

Chemoenzymatic stereoselective synthesis of *trans*-flavan-4-ols via lipase-catalyzed kinetic resolutions

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1. HPLC conditions

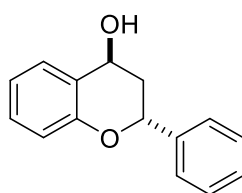
Table S1. HPLC conditions for the chiral analyses of *trans*-flavan-4-ols **2a-j** and their corresponding acetates **3a-j**.^a

Entry	(±)-Compound	Column	Hexane-2-PrOH (v/v)	Retention times (min) ^b
1	<i>trans</i> - 2a (H)	IA	92:8	10.3 (2 <i>S</i> ,4 <i>R</i>) and 10.9 (2<i>R</i>,4<i>S</i>)
2	<i>trans</i> - 3a (H)	OJ-H	92:8	16.6 (2<i>S</i>,4<i>R</i>) and 28.1 (2 <i>R</i> ,4 <i>S</i>)
3	<i>trans</i> - 2b (2-F)	OJ-H	92:8	15.3 (2 <i>S</i> ,4 <i>R</i>) and 19.0 (2<i>R</i>,4<i>S</i>)
4	<i>trans</i> - 3b (2-F)	AS	92:8	5.3 (2 <i>R</i> ,4 <i>S</i>) and 5.6 (2<i>S</i>,4<i>R</i>)
5	<i>trans</i> - 2c (3-F)	IA	92:8	9.9 (2 <i>S</i> ,4 <i>R</i>) and 10.8 (2<i>R</i>,4<i>S</i>)
6	<i>trans</i> - 2c (3-F)	OJ-H	92:8	9.9 (2<i>S</i>,4<i>R</i>) and 12.7 (2 <i>R</i> ,4 <i>S</i>)
7	<i>trans</i> - 2d (4-F)	IA	92:8	10.5 (2 <i>S</i> ,4 <i>R</i>) and 12.3 (2<i>R</i>,4<i>S</i>)
8	<i>trans</i> - 3d (4-F)	OJ-H	92:8	13.5 (2<i>S</i>,4<i>R</i>) and 16.0 (2 <i>R</i> ,4 <i>S</i>)
9	<i>trans</i> - 2e (4-Cl)	IA	92:8	11.1 (2 <i>S</i> ,4 <i>R</i>) and 13.1 (2<i>R</i>,4<i>S</i>)
10	<i>trans</i> - 3e (4-Cl)	AS	92:8	5.7 (2 <i>R</i> ,4 <i>S</i>) and 6.2 (2<i>S</i>,4<i>R</i>)
11	<i>trans</i> - 2f (4-Br)	IA	92:8	11.6 (2 <i>S</i> ,4 <i>R</i>) and 13.8 (2<i>R</i>,4<i>S</i>)
12	<i>trans</i> - 3f (4-Br)	OD	98:2	8.8 (2 <i>R</i> ,4 <i>S</i>) and 9.6 (2<i>S</i>,4<i>R</i>)
13	<i>trans</i> - 2g (2-OMe)	OJ-H	92:8	17.7 (2 <i>S</i> ,4 <i>R</i>) and 20.0 (2<i>R</i>,4<i>S</i>)
14	<i>trans</i> - 3g (2-OMe)	OJ-H	92:8	13.4 (2 <i>R</i> ,4 <i>S</i>) and 14.6 (2<i>S</i>,4<i>R</i>)
15	<i>trans</i> - 2h (3-OMe)	OJ-H	92:8	26.0 (2 <i>S</i> ,4 <i>R</i>) and 28.8 (2<i>R</i>,4<i>S</i>)
16	<i>trans</i> - 3h (3-OMe)	OJ-H	92:8	16.6 (2<i>S</i>,4<i>R</i>) and 23.2 (2 <i>R</i> ,4 <i>S</i>)
17	<i>trans</i> - 2i (4-OMe)	IA	92:8	15.0 (2 <i>S</i> ,4 <i>R</i>) and 16.6 (2<i>R</i>,4<i>S</i>)
18	<i>trans</i> - 3i (4-OMe)	IB	92:8	6.5 (2<i>S</i>,4<i>R</i>) and 6.8 (2 <i>R</i> ,4 <i>S</i>)
19	<i>trans</i> - 2j (4-Me)	IA	92:8	10.4 (2 <i>S</i> ,4 <i>R</i>) and 11.4 (2<i>R</i>,4<i>S</i>)
20	<i>trans</i> - 3j (4-Me)	OD	98:2	7.1 (2<i>S</i>,4<i>R</i>) and 7.9 (2 <i>R</i> ,4 <i>S</i>)

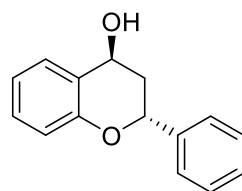
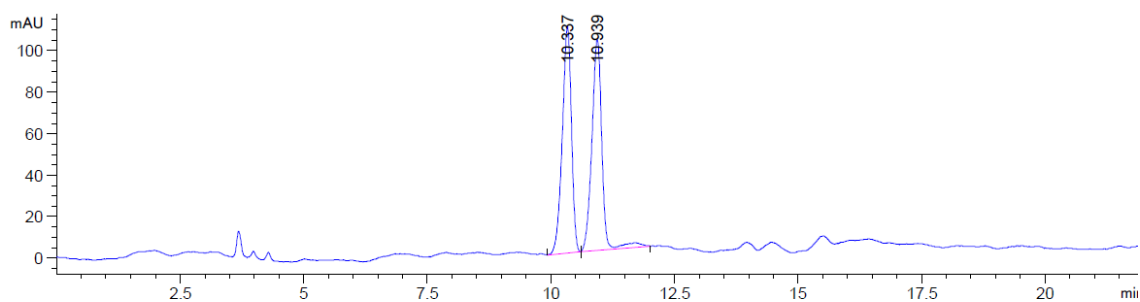
^a The temperature column was 30 °C and the flow 0.8 mL/min. Analyses were performