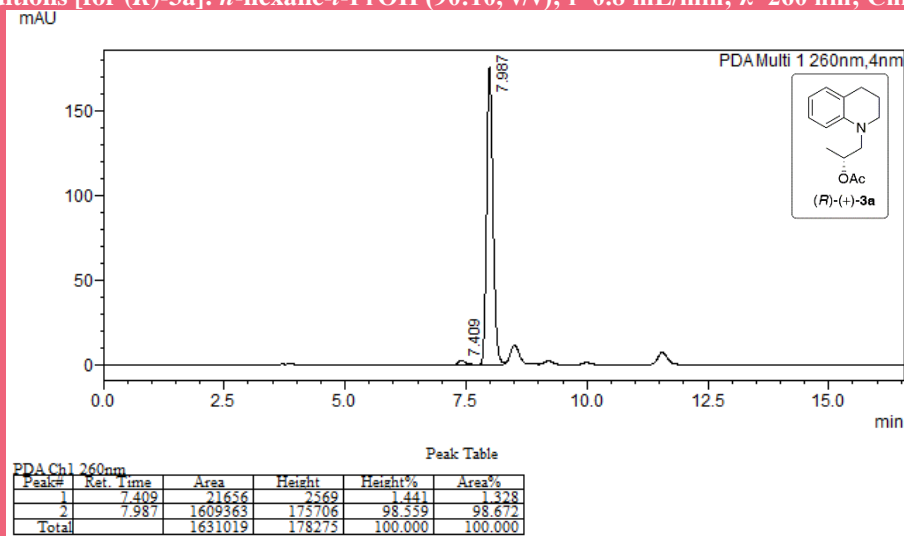
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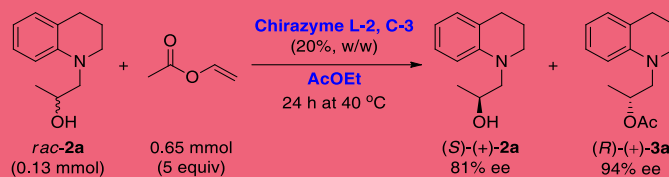
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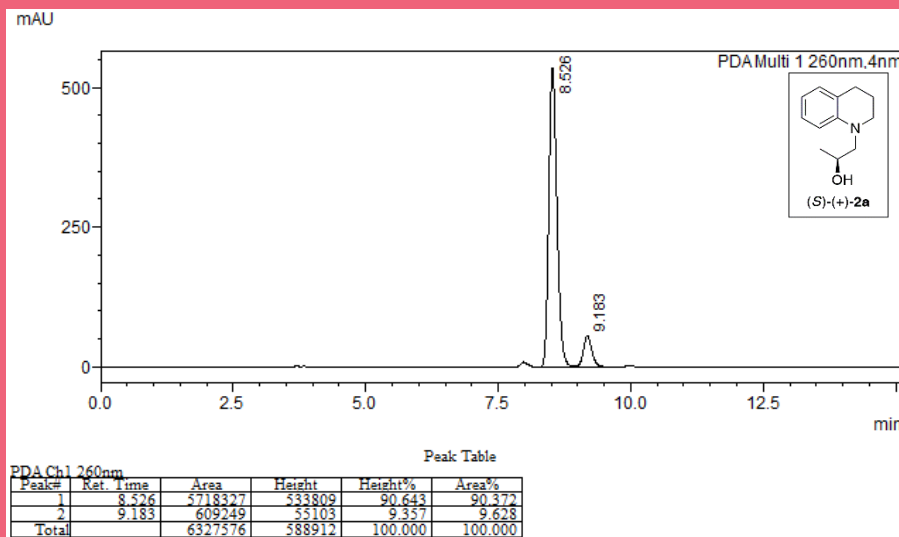
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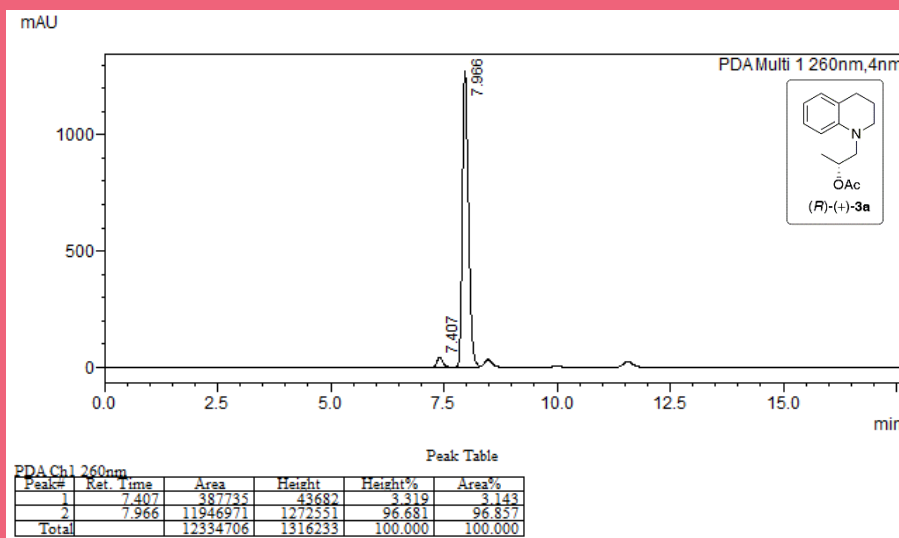
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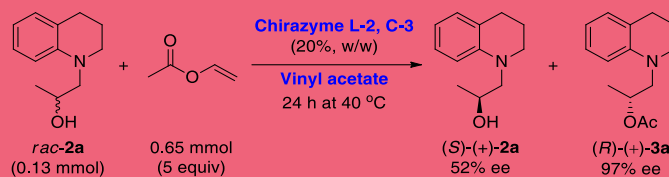
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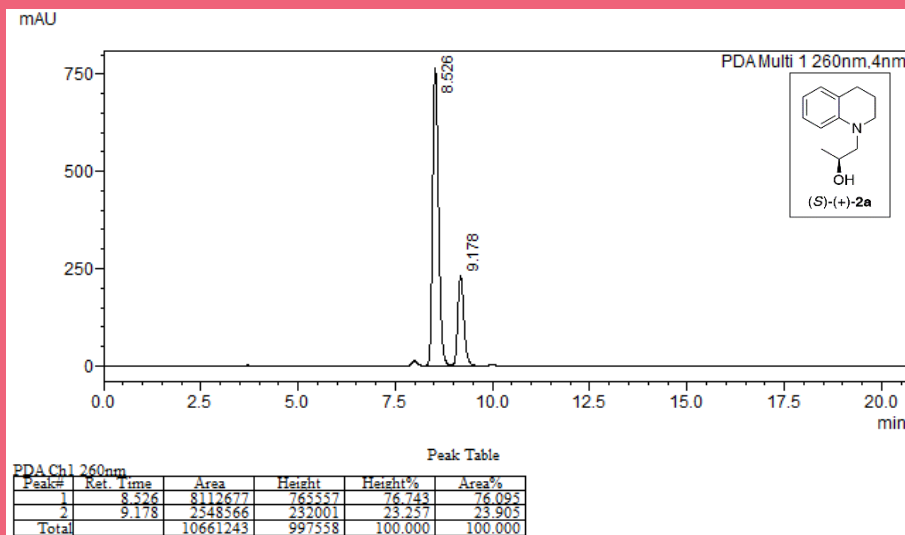
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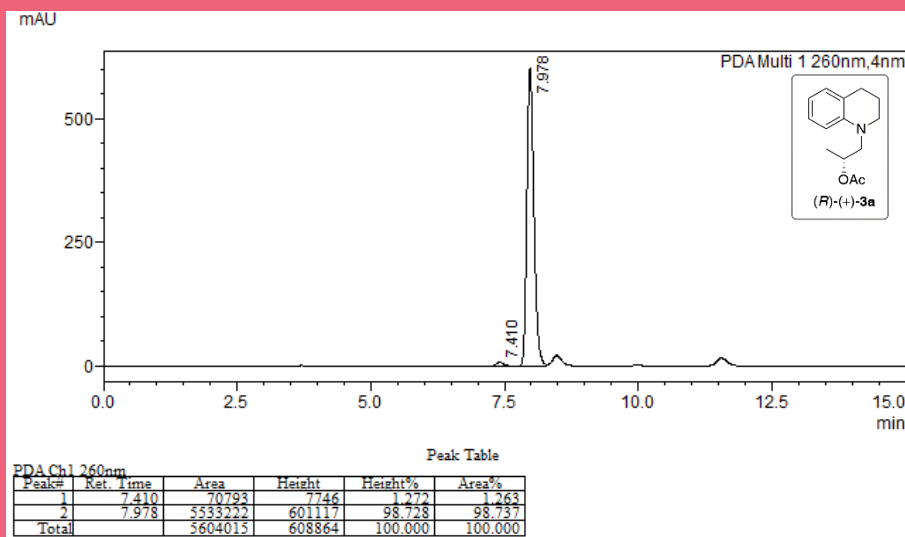
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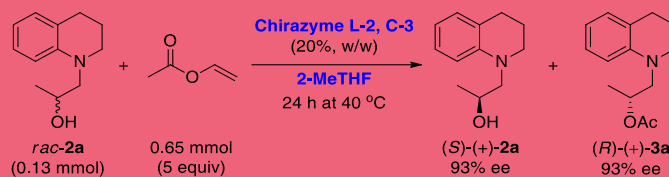
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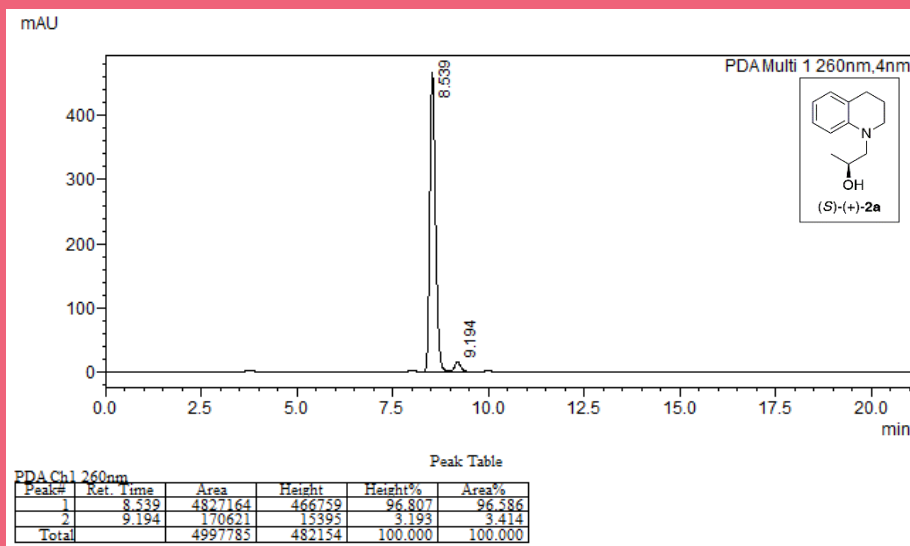
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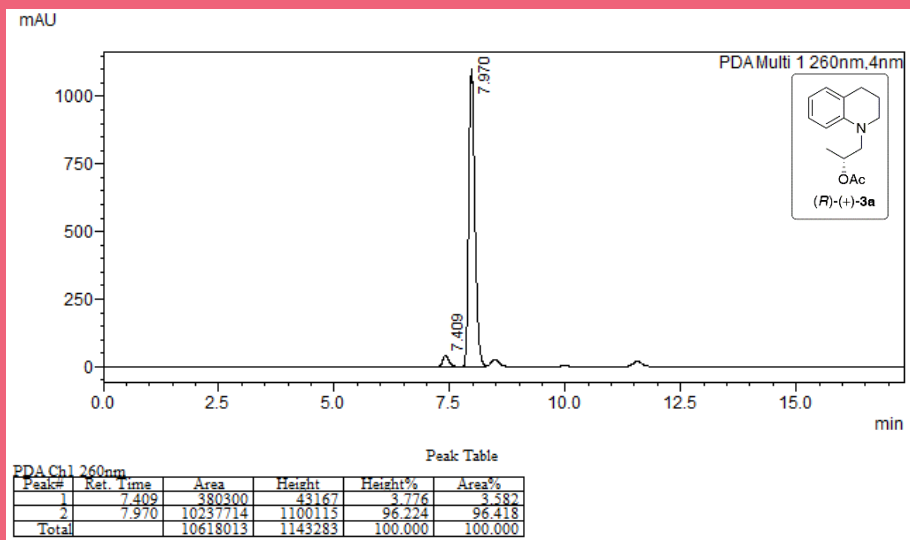
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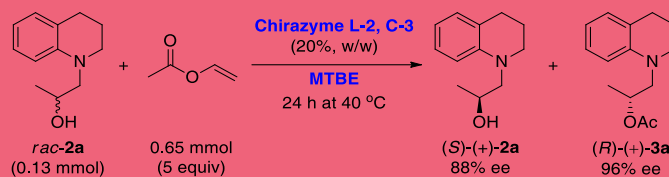
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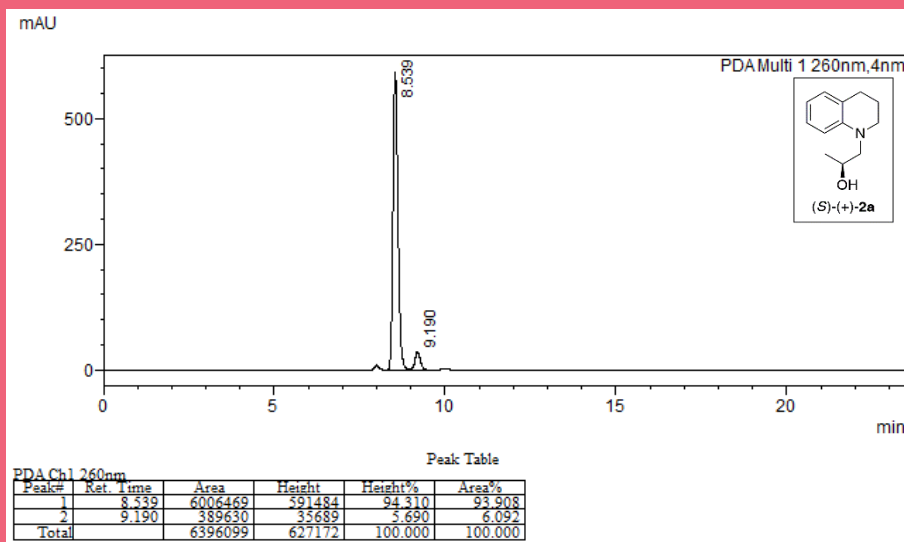
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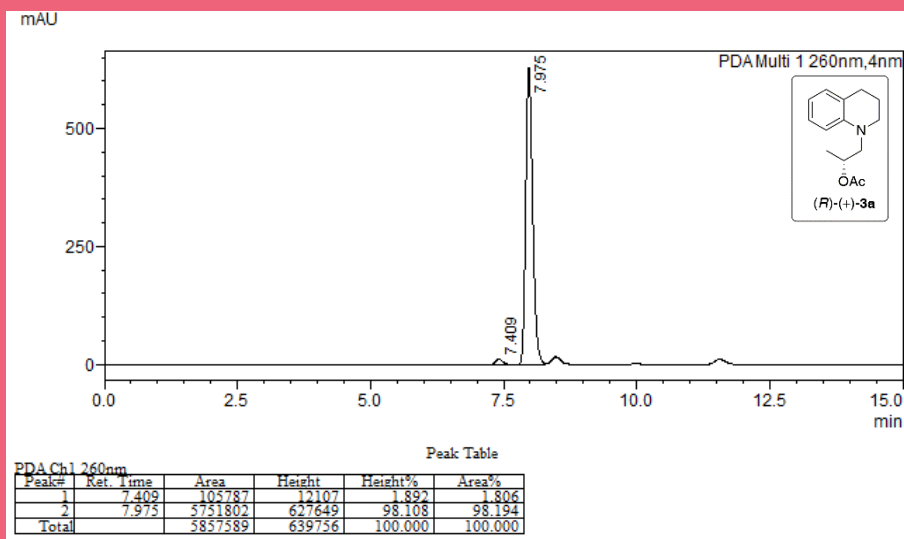
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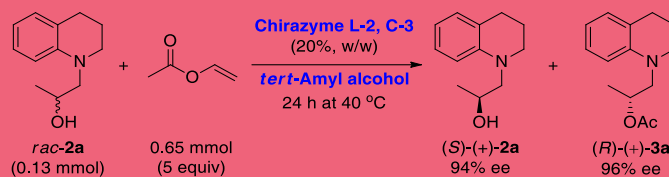
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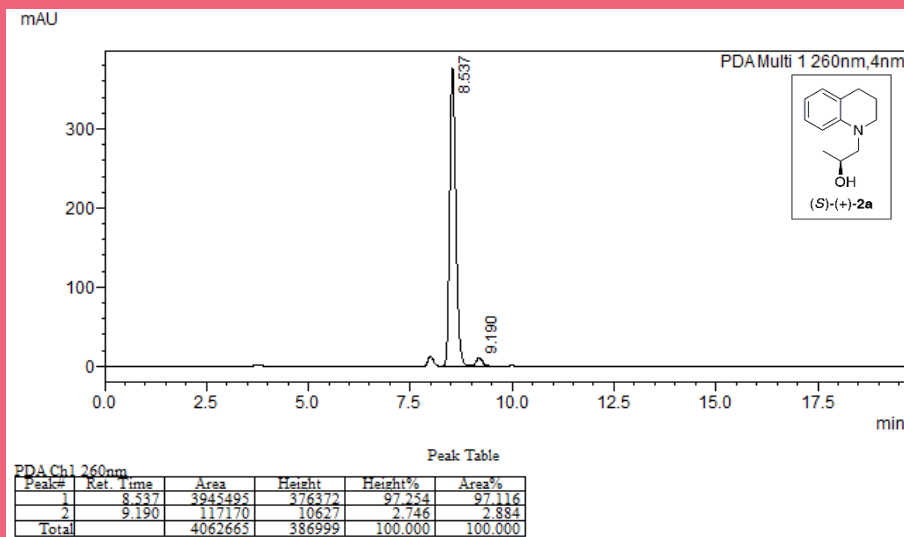
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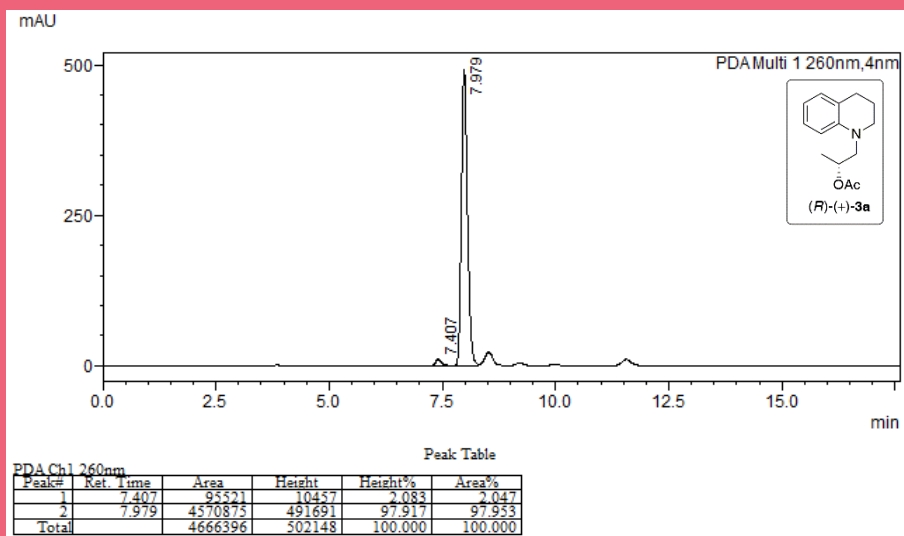
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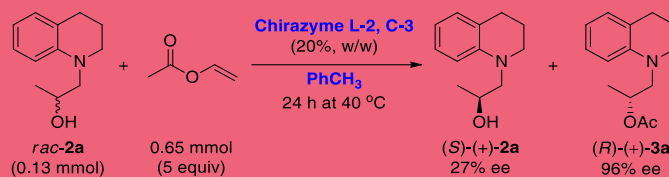
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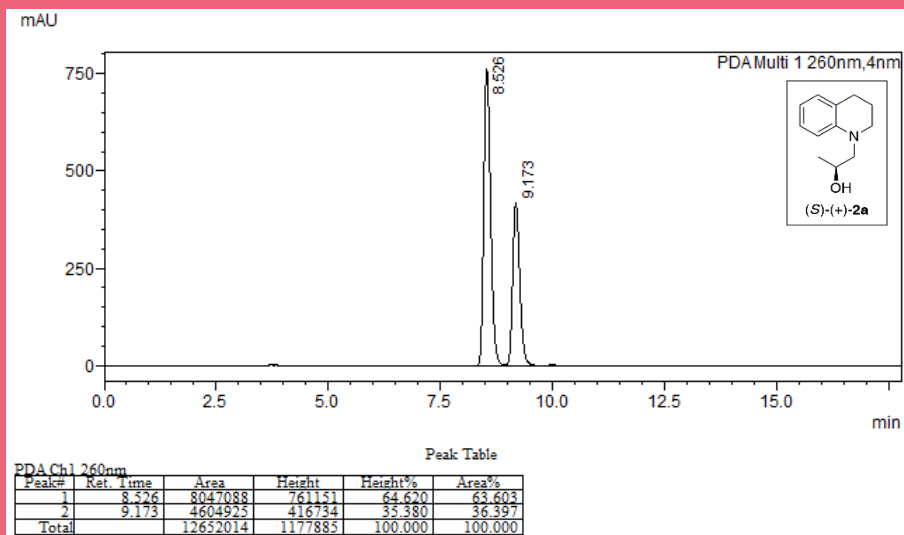
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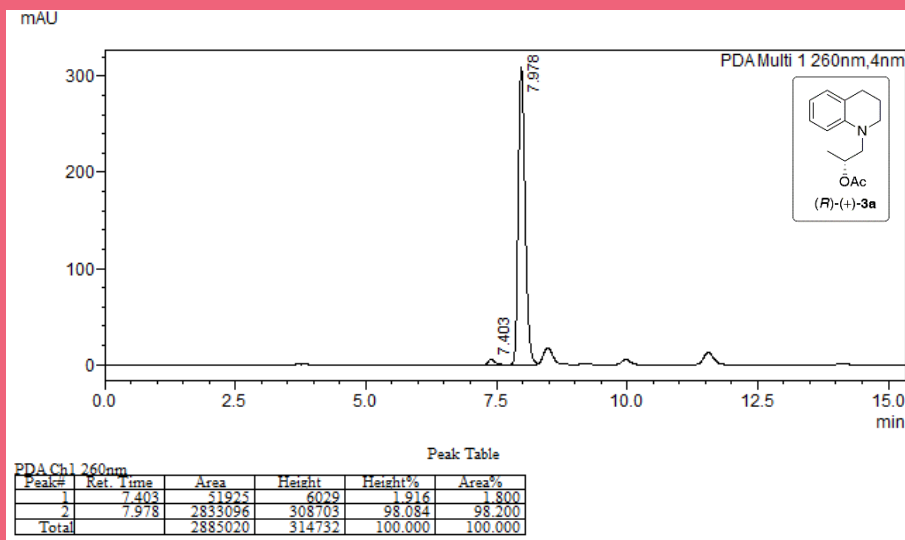
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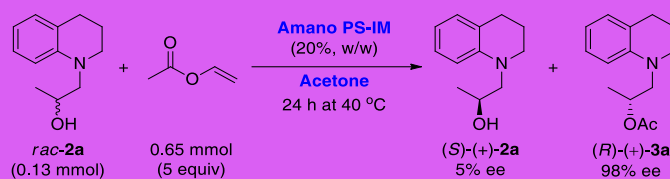
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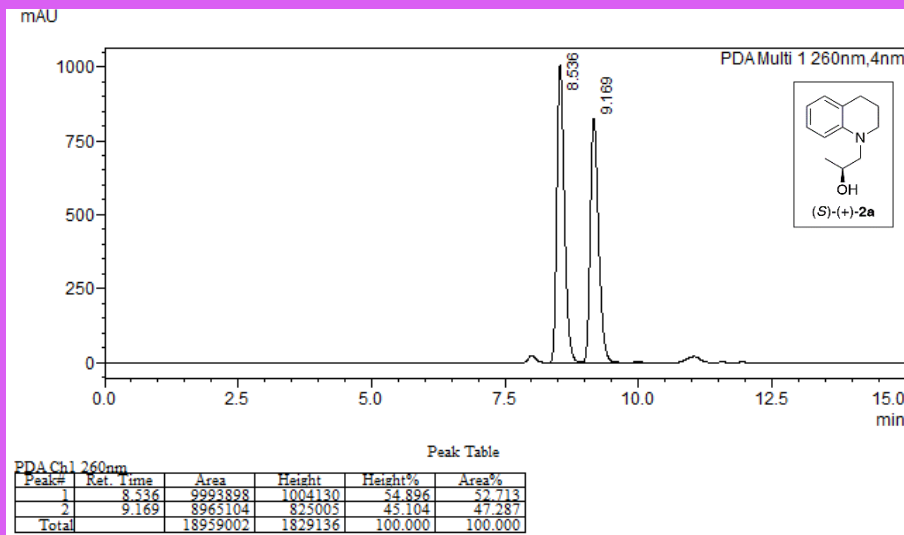
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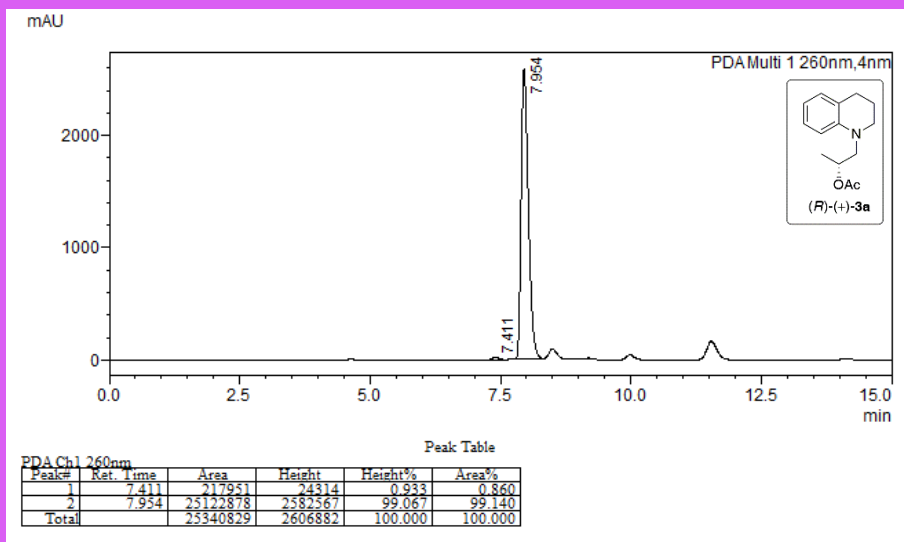
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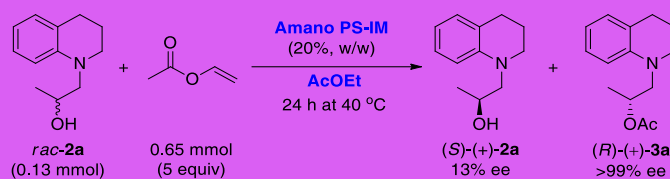
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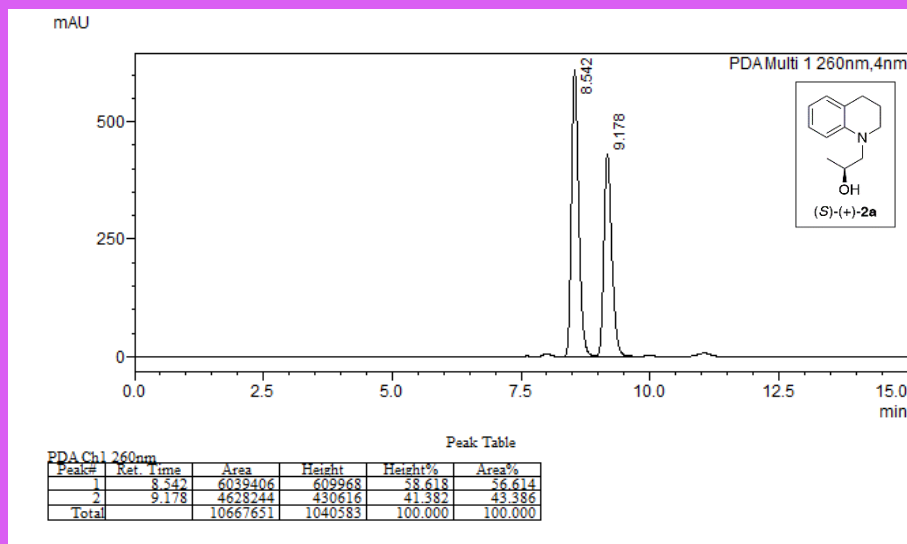
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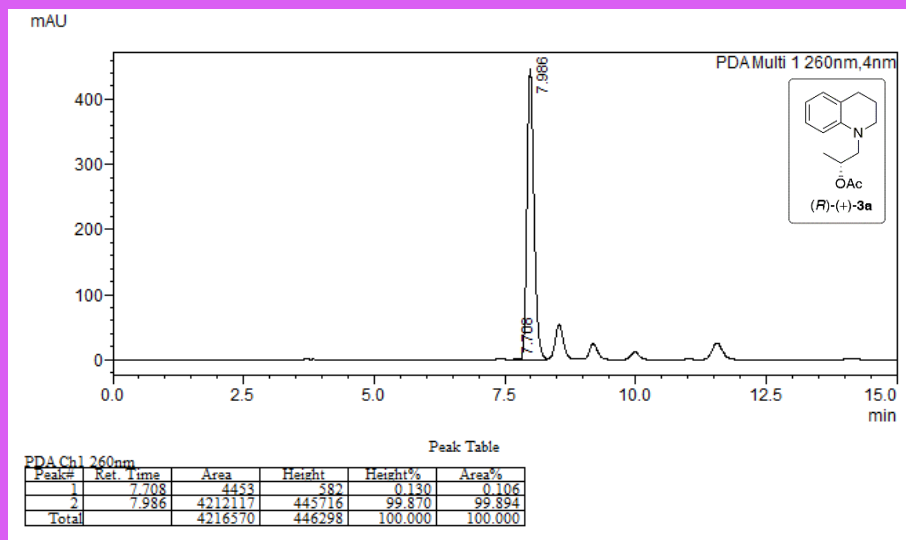
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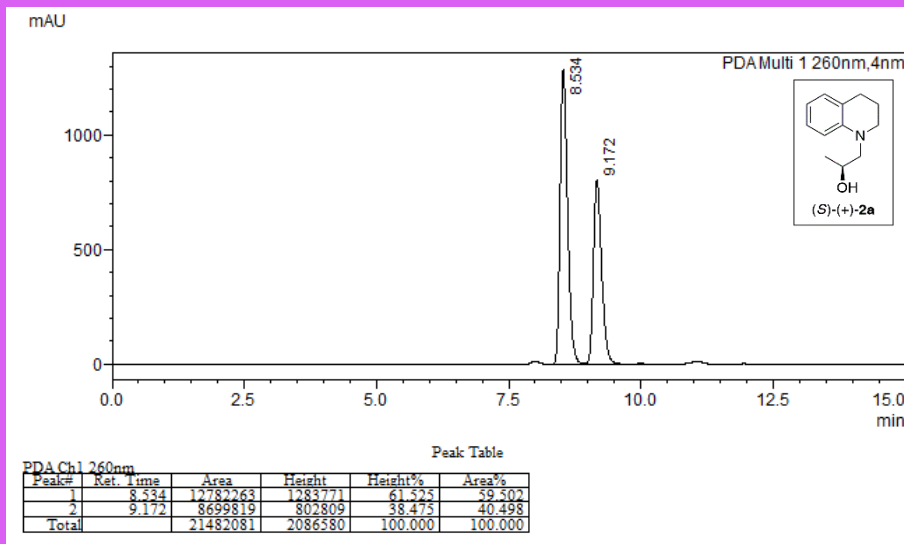
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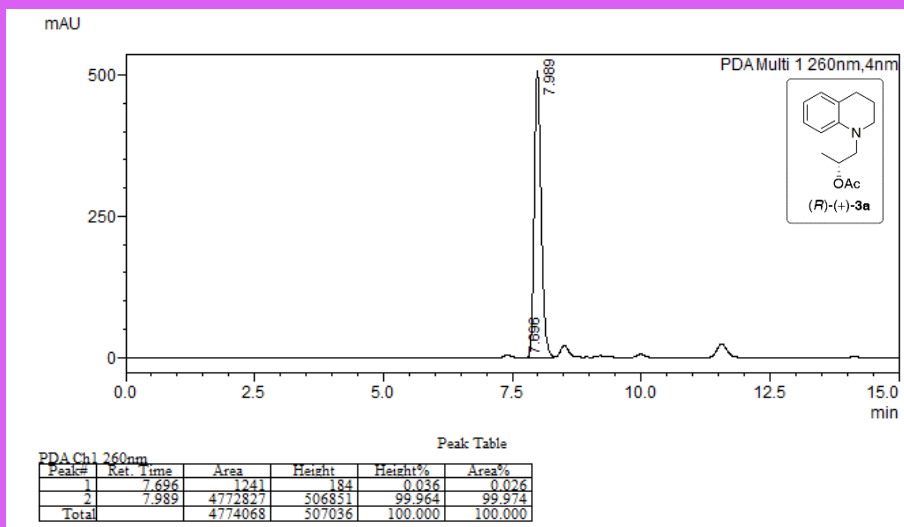
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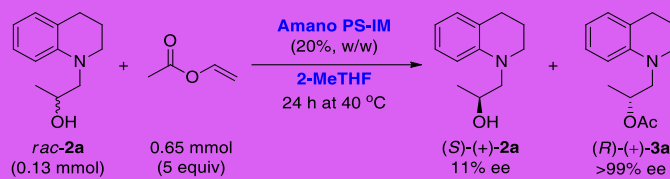
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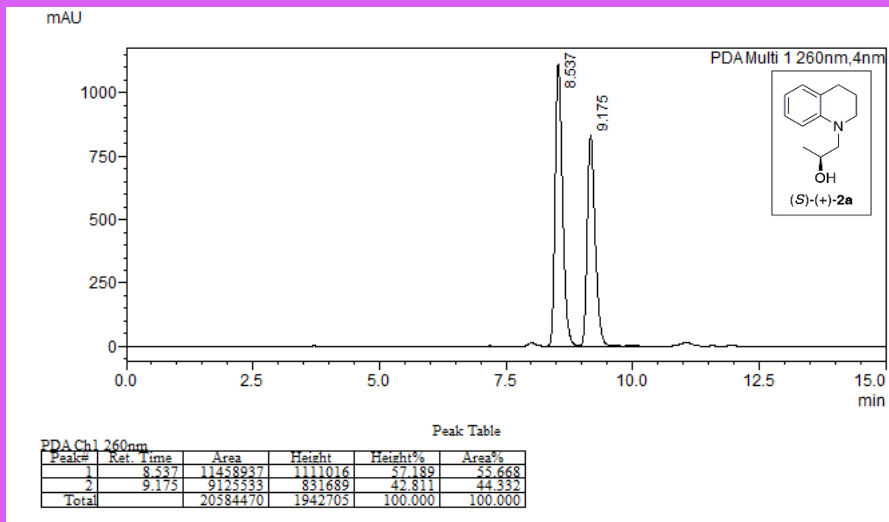
HPLC conditions [for (*R*)-**3a**]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



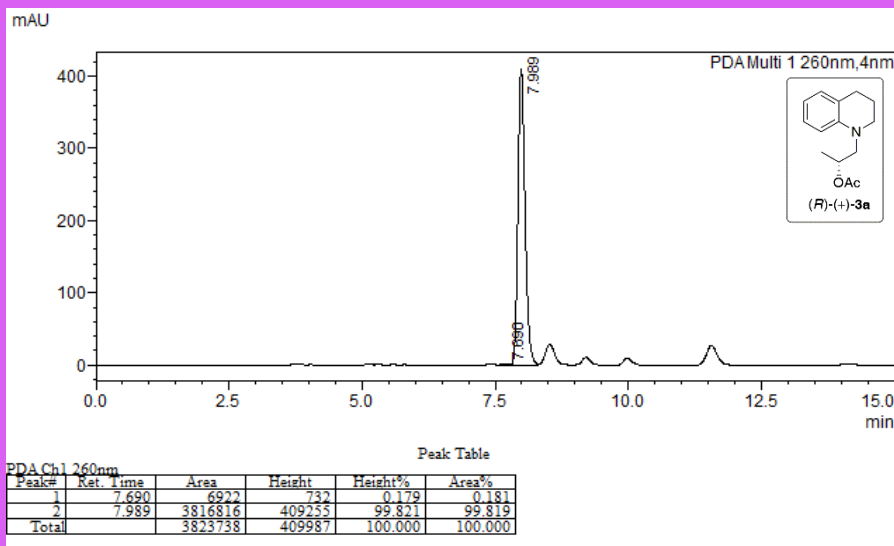
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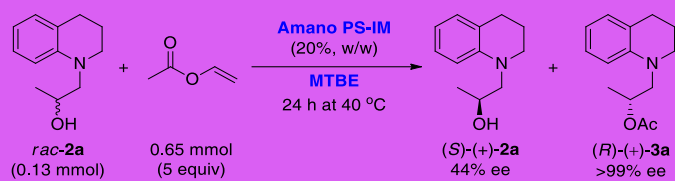
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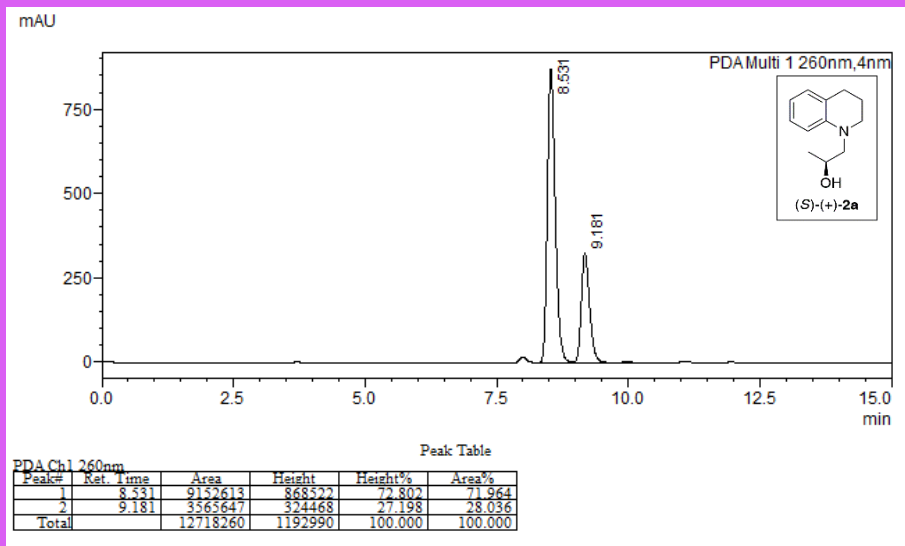
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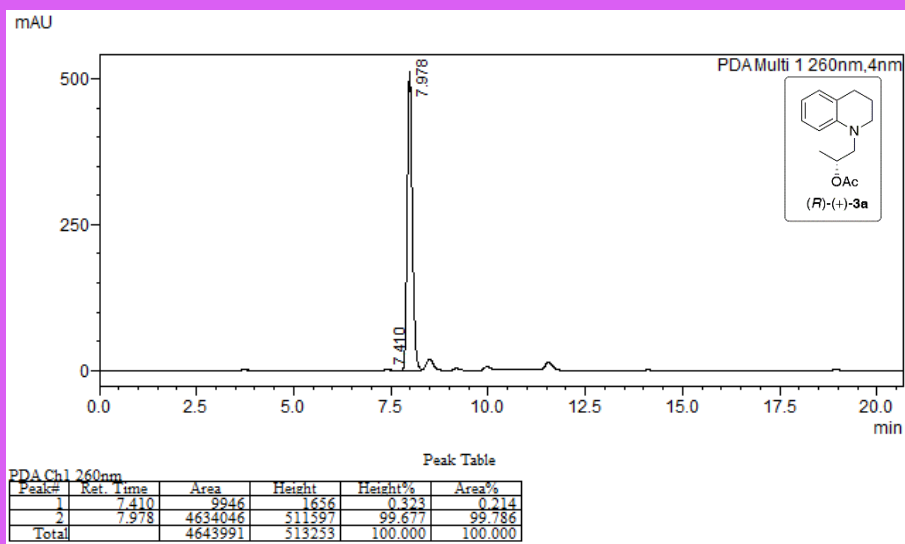
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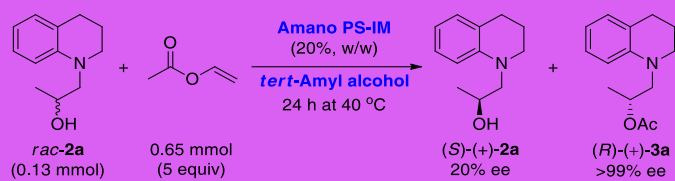
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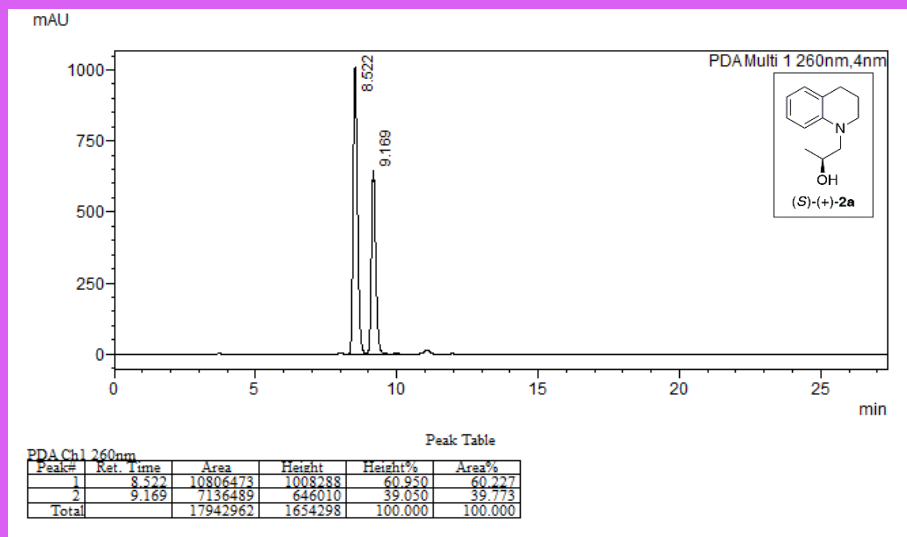
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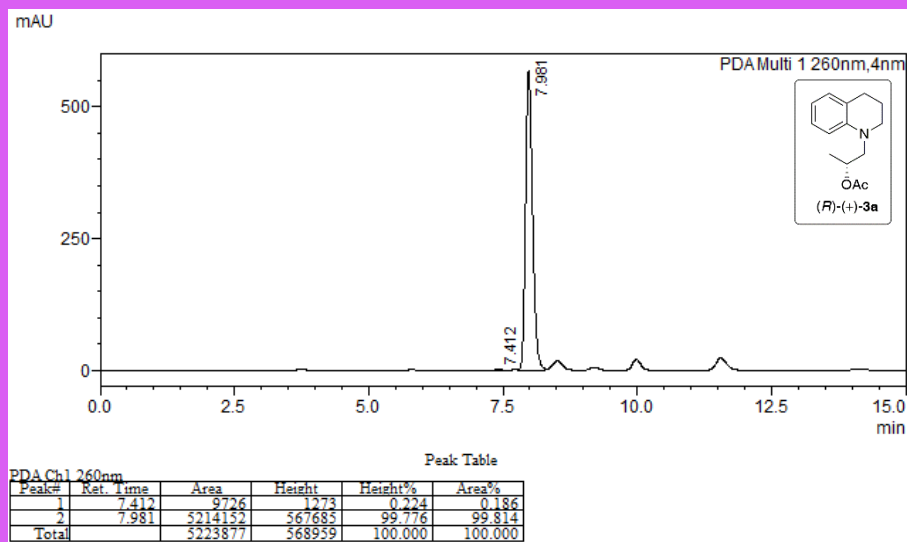
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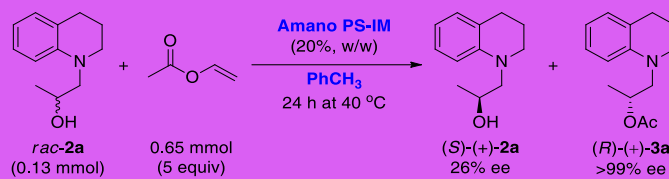
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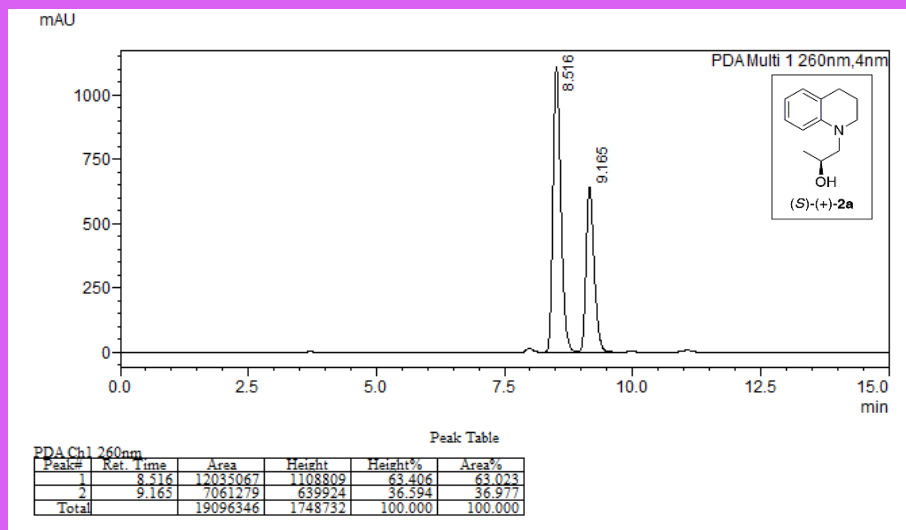
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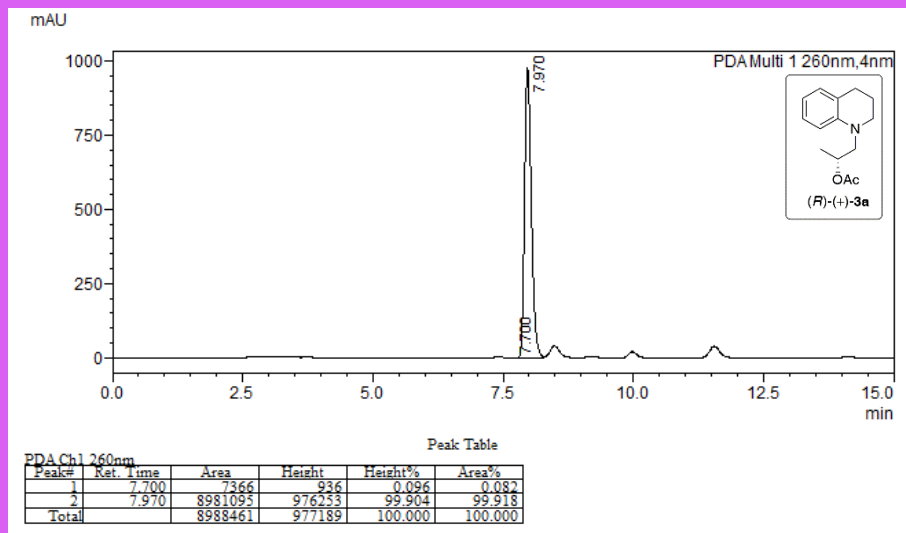
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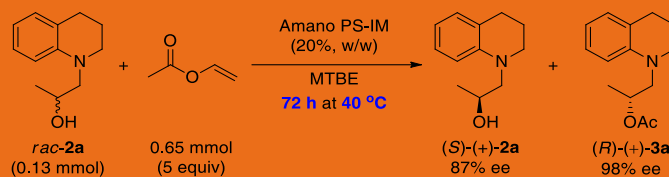
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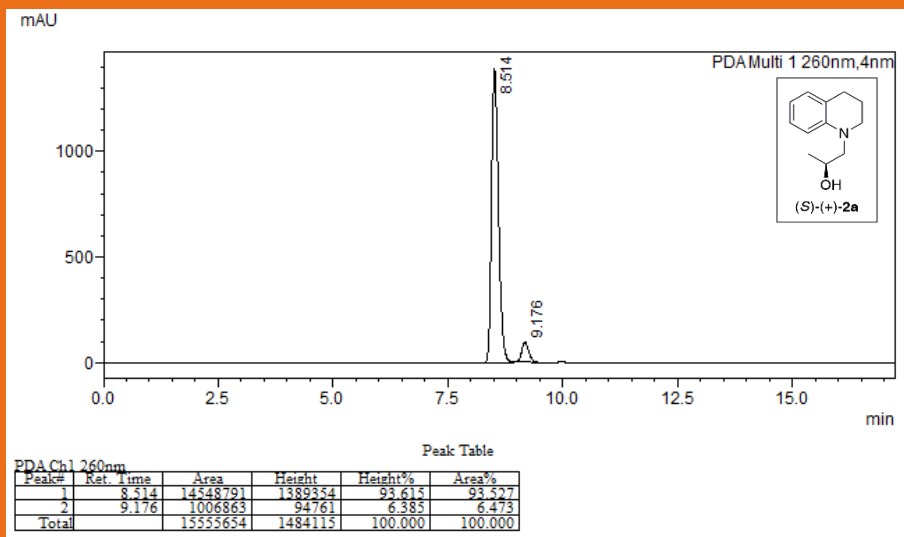
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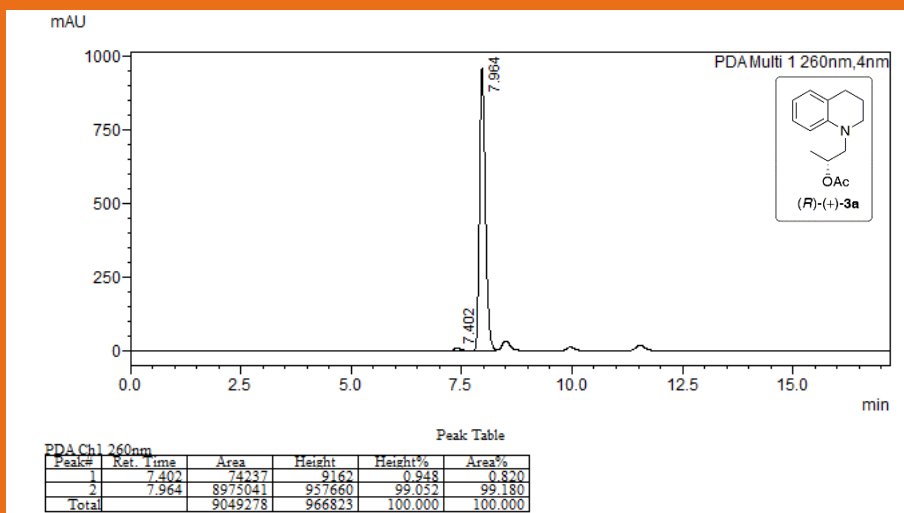
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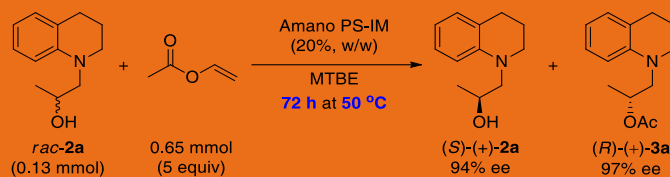
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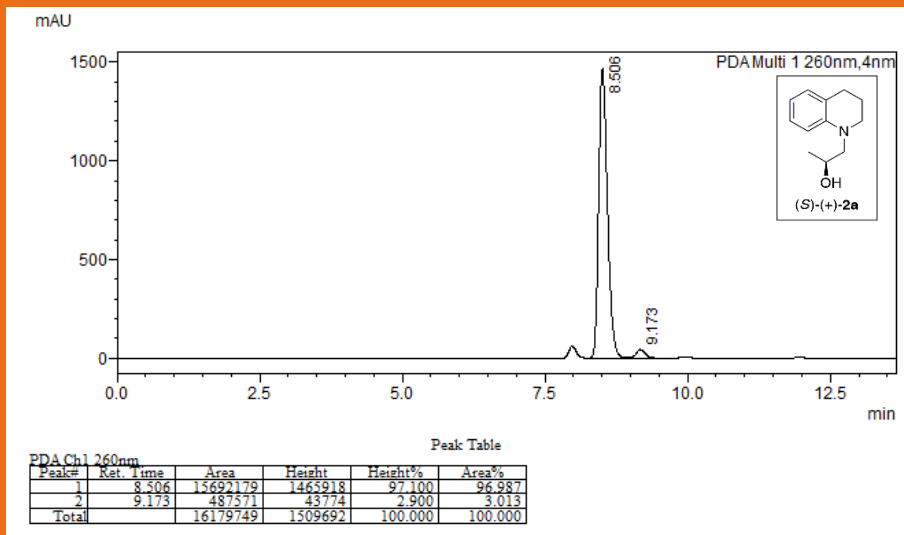
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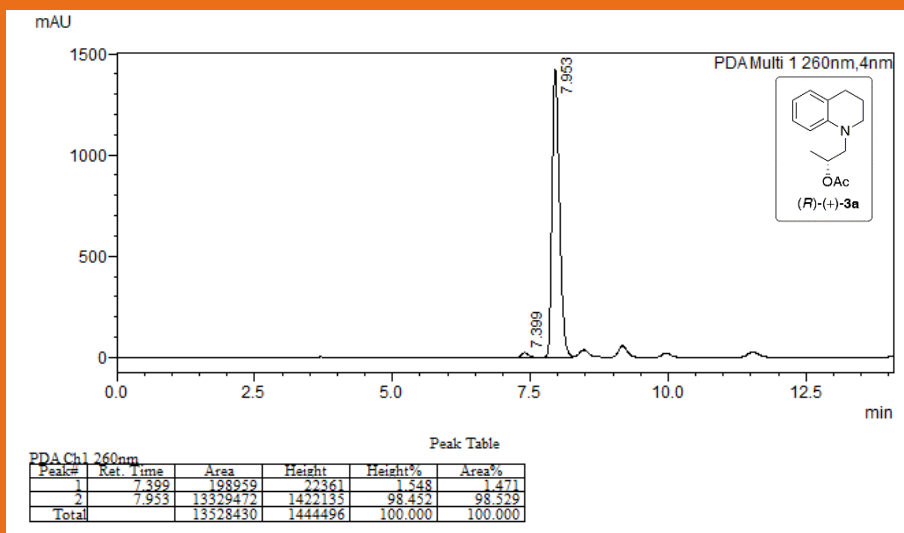
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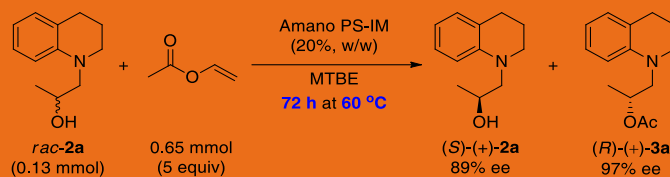
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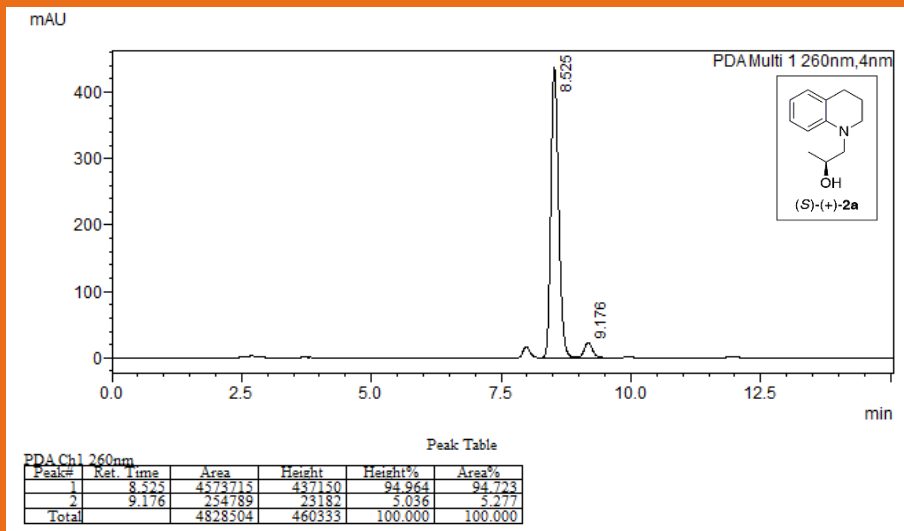
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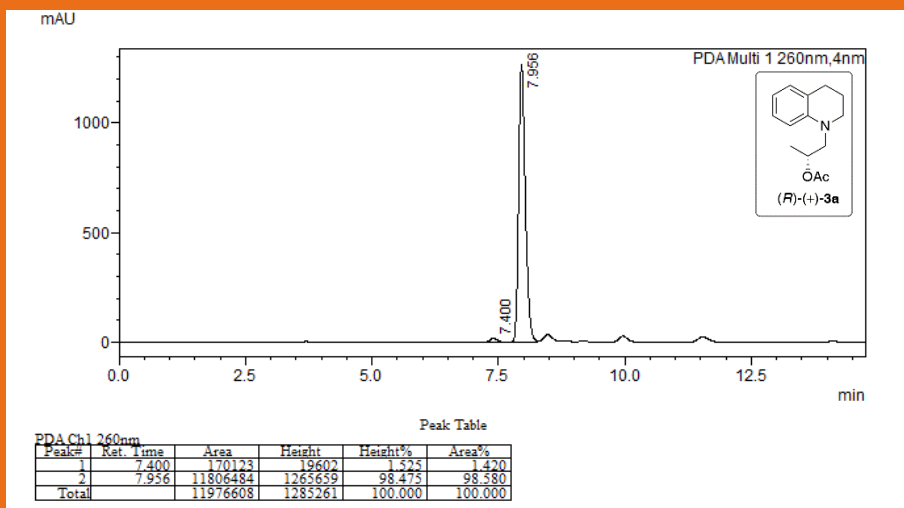
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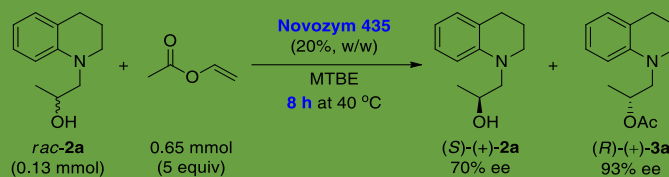
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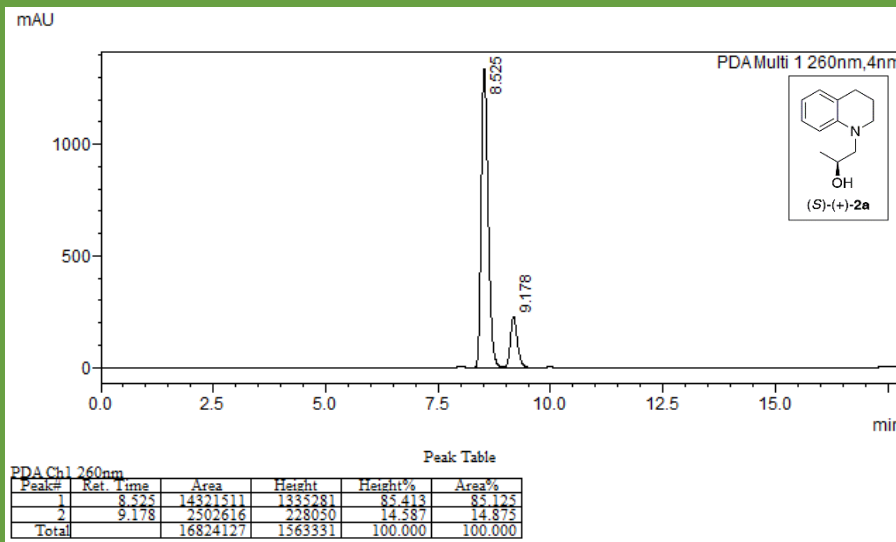
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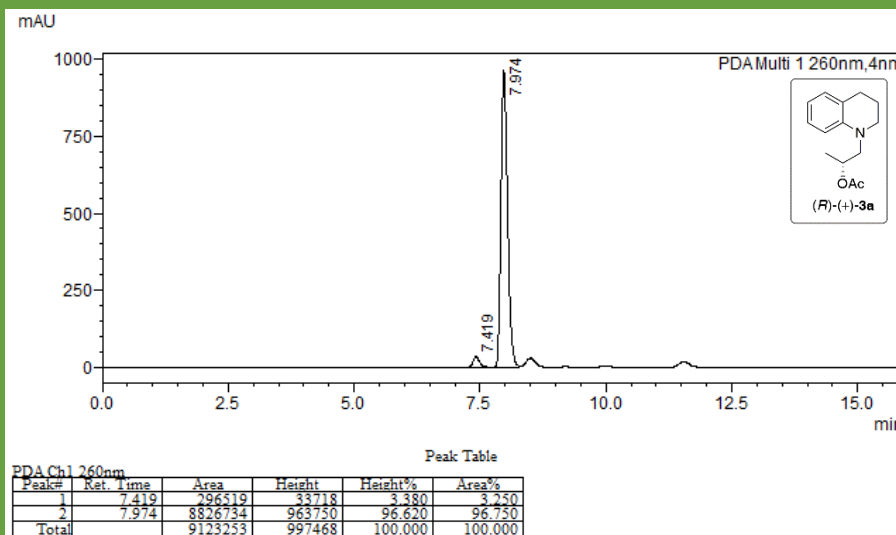
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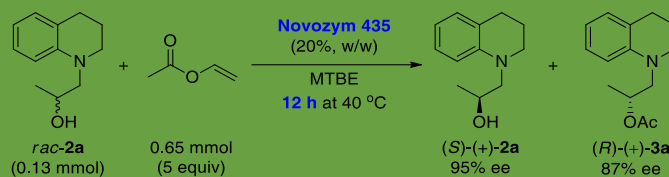
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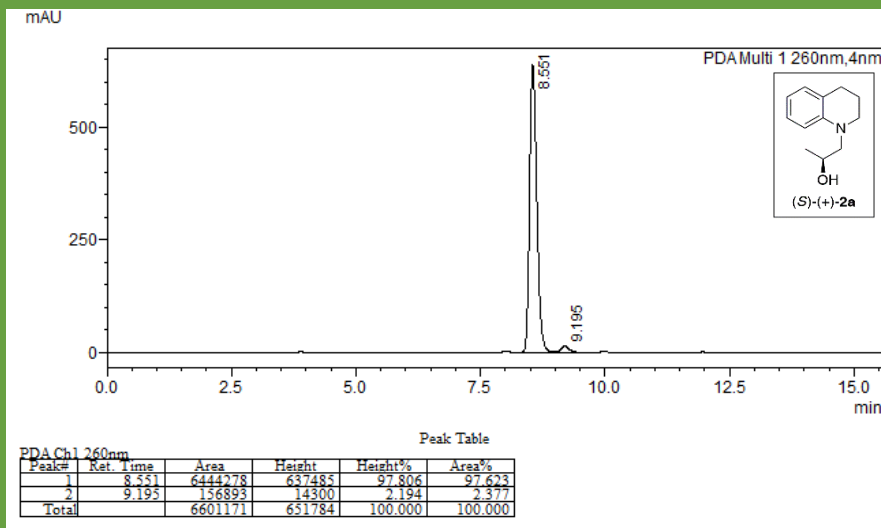
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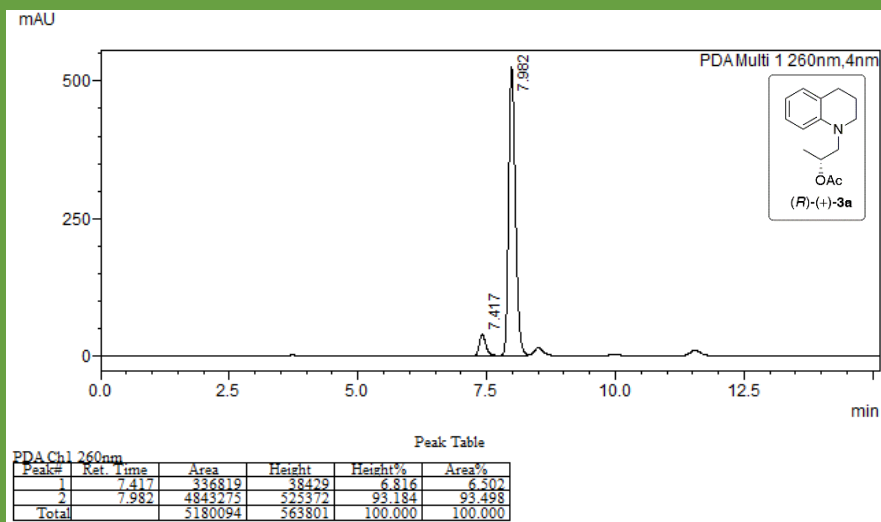
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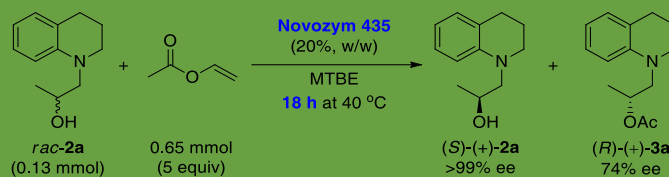
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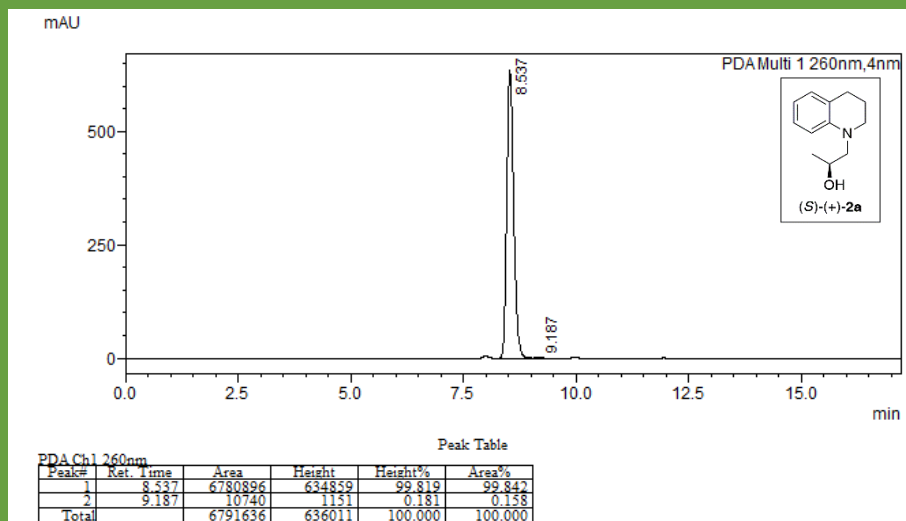
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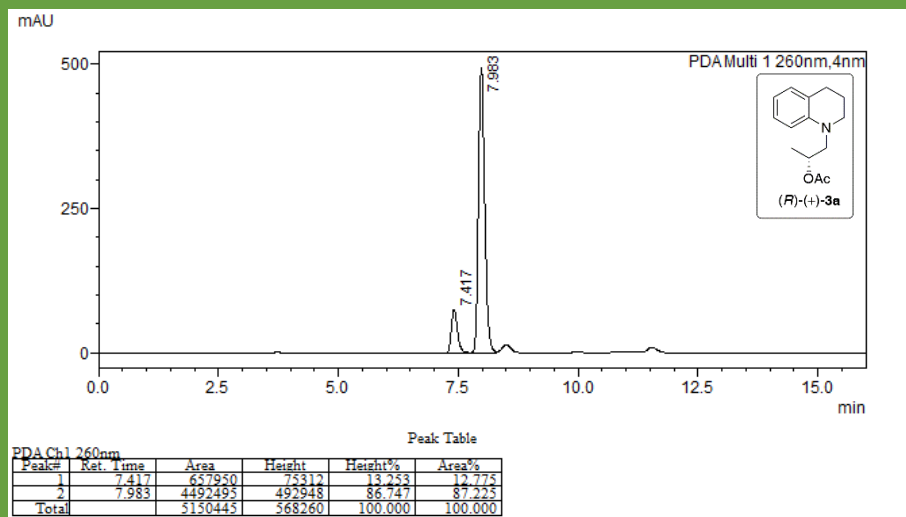
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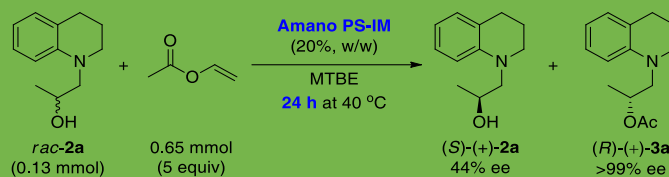
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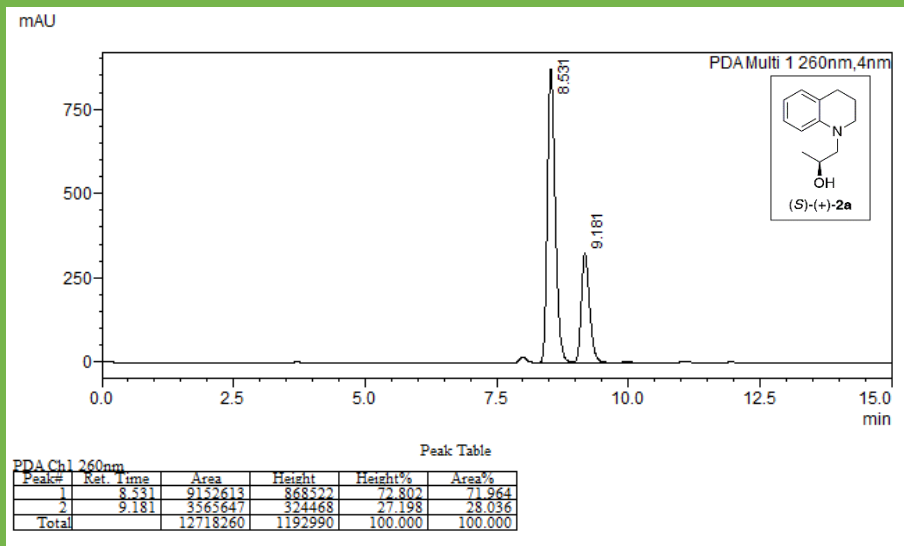
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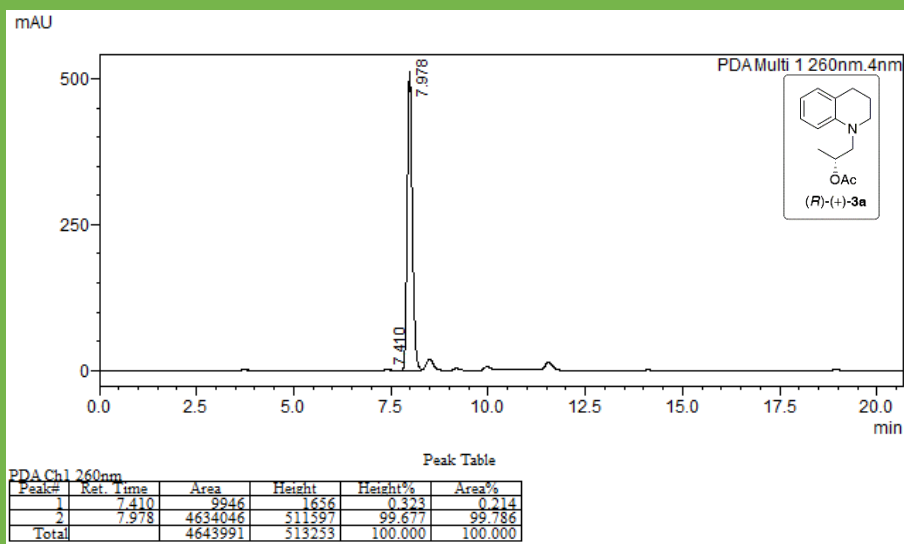
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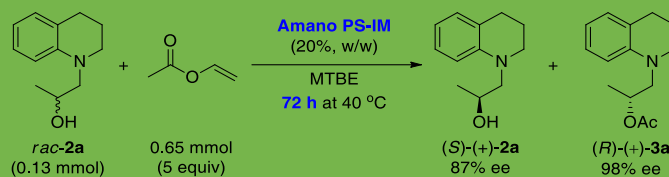
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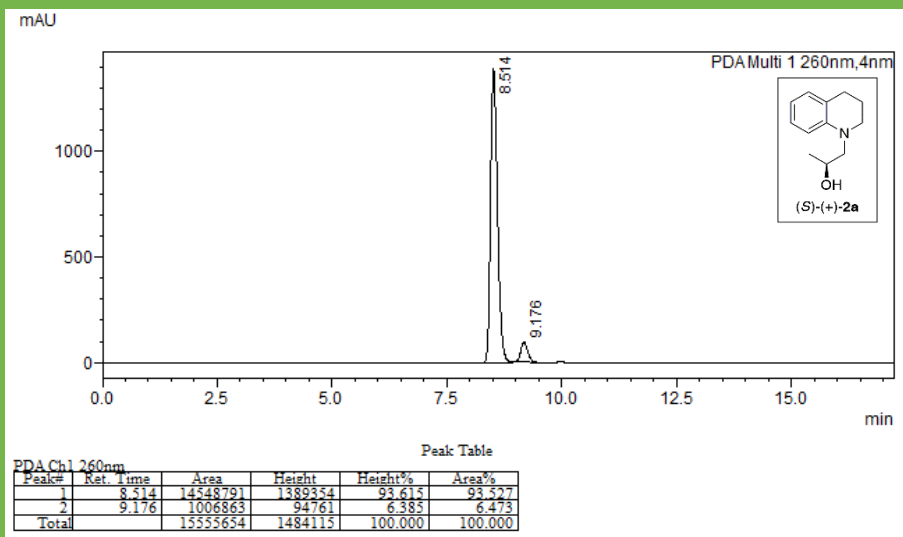
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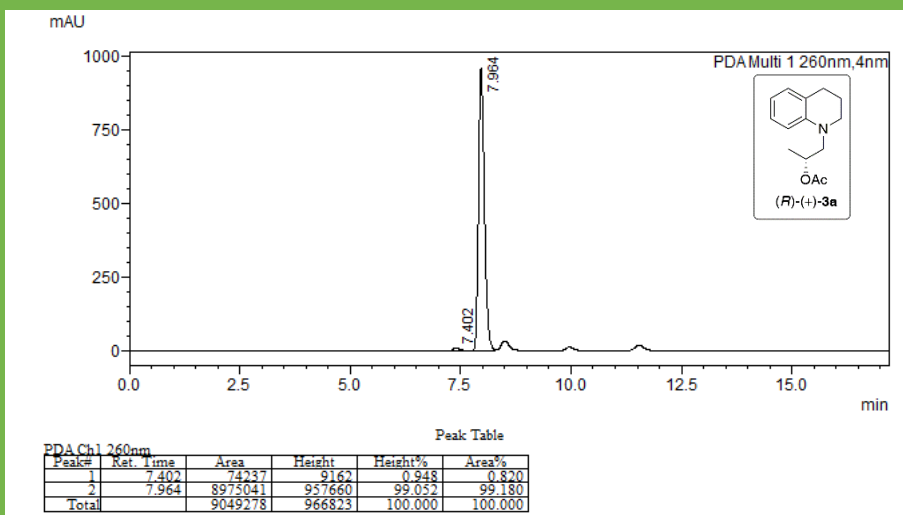
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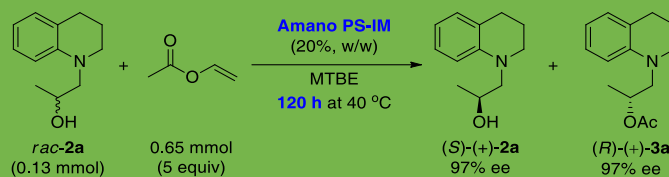
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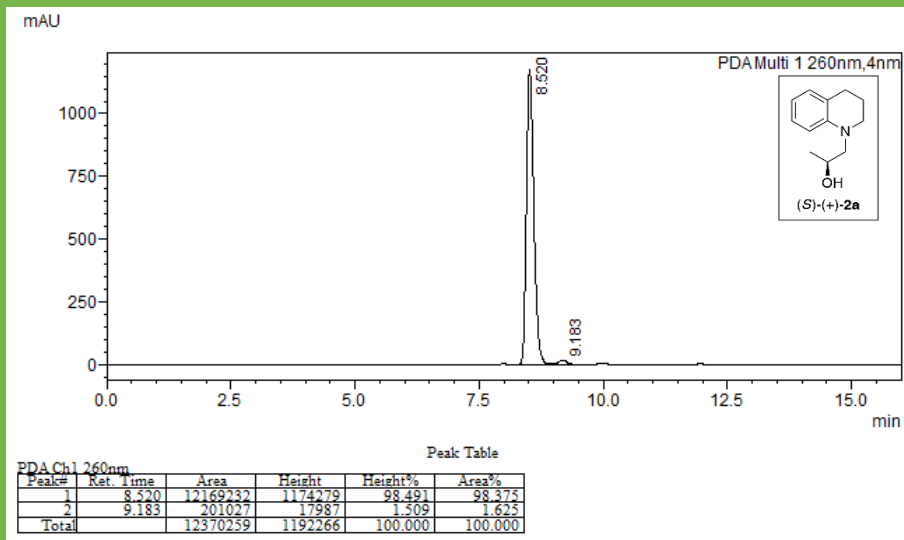
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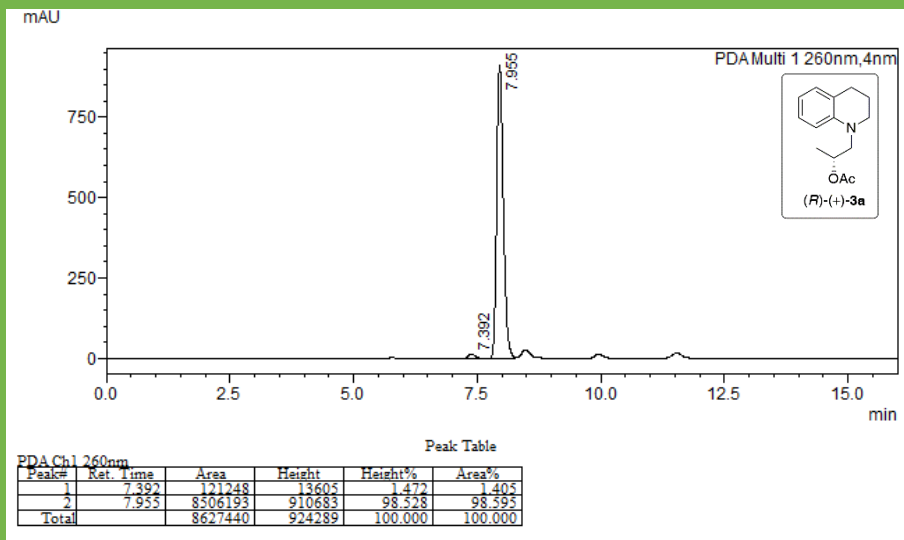
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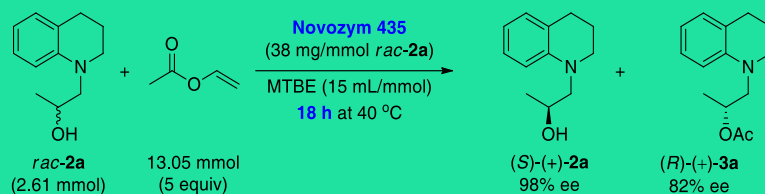
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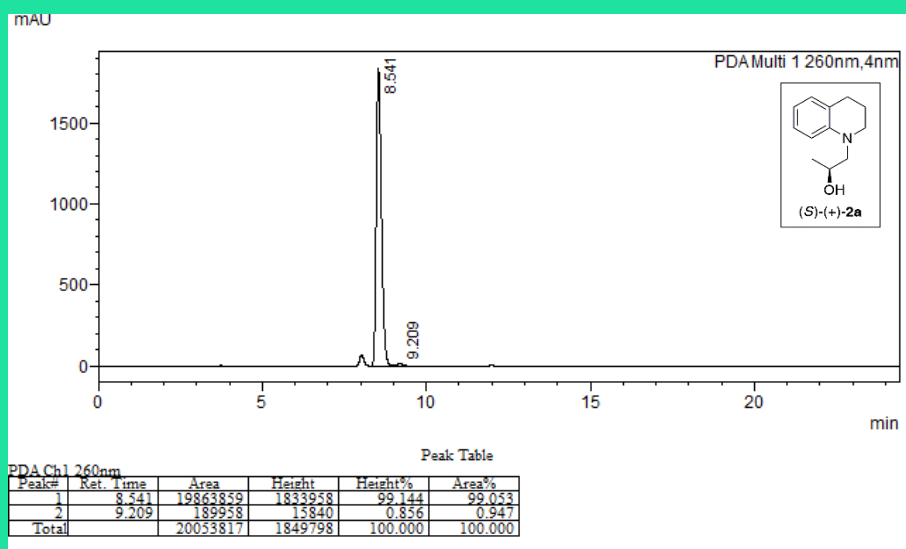
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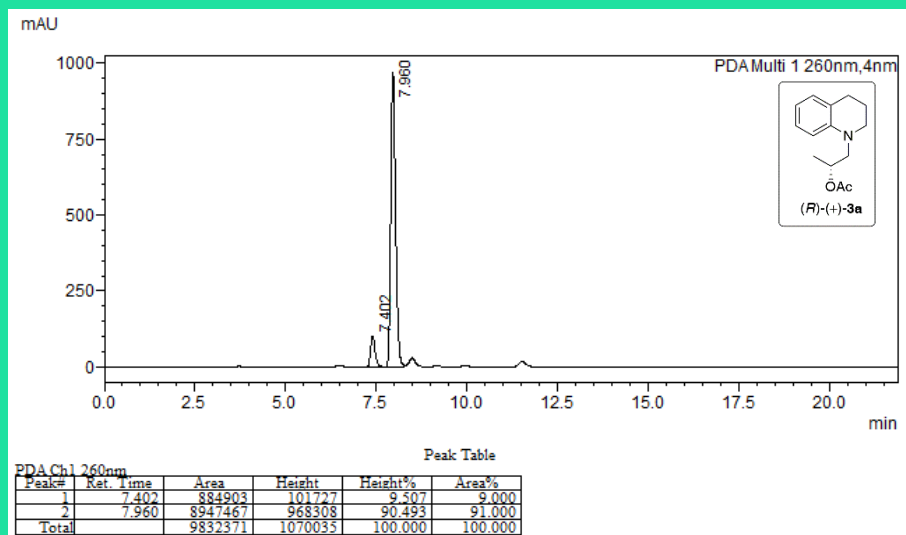
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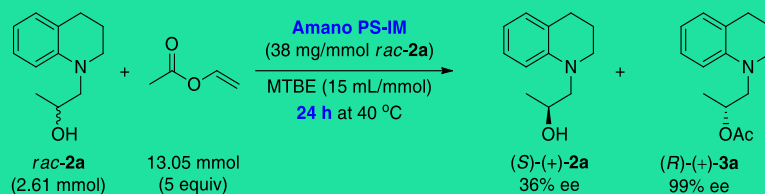
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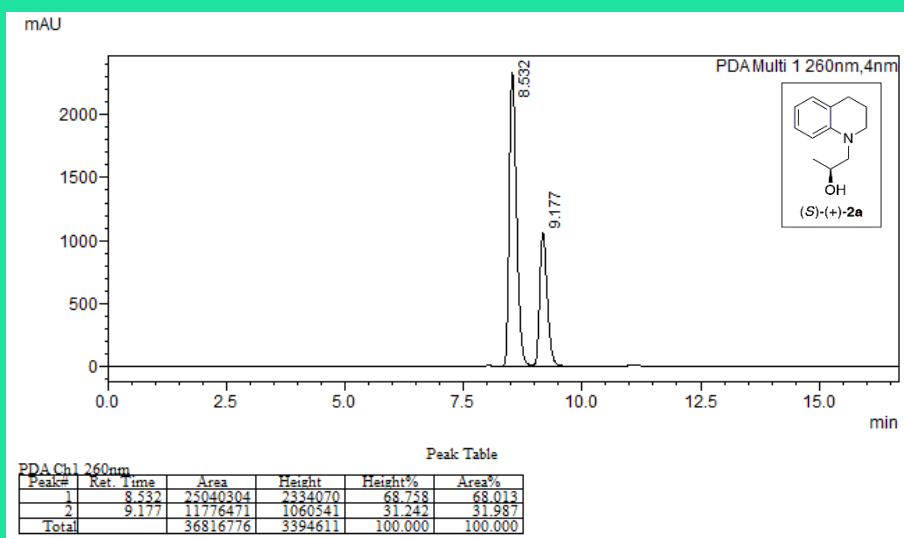
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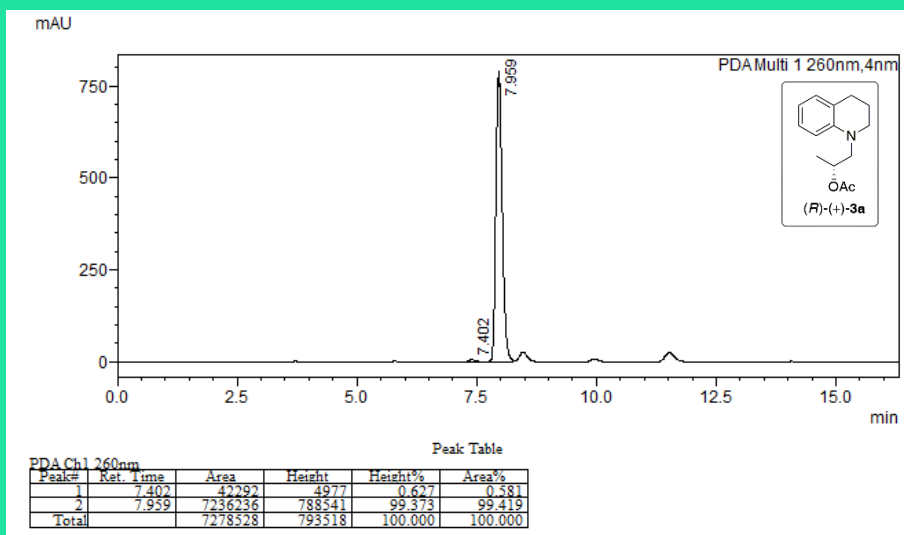
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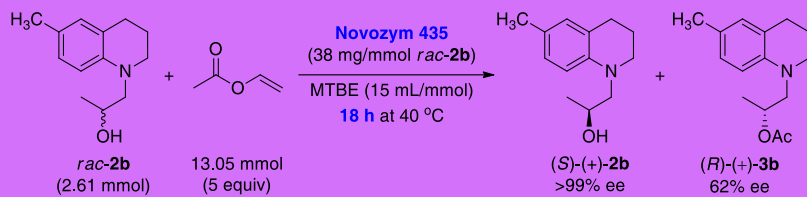
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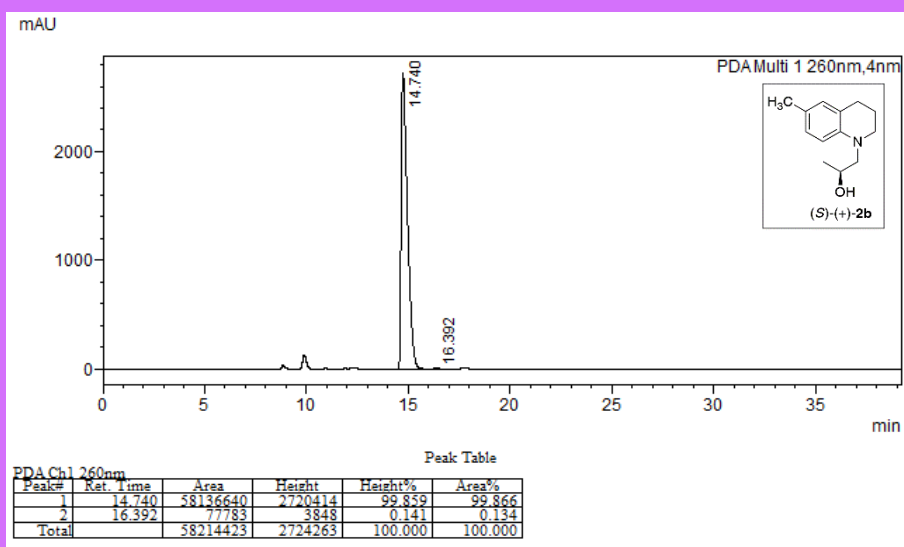
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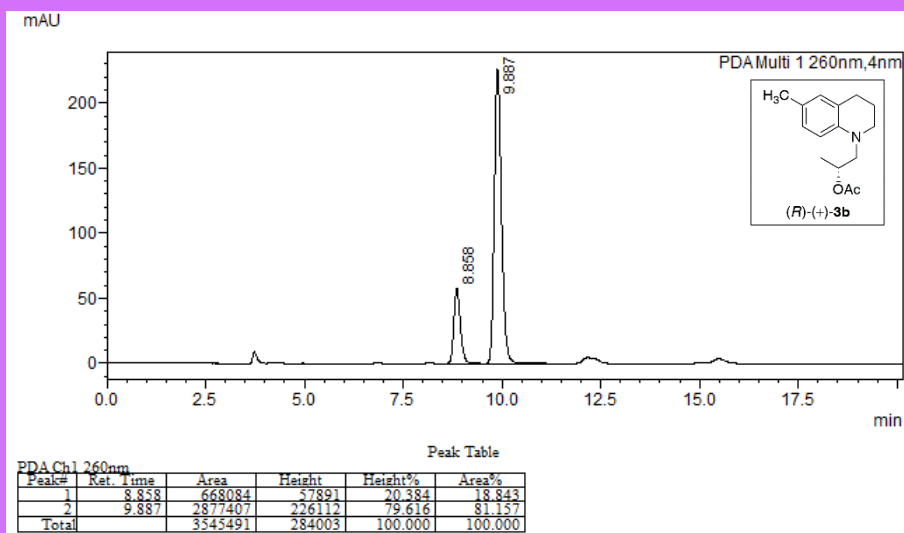
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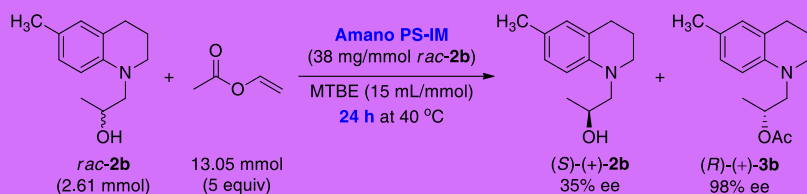
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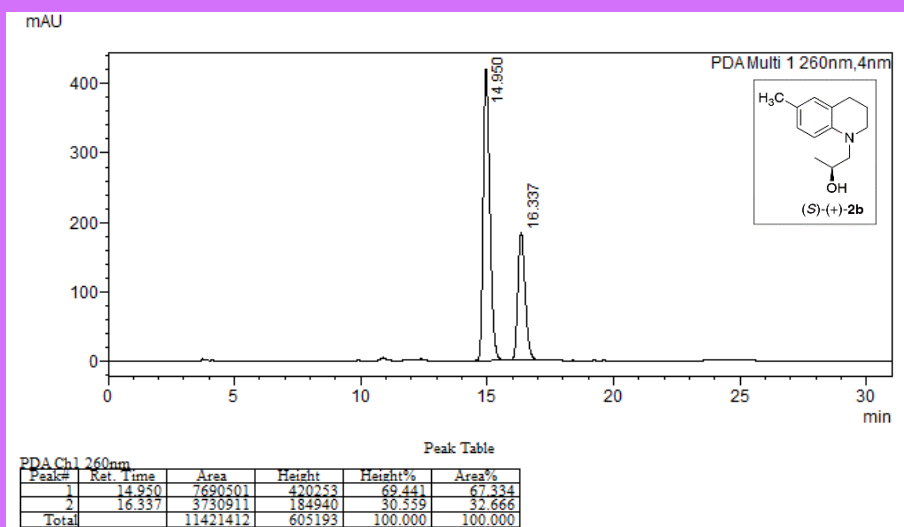
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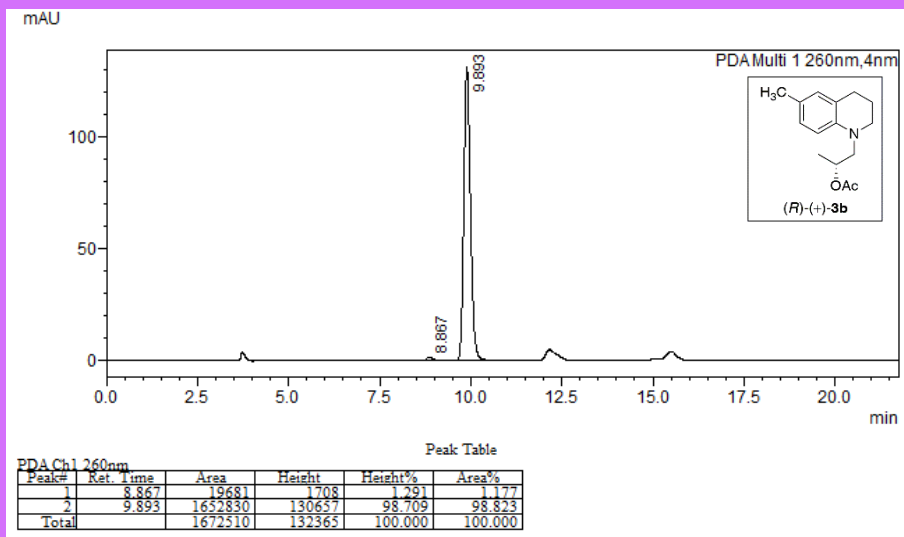
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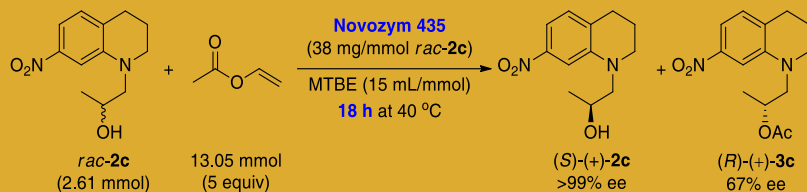
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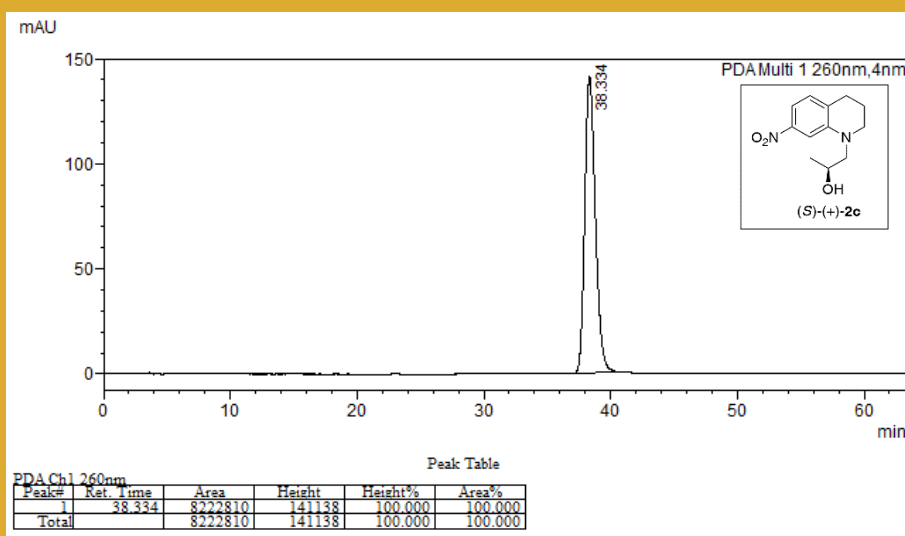
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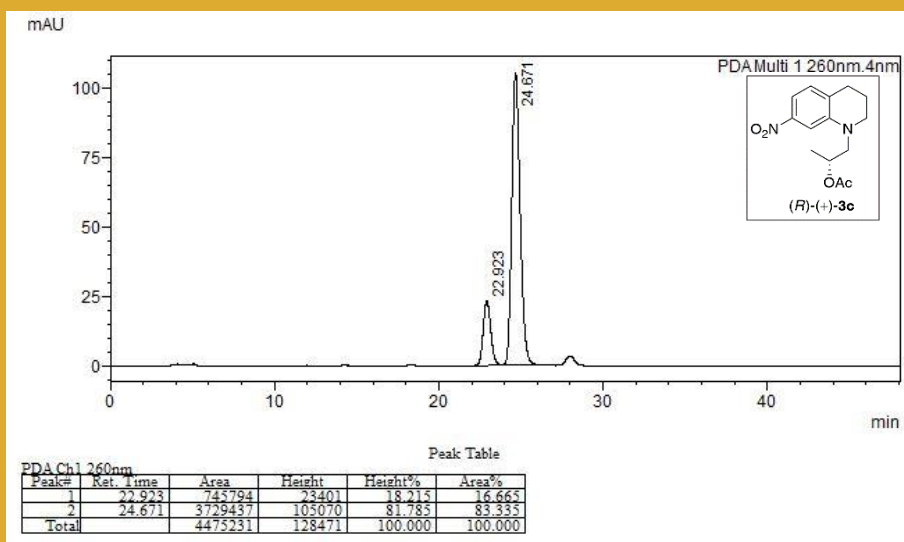
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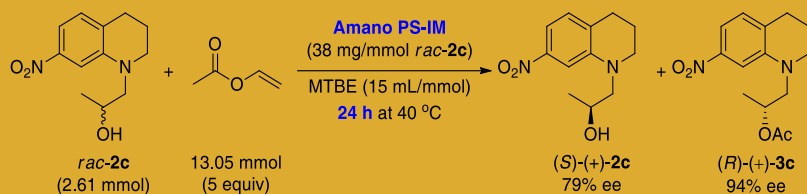
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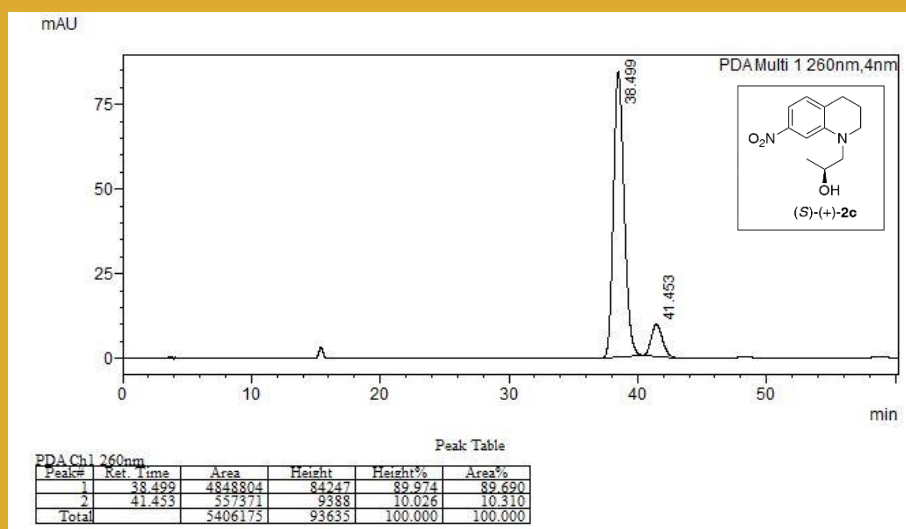
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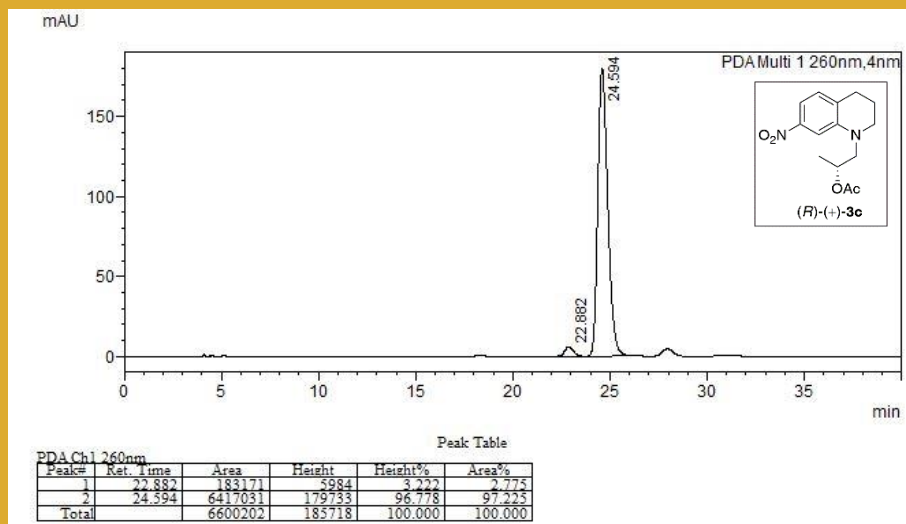
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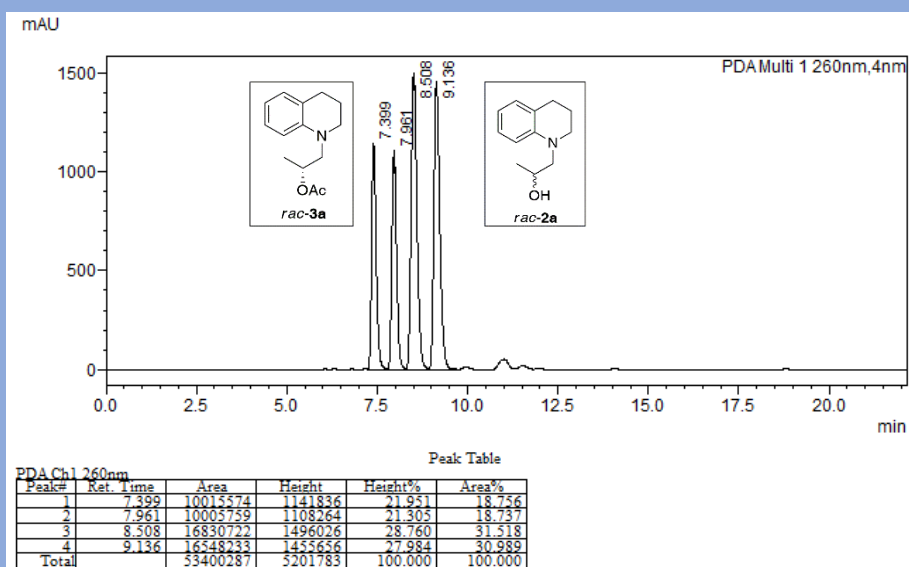
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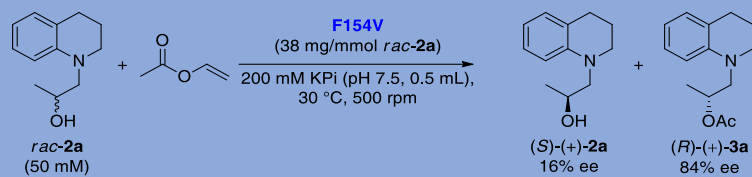
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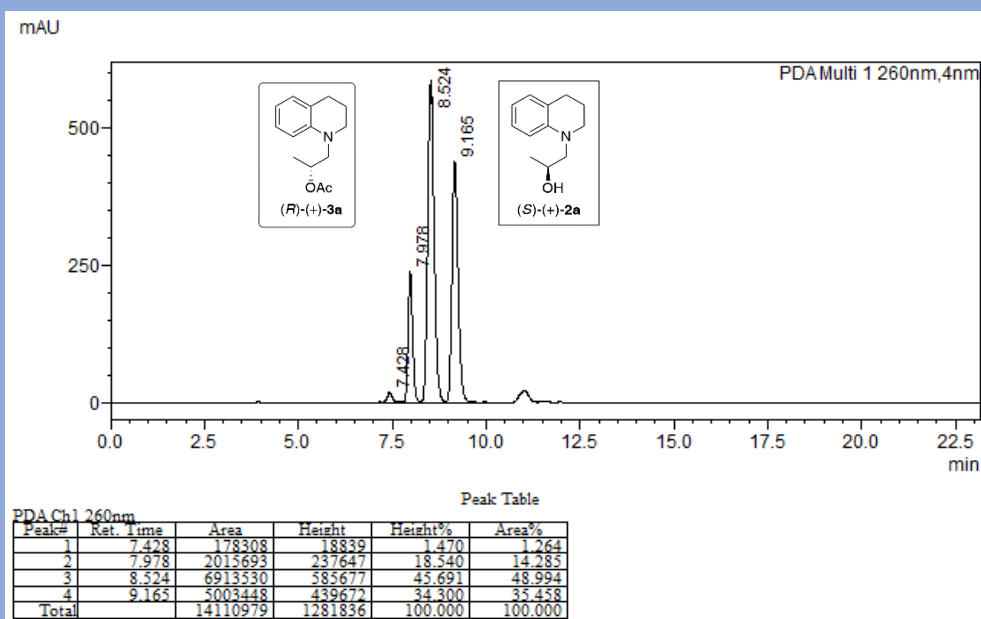
HPLC conditions [for *rac*-2a and *rac*-3a]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



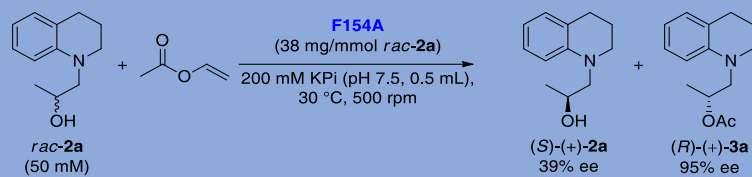
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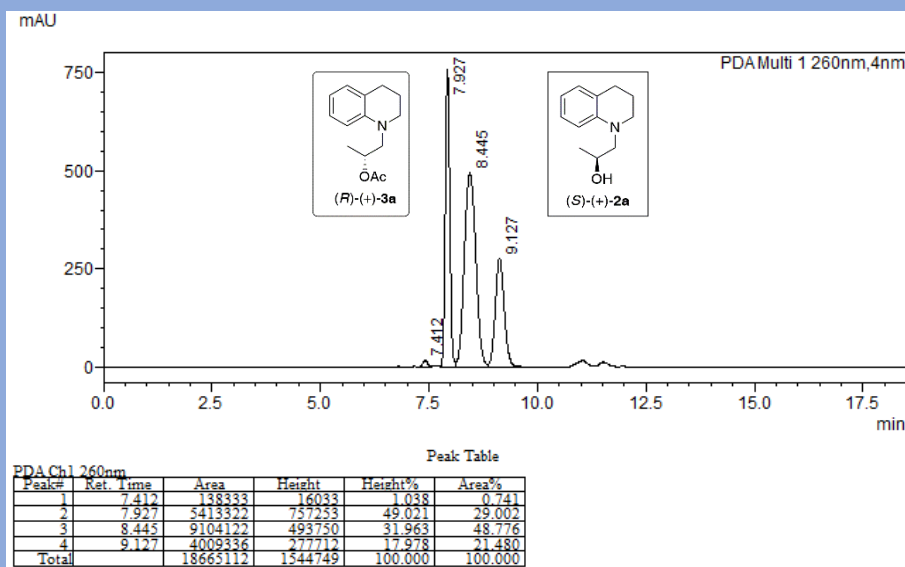
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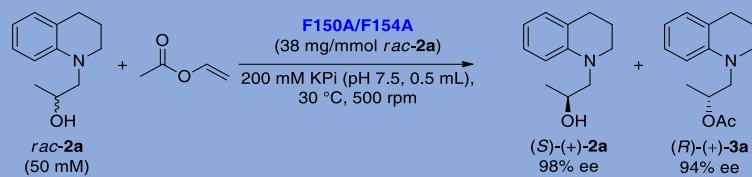
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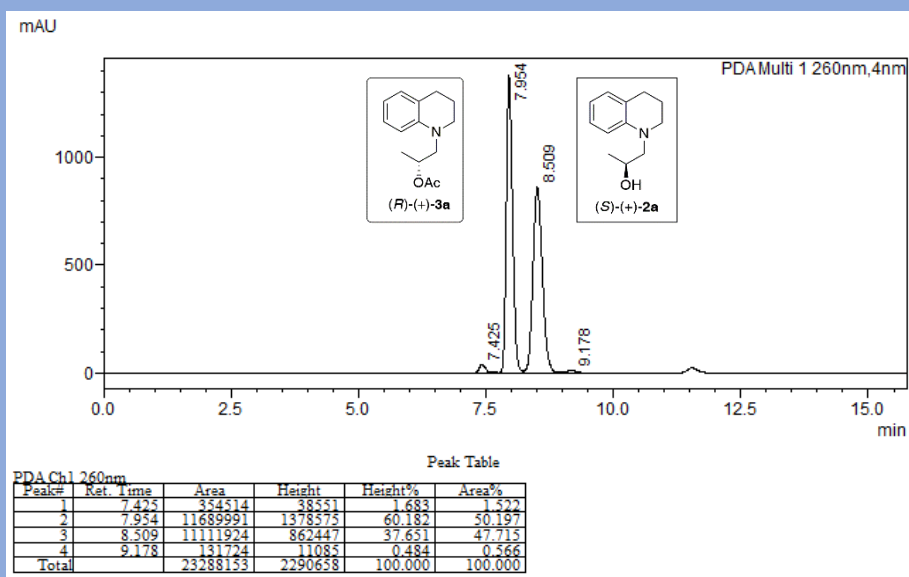
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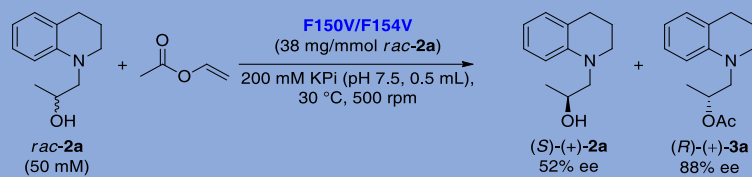
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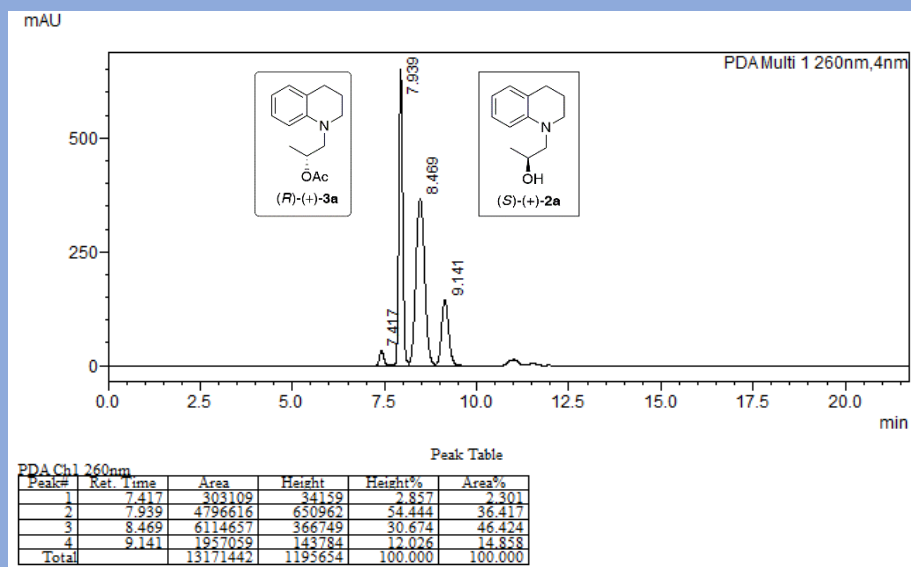
HPLC conditions [for (*S*)-2a and (*R*)-3a]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



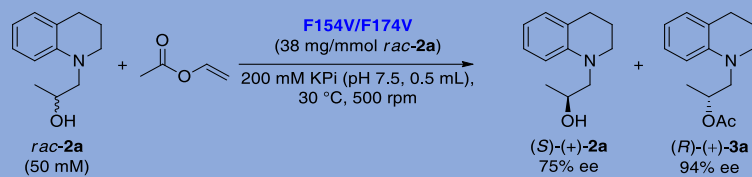
HPLC analysis for the subsequent biocatalytic reaction:



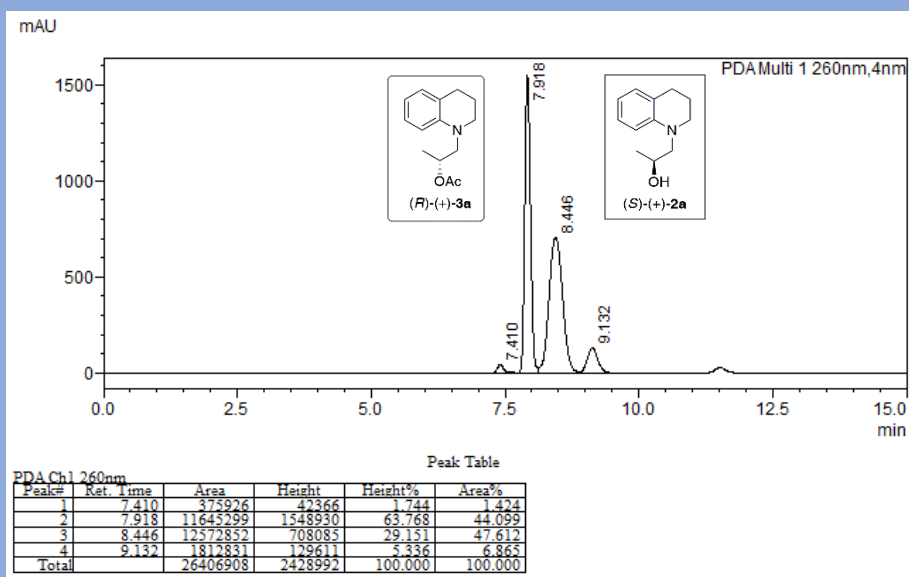
HPLC conditions [for (S)-2a and (R)-3a]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



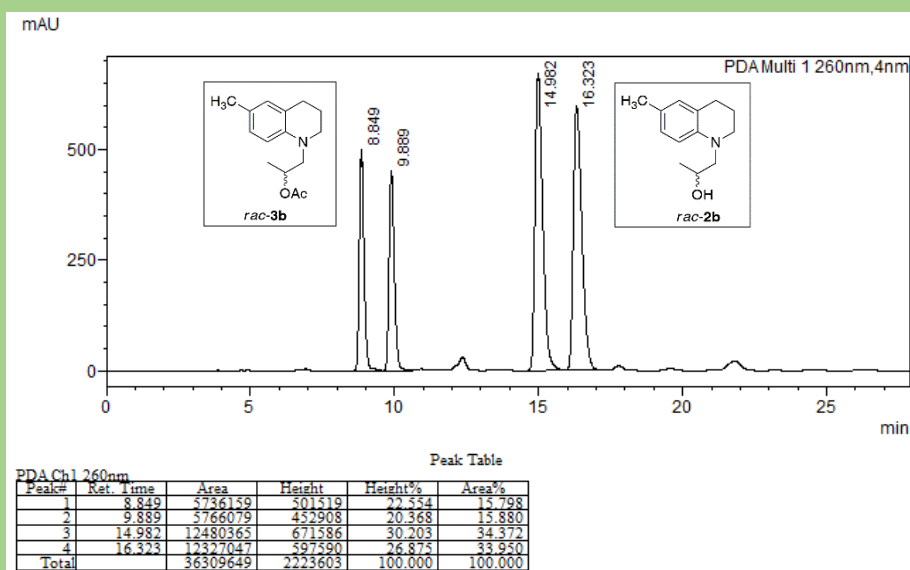
HPLC analysis for the subsequent biocatalytic reaction:



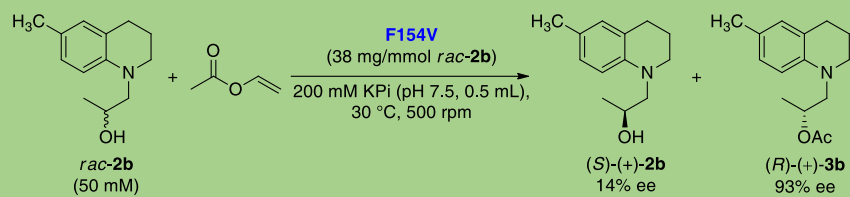
HPLC conditions [for (*S*)-2a and (*R*)-3a]: *n*-hexane-*i*-PrOH (90:10, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



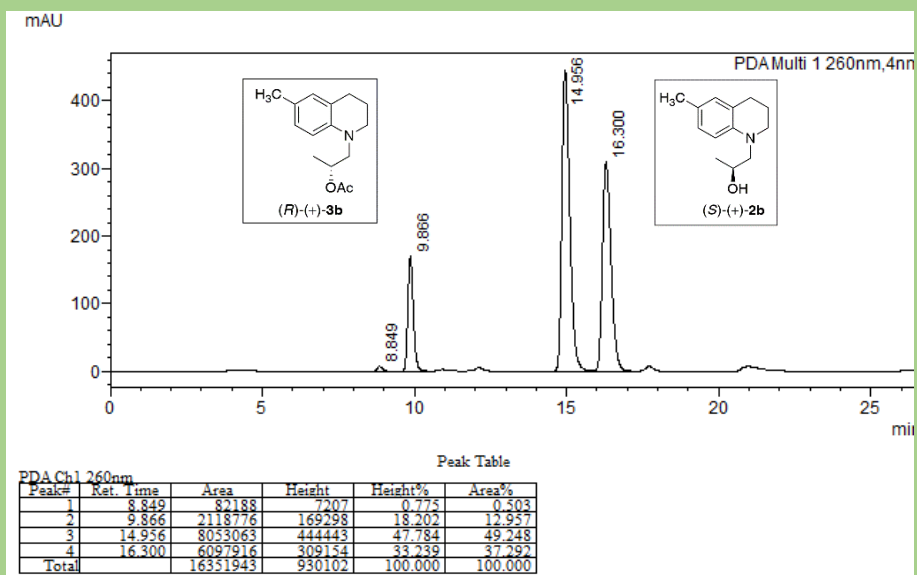
HPLC conditions [for *rac*-2b and *rac*-3b]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



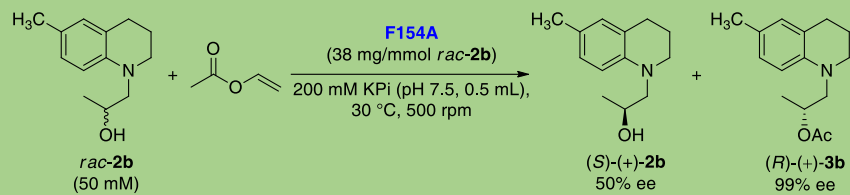
HPLC analysis for the subsequent biocatalytic reaction:



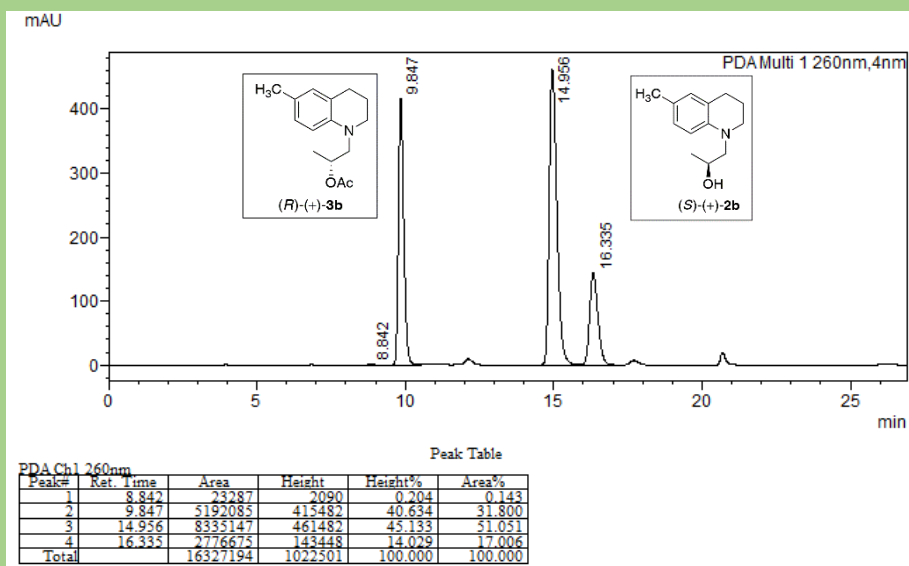
HPLC conditions [for (*S*)-**2b** and (*R*)-**3b**]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



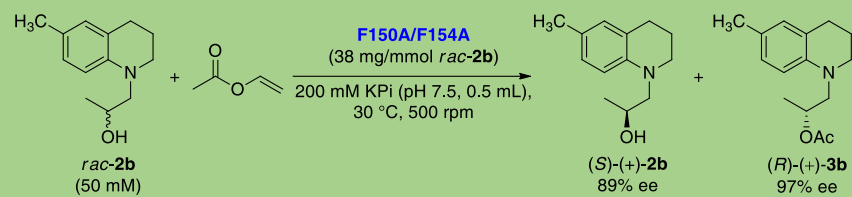
HPLC analysis for the subsequent biocatalytic reaction:



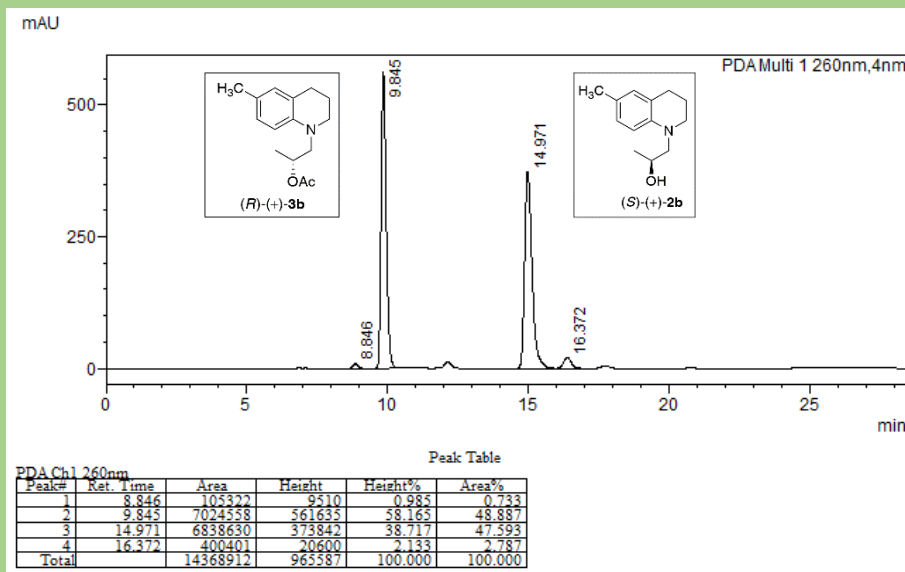
HPLC conditions [for (S)-**2b** and (R)-**3b**]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



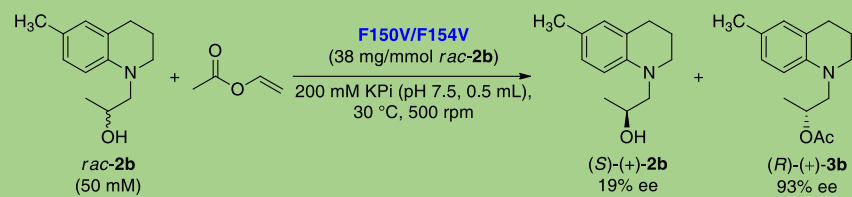
HPLC analysis for the subsequent biocatalytic reaction:



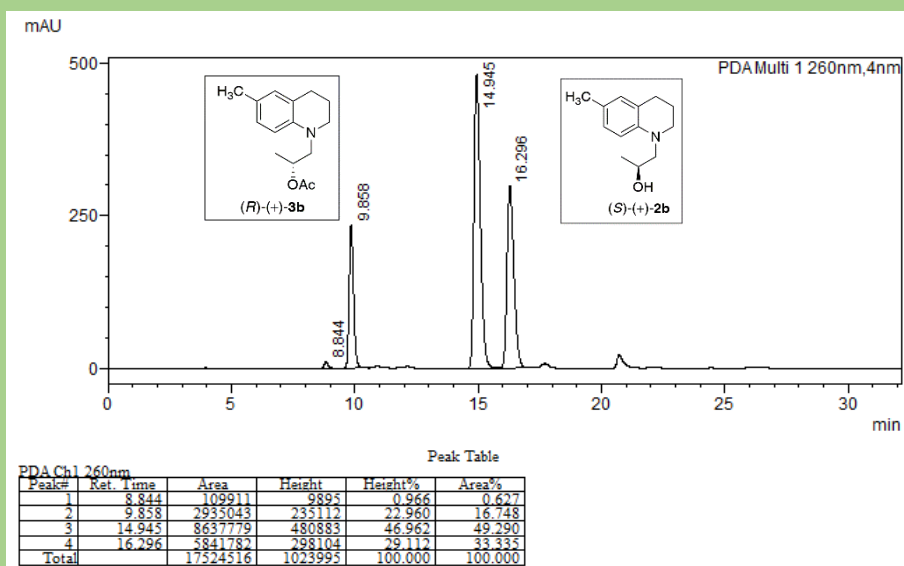
HPLC conditions [for (S)-**2b** and (R)-**3b**]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



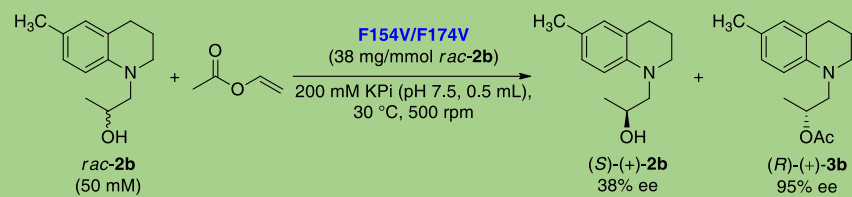
HPLC analysis for the subsequent biocatalytic reaction:



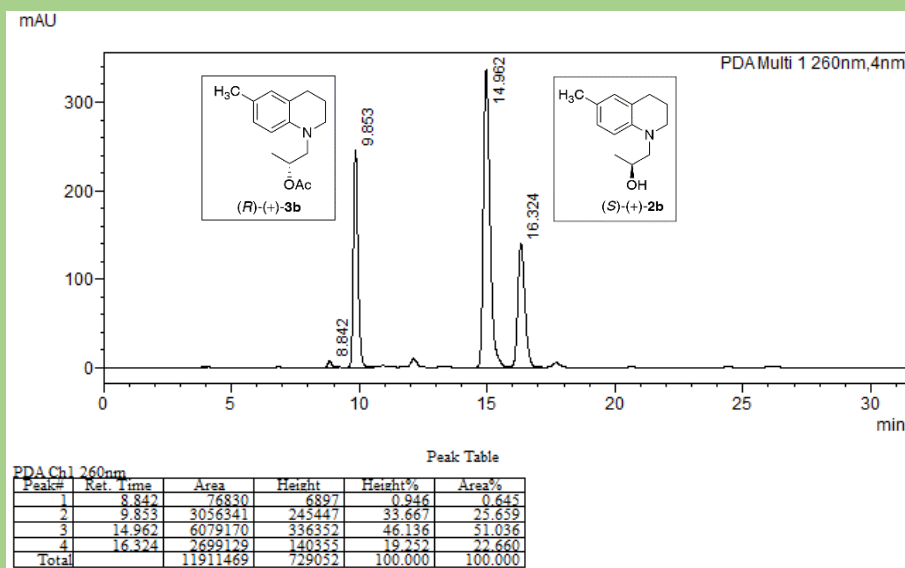
HPLC conditions [for (S)-**2b** and (R)-**3b**]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



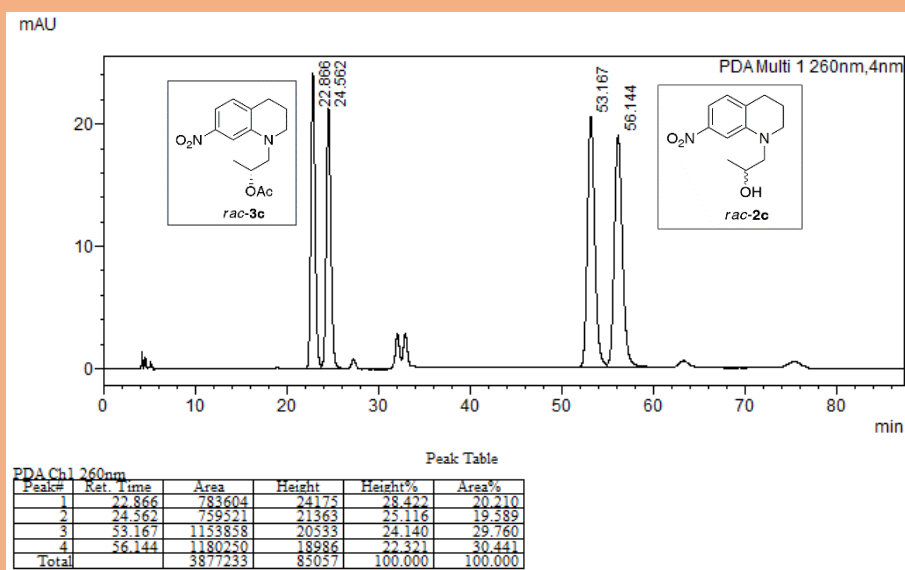
HPLC analysis for the subsequent biocatalytic reaction:



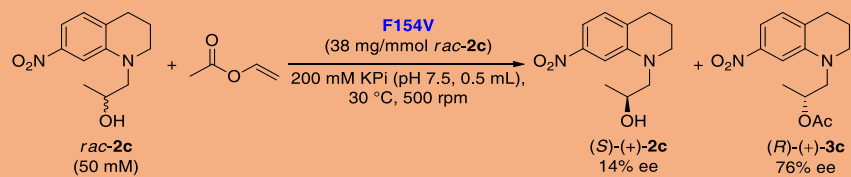
HPLC conditions [for (S)-**2b** and (R)-**3b**]: *n*-hexane-*i*-PrOH (97:3, v/v); *f*=0.8 mL/min; λ =260 nm; Chiralcel OJ-H



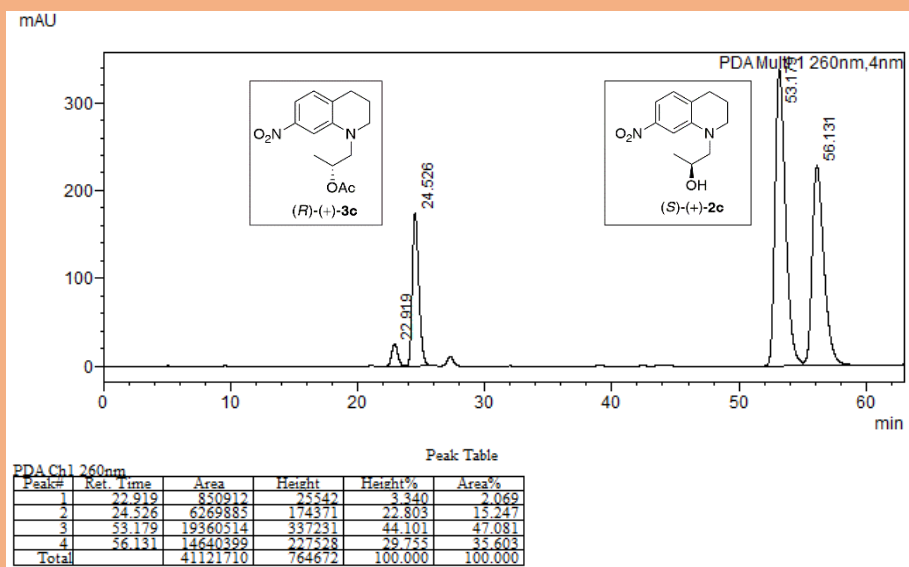
HPLC conditions [for *rac*-2c and *rac*-3c]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ =260 nm; Chiralcel OD-H



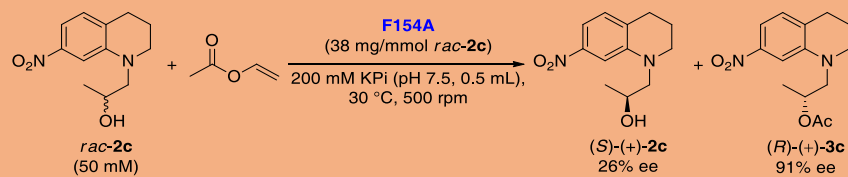
HPLC analysis for the subsequent biocatalytic reaction:



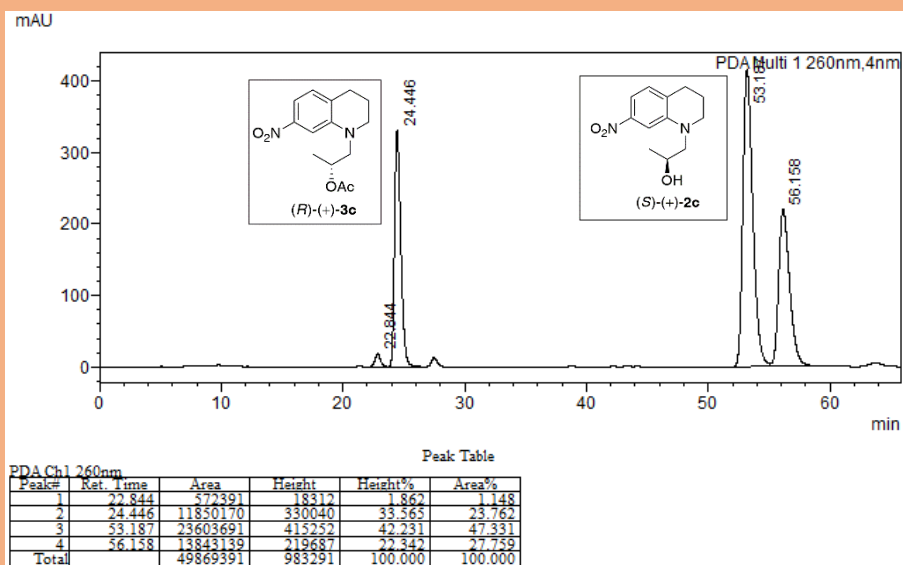
HPLC conditions [for (*S*)-**2c** and (*R*)-**3c**]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ=260 nm; Chiralcel OD-H



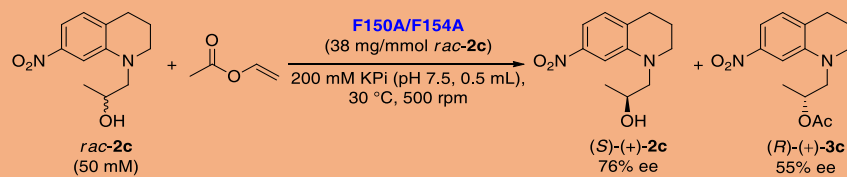
HPLC analysis for the subsequent biocatalytic reaction:



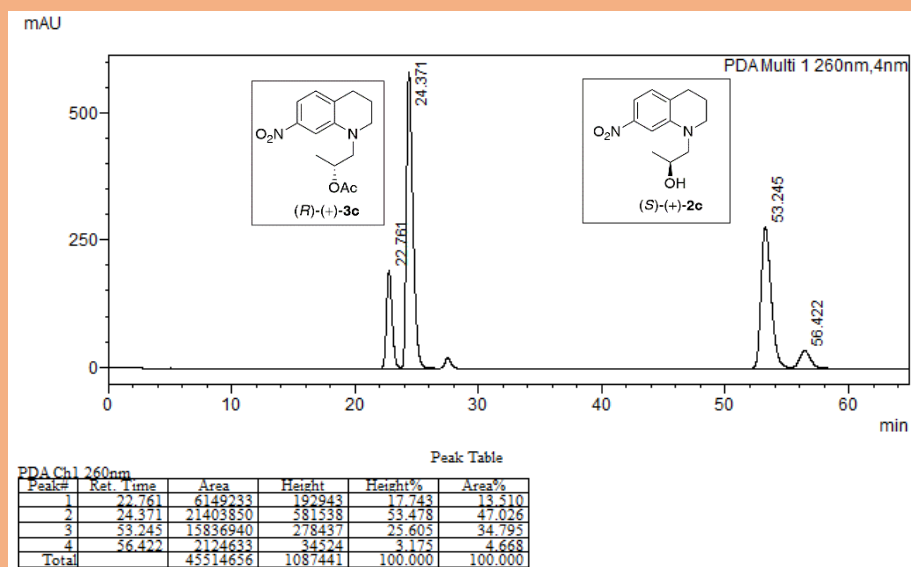
HPLC conditions [for $(S)\text{-2c}$ and $(R)\text{-3c}$]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ =260 nm; Chiralcel OD-H



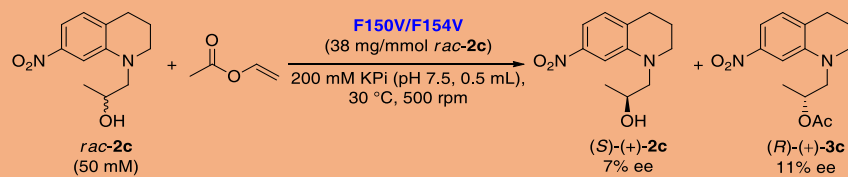
HPLC analysis for the subsequent biocatalytic reaction:



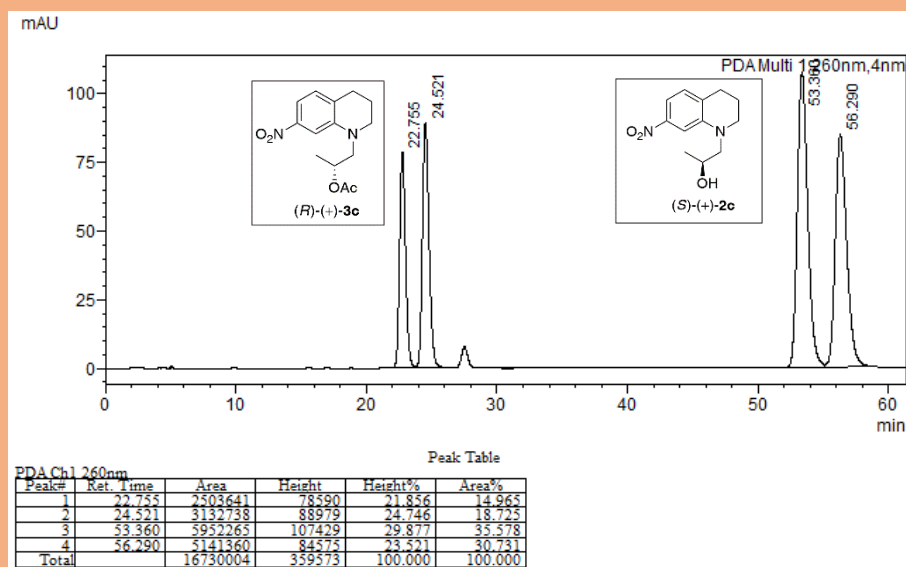
HPLC conditions [for (*S*)-**2c** and (*R*)-**3c**]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ=260 nm; Chiralcel OD-H



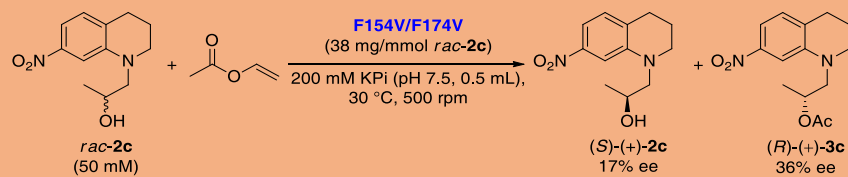
HPLC analysis for the subsequent biocatalytic reaction:



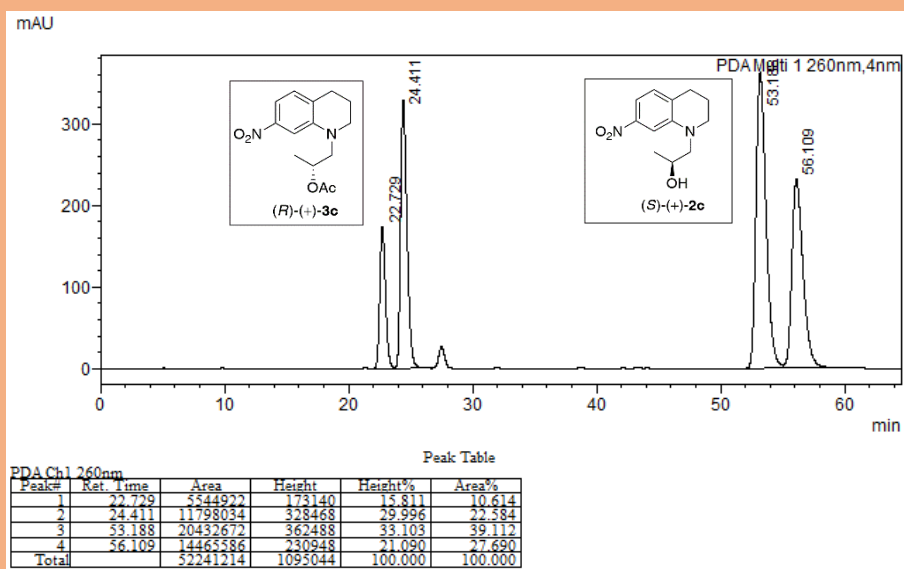
HPLC conditions [for (*S*)-**2c** and (*R*)-**3c**]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ=260 nm; Chiralcel OD-H



HPLC analysis for the subsequent biocatalytic reaction:

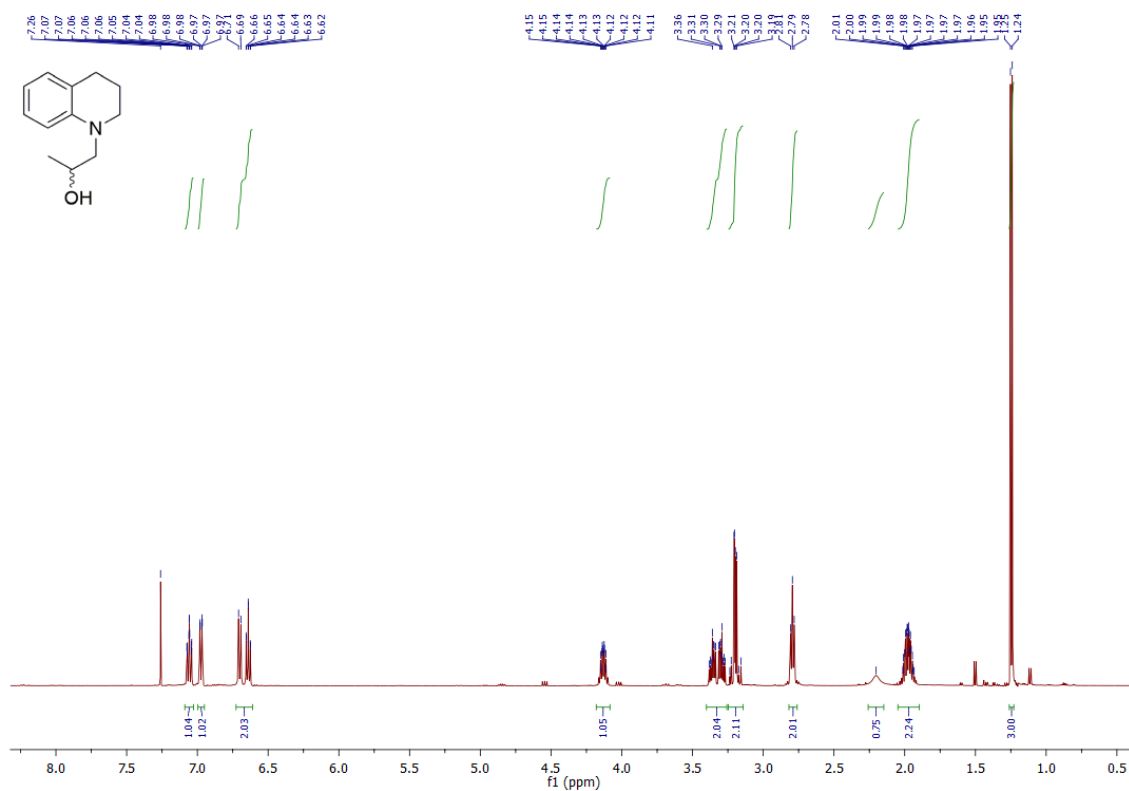


HPLC conditions [for $(S)\text{-2c}$ and $(R)\text{-3c}$]: 0-25 min: *n*-hexane-*i*-PrOH (99:1, v/v); f=0.7 mL/min; 25-70 min: *n*-hexane-*i*-PrOH (98:2, v/v); f=0.8 mL/min; λ =260 nm; Chiralcel OD-H

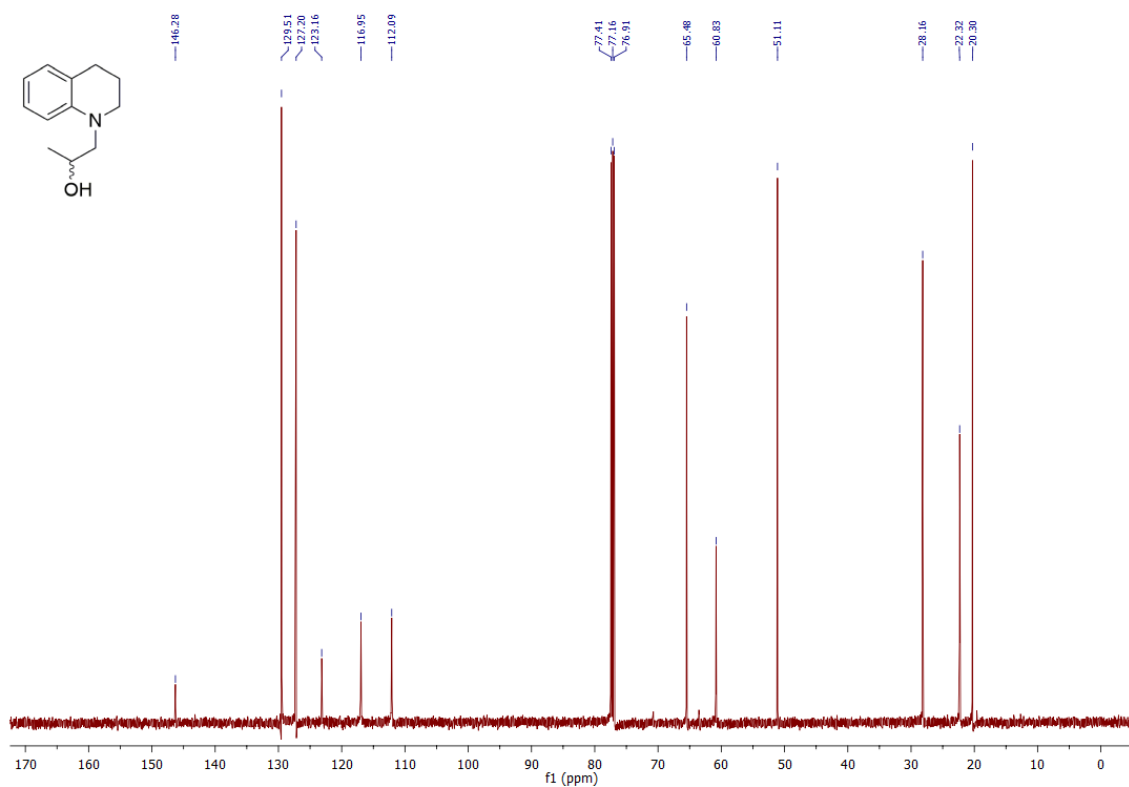


1-(3,4-Dihydroquinolin-1(2H)-yl)propan-2-ol (rac-2a)

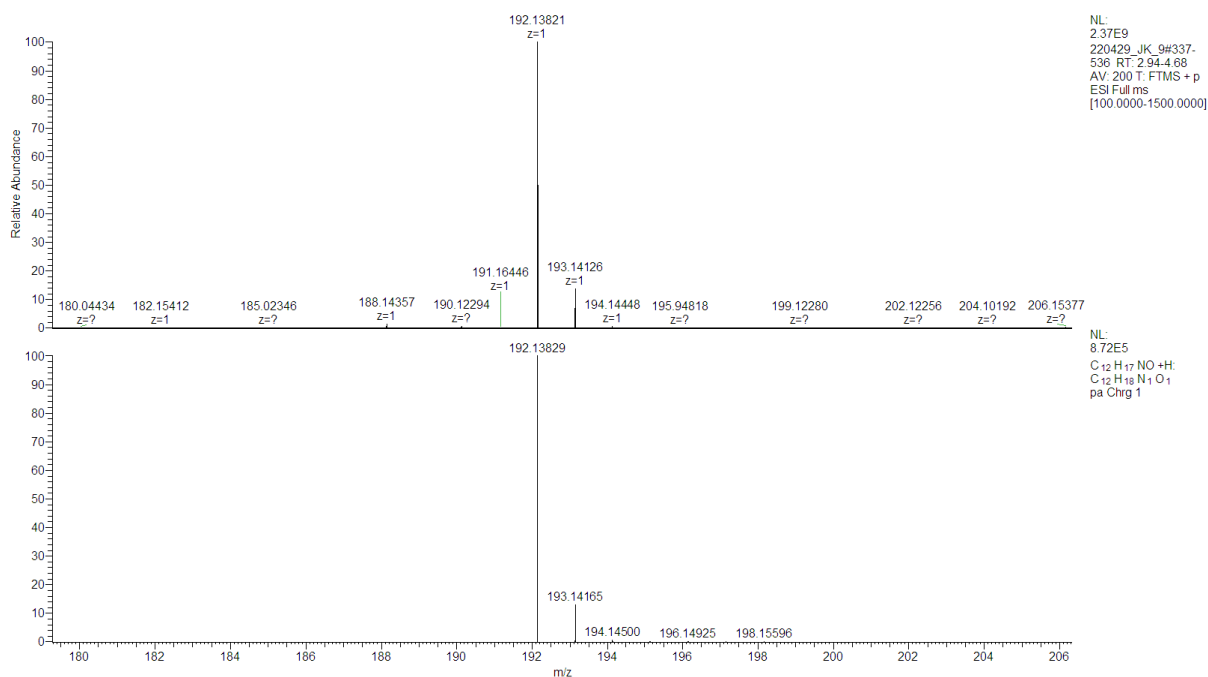
¹H NMR spectrum of *rac-2a* (500 MHz, CDCl₃)



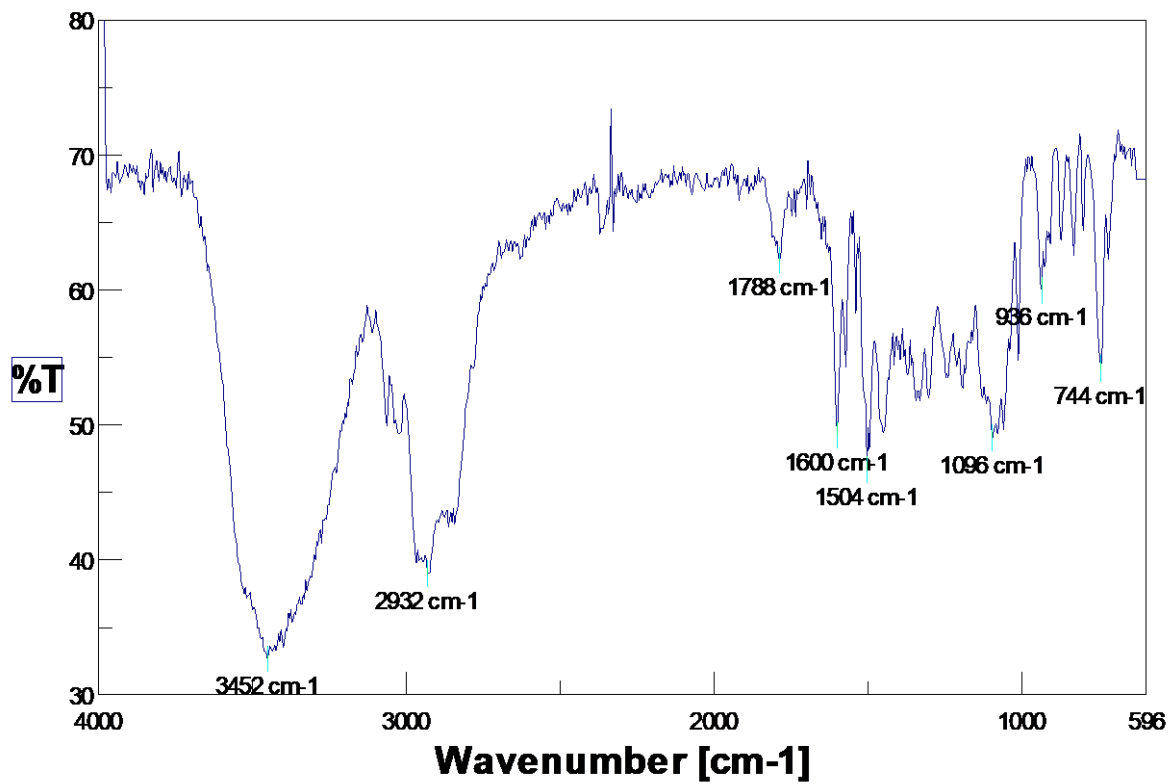
¹³C NMR spectrum of *rac-2a* (126 MHz, CDCl₃)



FTMS spectrum of *rac-2a* (ESI-TOF)

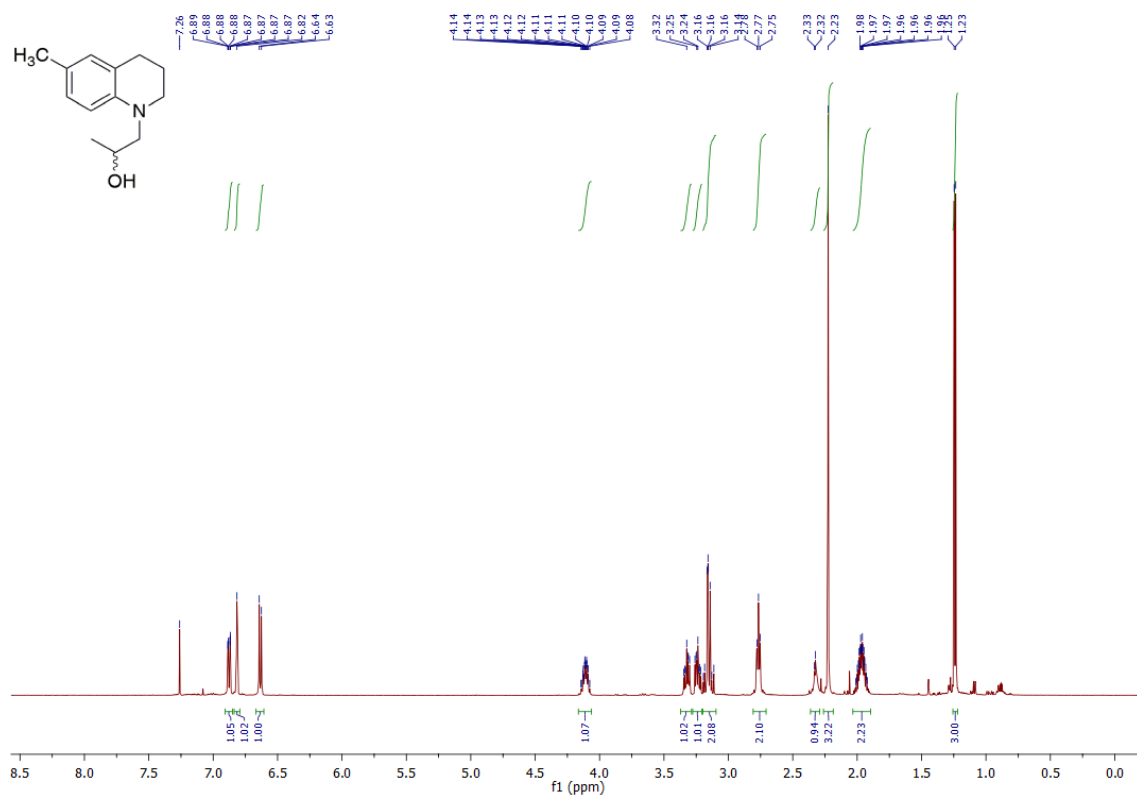


IR spectrum of *rac-2a* (Mineral oil, Nujol)

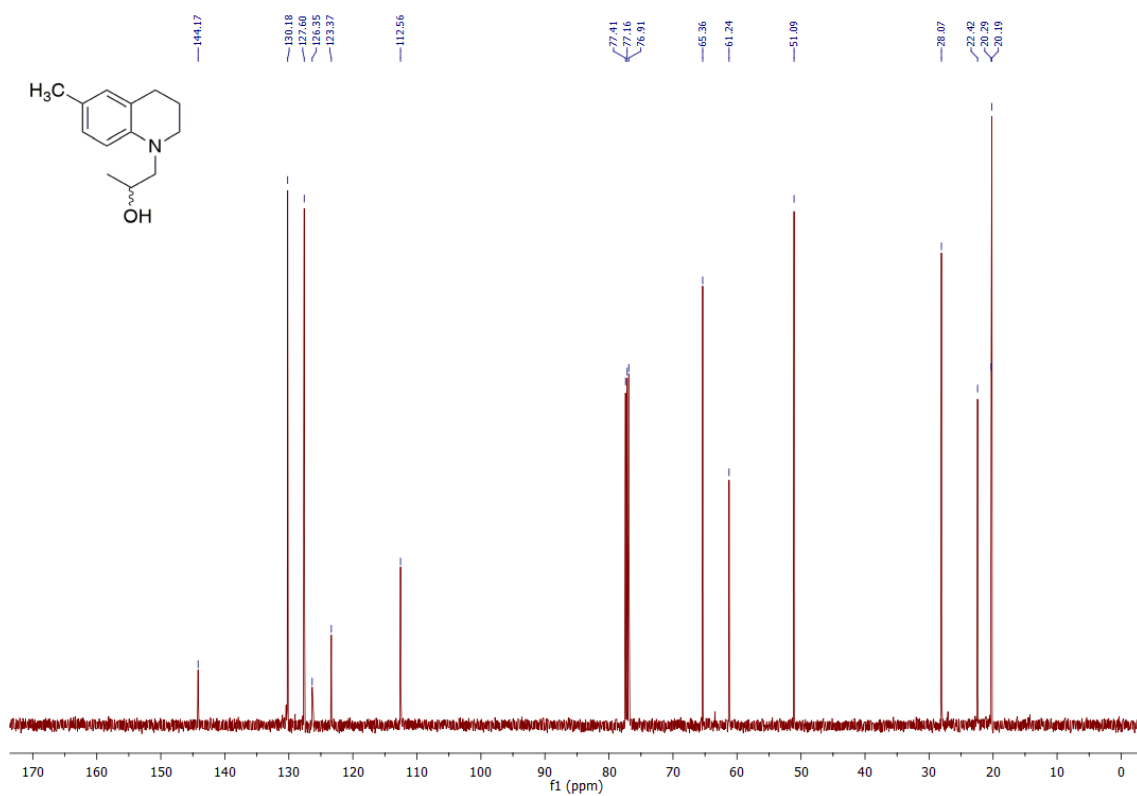


1-(6-Methyl-3,4-dihydroquinolin-1(2H)-yl)propan-2-ol (rac-2b)

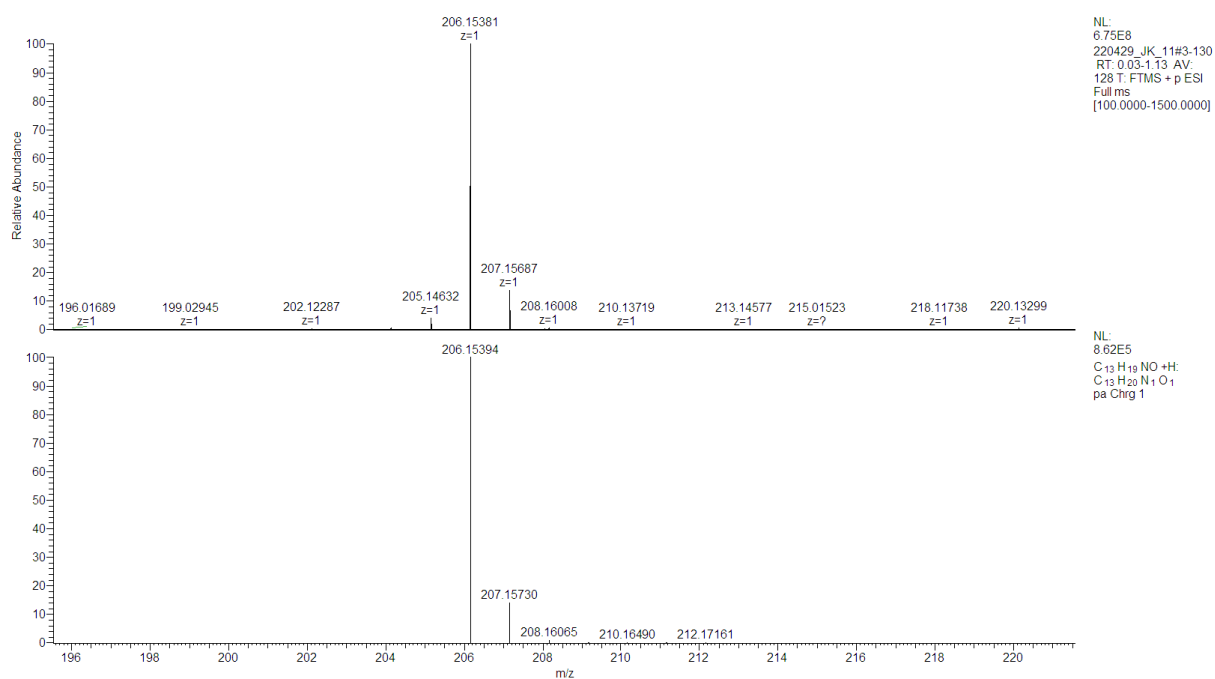
¹H NMR spectrum of *rac-2b* (500 MHz, CDCl₃)



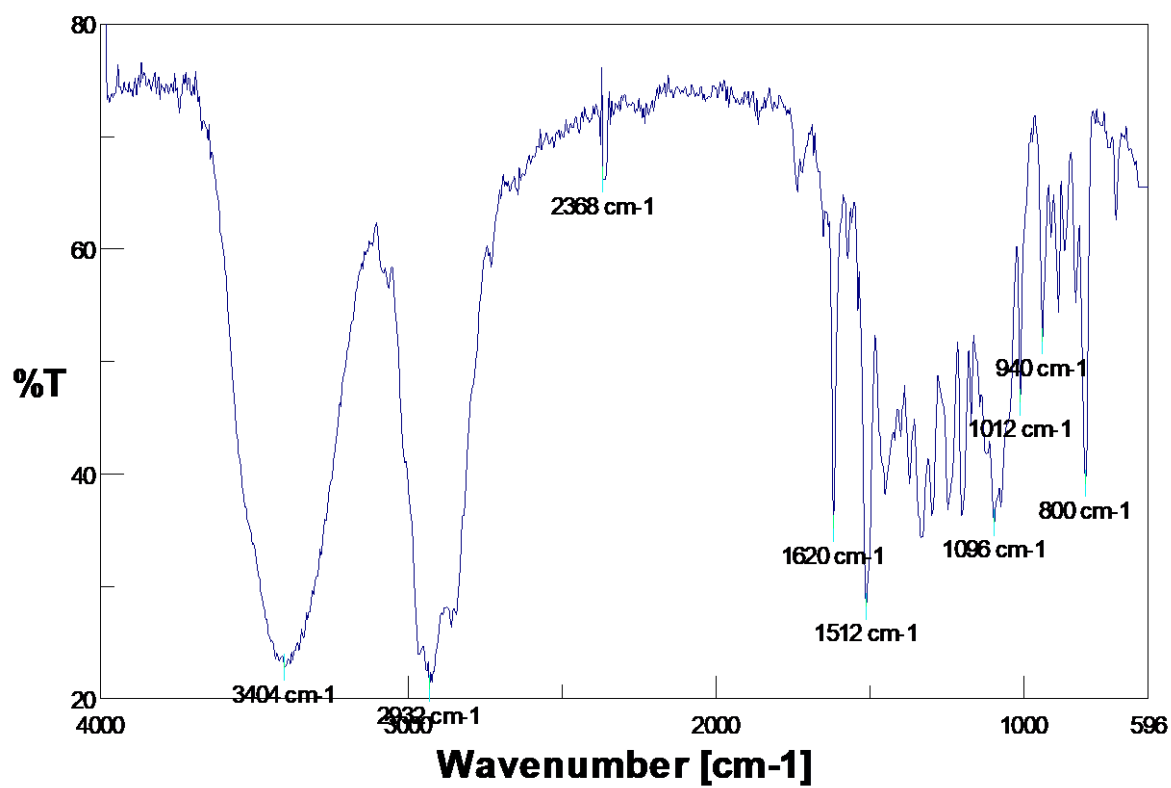
¹³C NMR spectrum of *rac-2b* (126 MHz, CDCl₃)



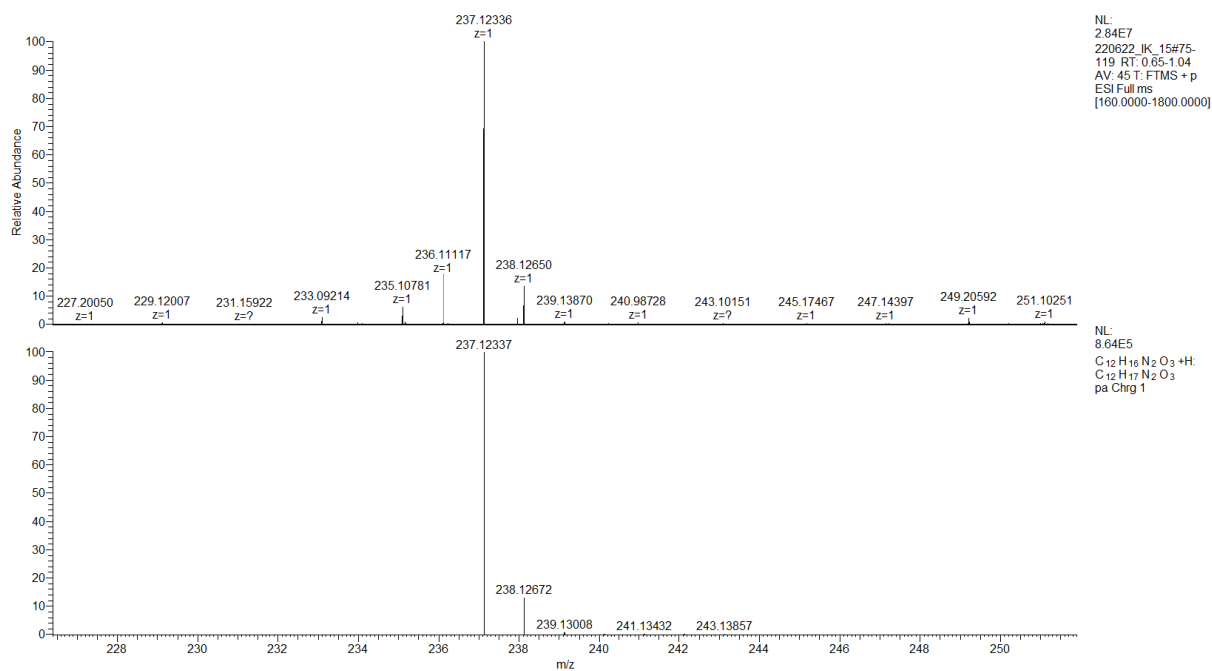
FTMS spectrum of *rac*-**2b** (ESI-TOF)



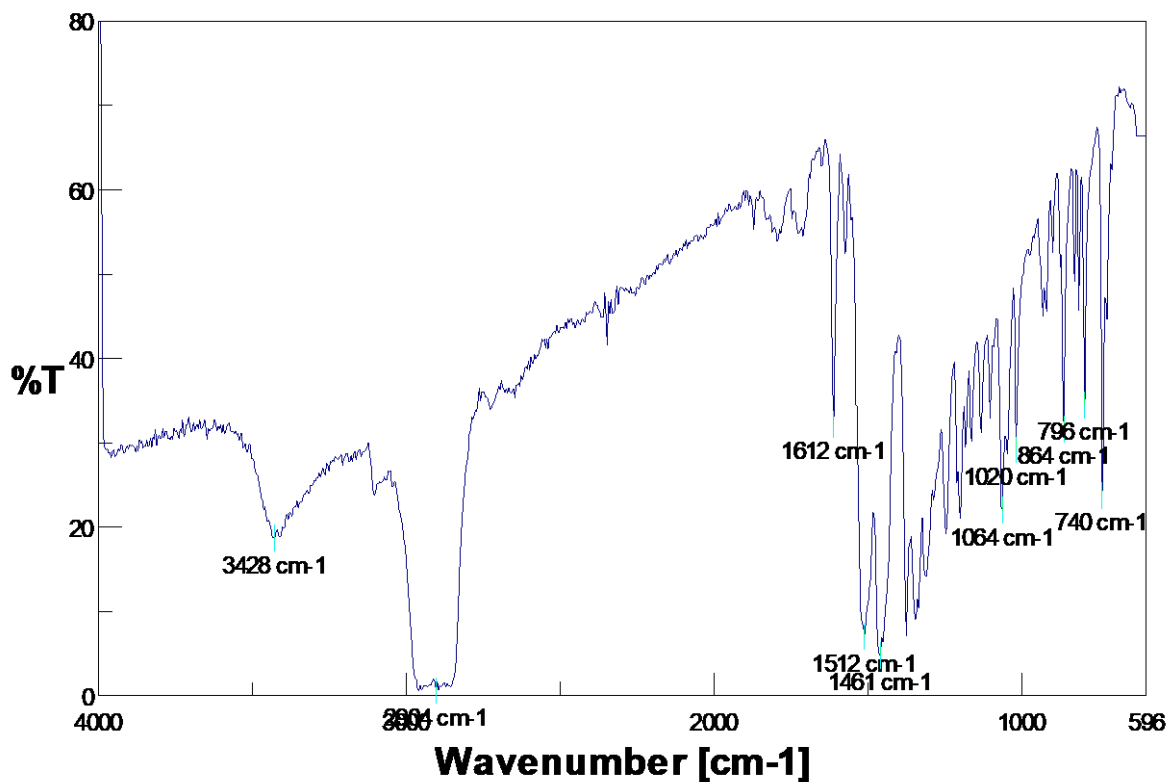
IR spectrum of *rac*-**2b** (Mineral oil, Nujol)



FTMS spectrum of *rac-2c* (ESI-TOF)

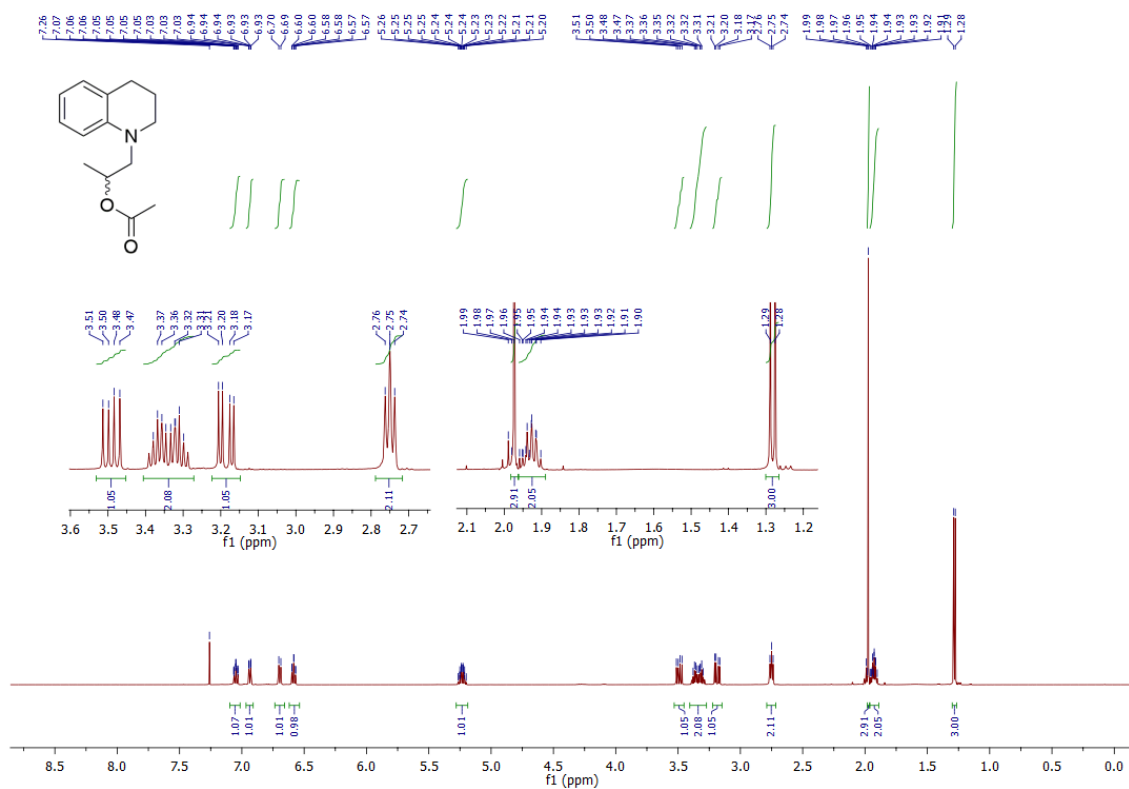


IR spectrum of *rac-2c* (Mineral oil, Nujol)

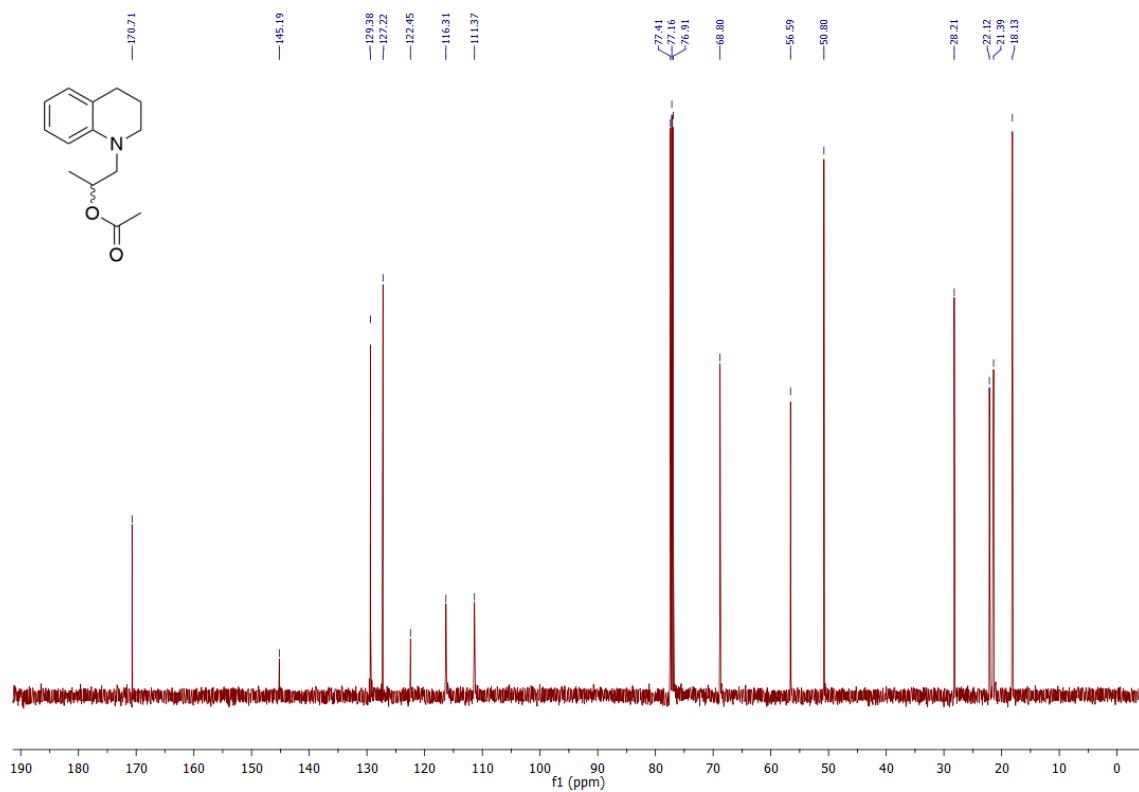


1-(3,4-Dihydroquinolin-1(2H)-yl)propan-2-yl acetate (rac-3a)

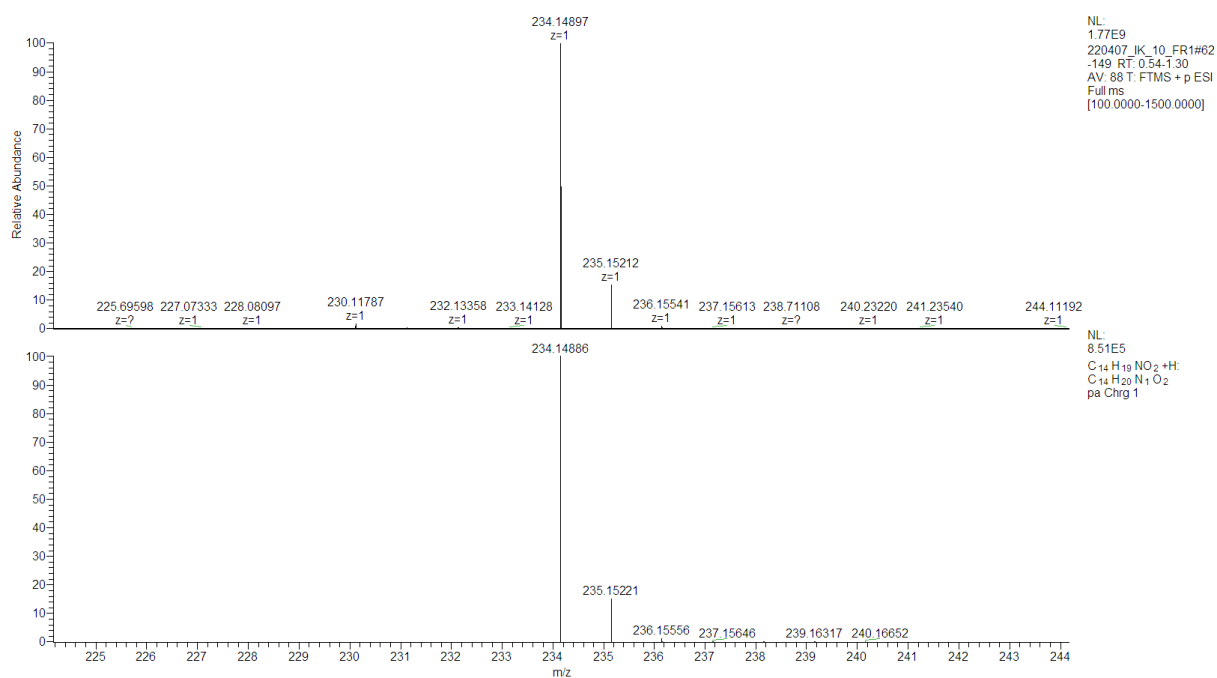
¹H NMR spectrum of *rac-3a* (500 MHz, CDCl₃)



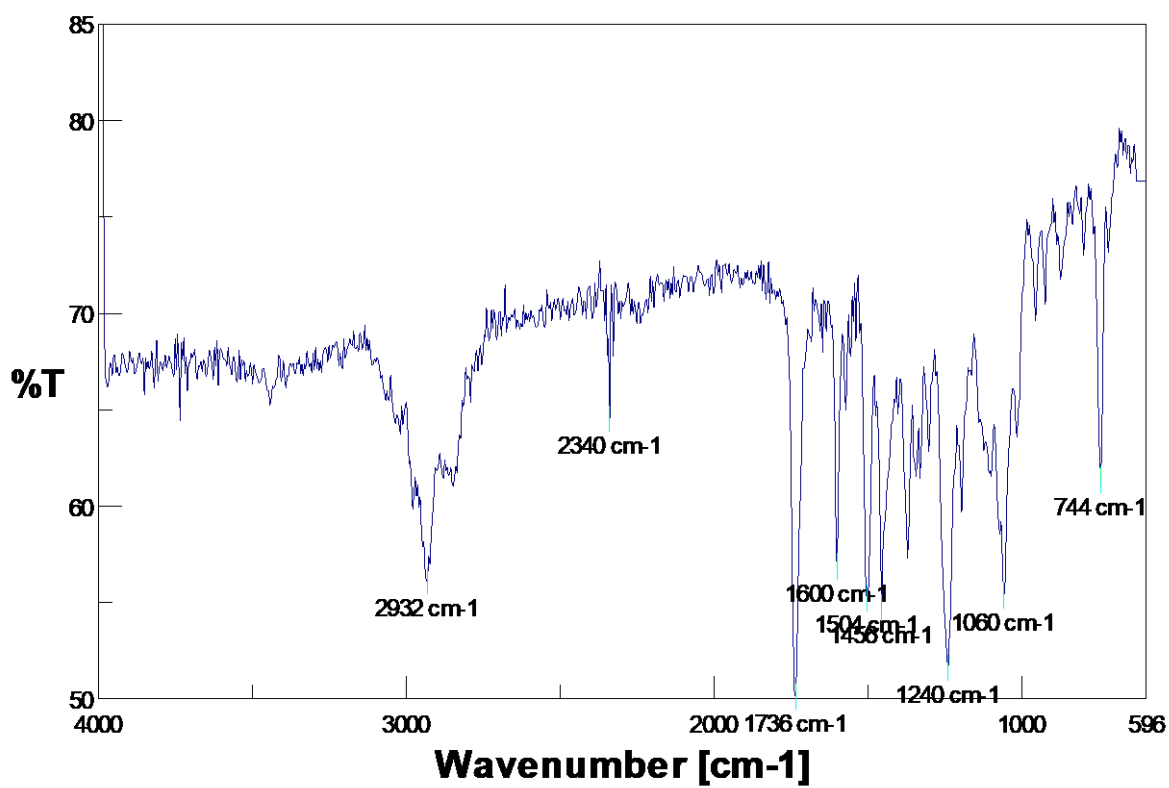
¹³C NMR spectrum of *rac-3a* (126 MHz, CDCl₃)



FTMS spectrum of *rac*-**3a** (ESI-TOF)

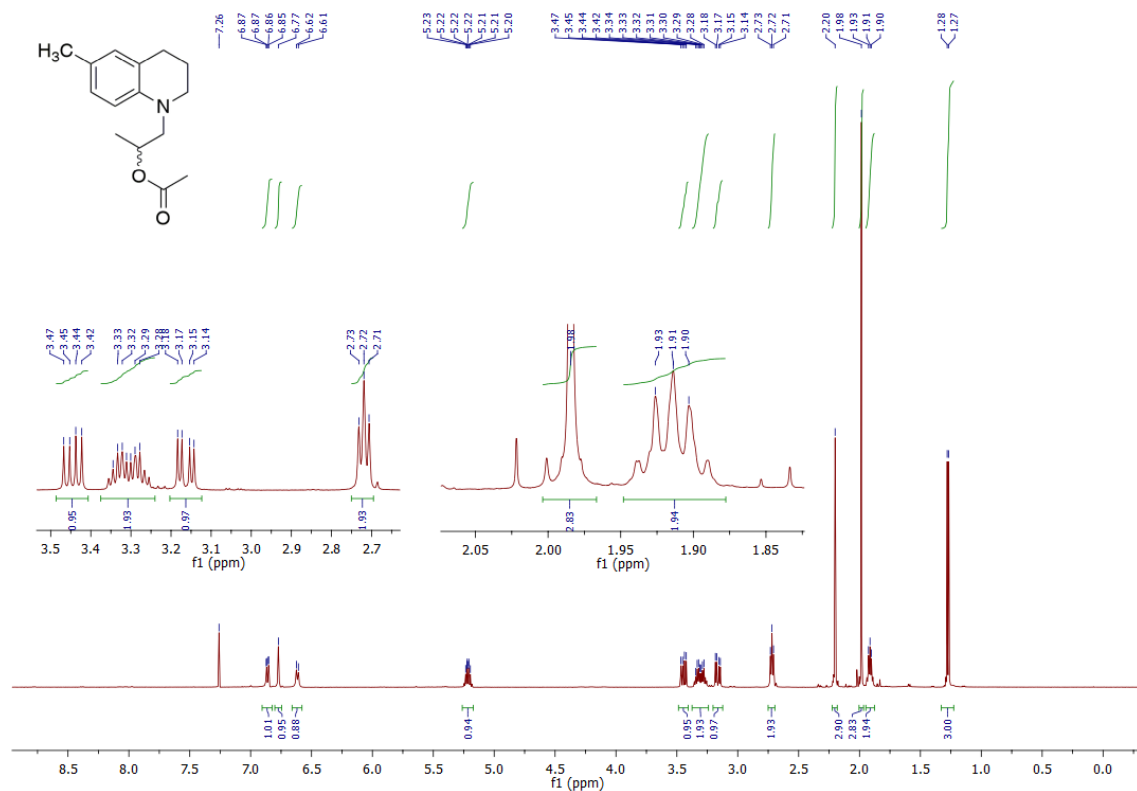


IR spectrum of *rac*-**3a** (Mineral oil, Nujol)

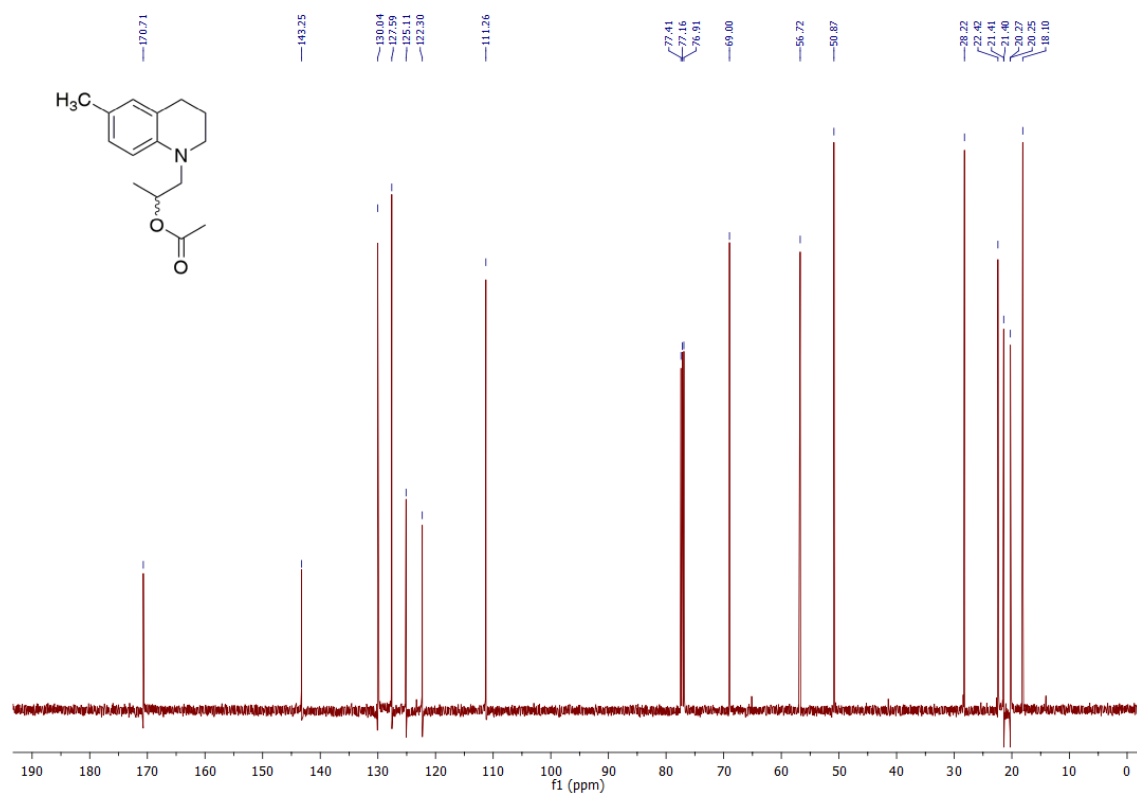


1-(6-Methyl-3,4-dihydroquinolin-1(2H)-yl)propan-2-yl acetate (rac-3b)

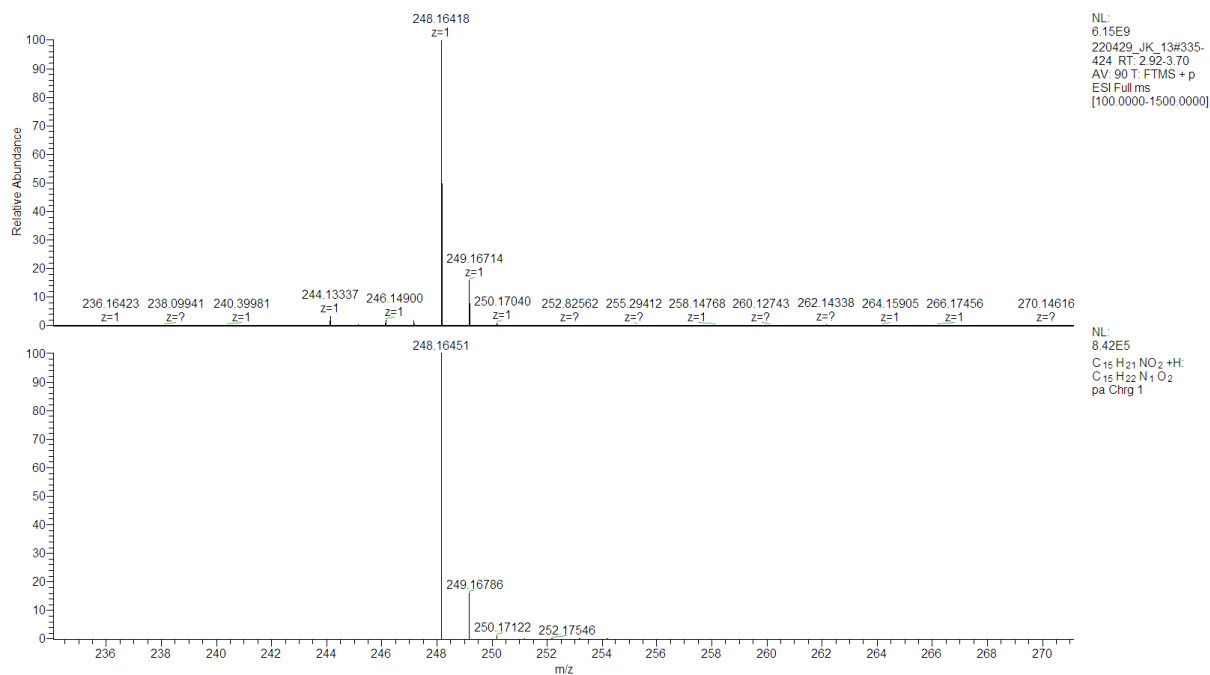
¹H NMR spectrum of *rac-3b* (500 MHz, CDCl₃)



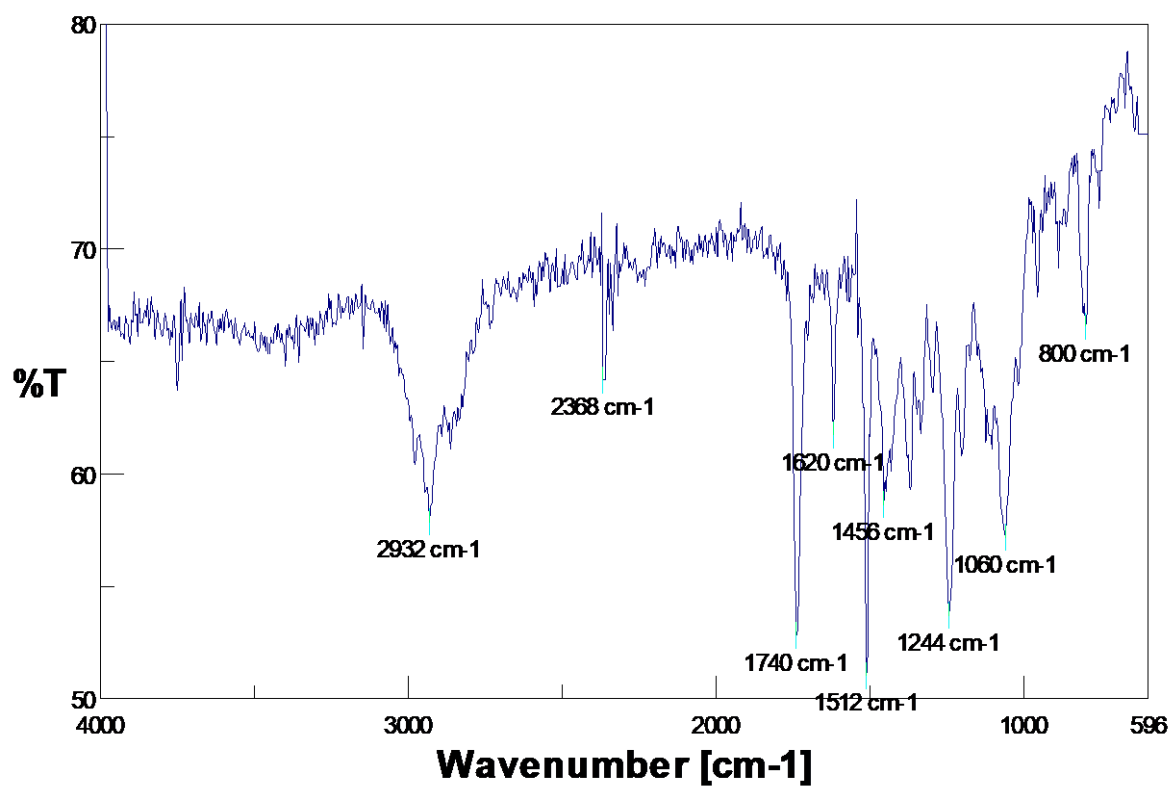
¹³C NMR spectrum of *rac-3b* (126 MHz, CDCl₃)



FTMS spectrum of *rac*-**3b** (ESI-TOF)

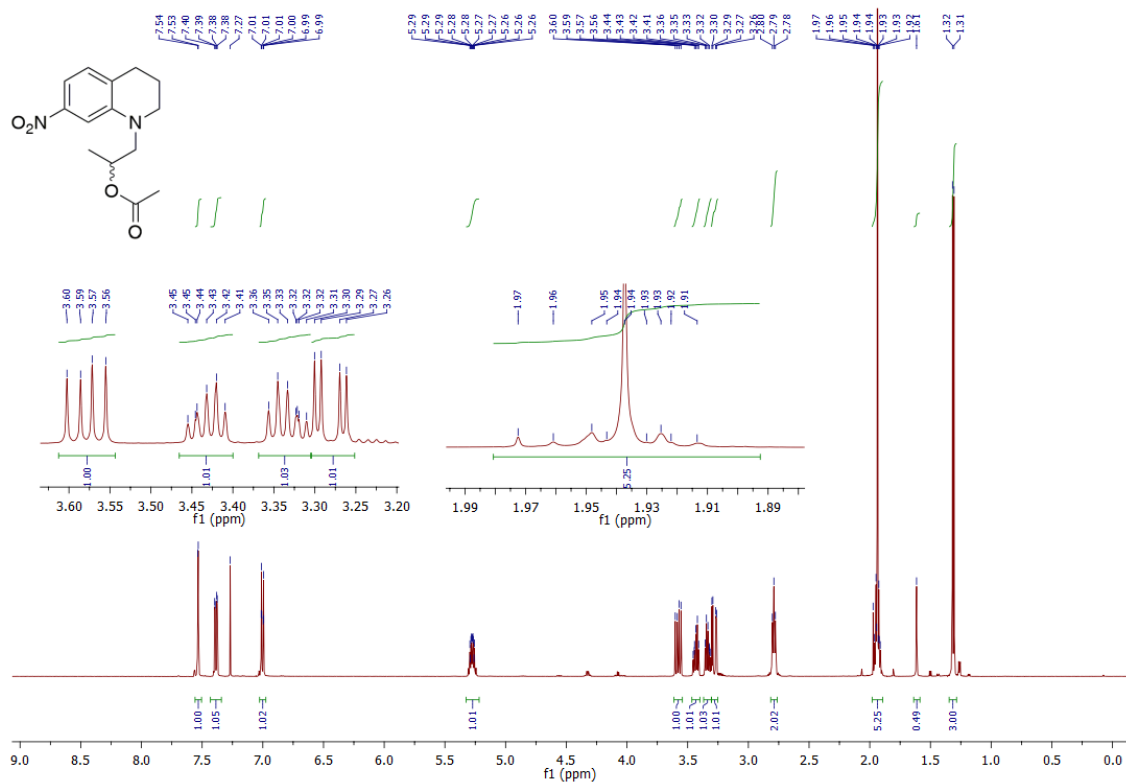


IR spectrum of *rac*-**3b** (Mineral oil, Nujol)

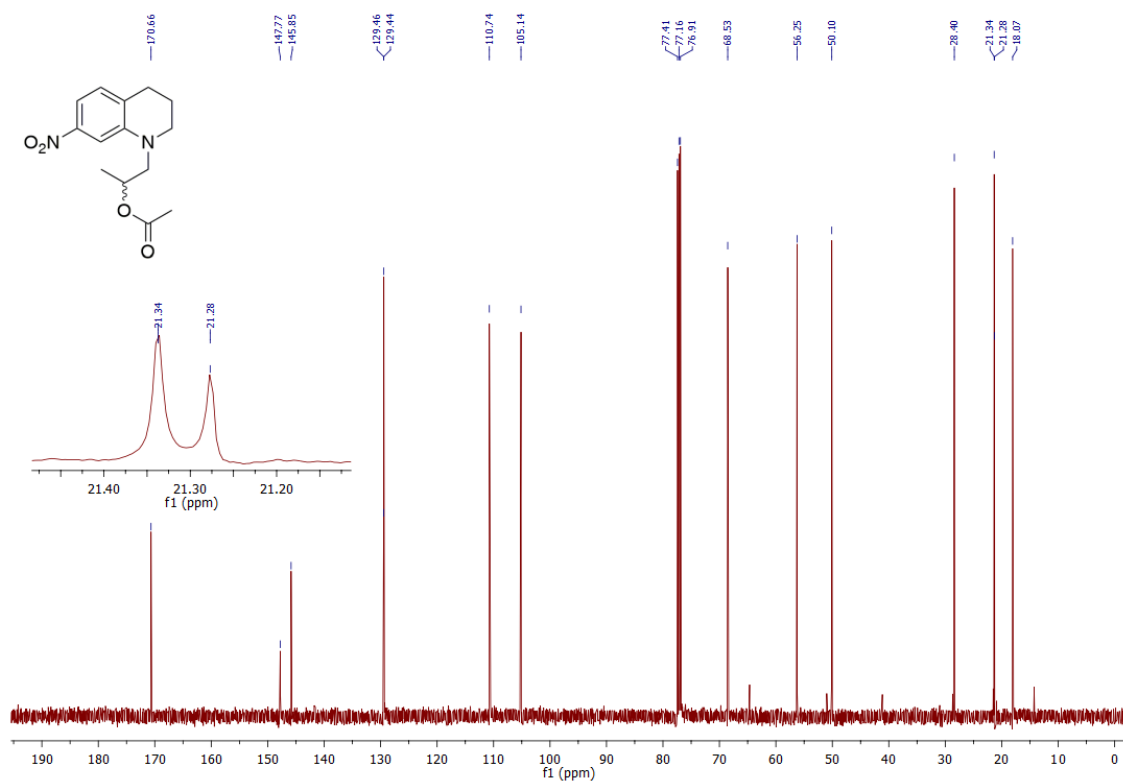


1-(7-Nitro-3,4-dihydroquinolin-1(2H)-yl)propan-2-yl acetate (rac-3c)

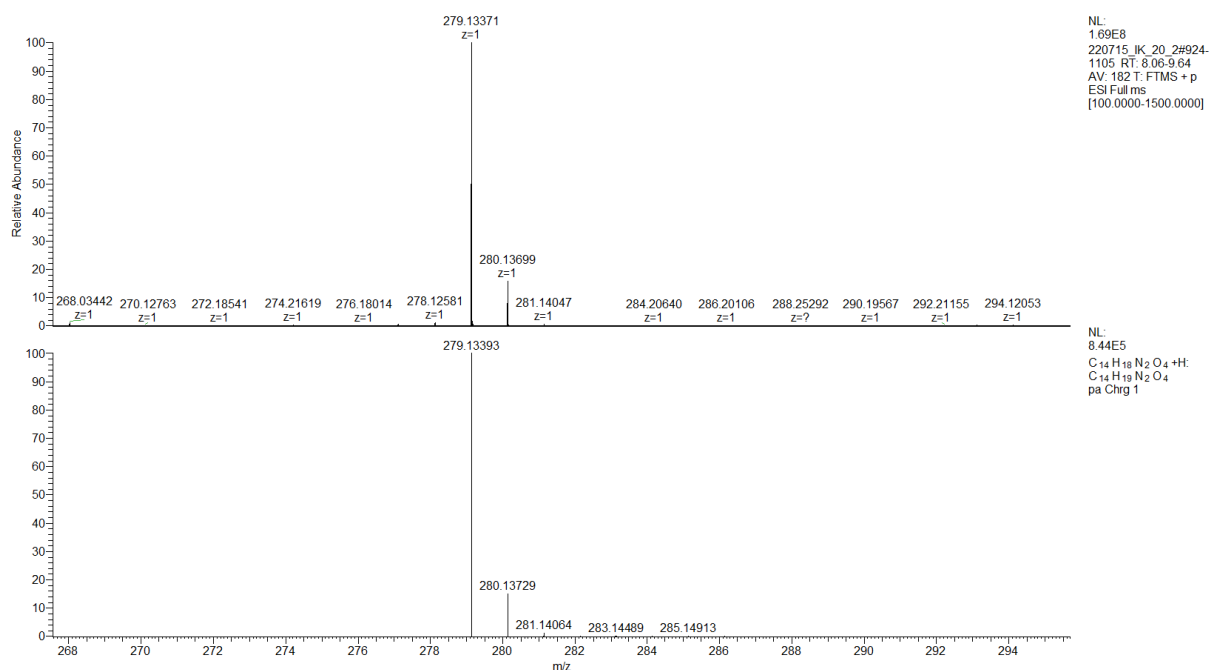
¹H NMR spectrum of *rac-3c* (500 MHz, CDCl₃)



¹³C NMR spectrum of *rac-3c* (126 MHz, CDCl₃)



FTMS spectrum of *rac*-**3c** (ESI-TOF)



IR spectrum of *rac*-**3c** (Mineral oil, Nujol)

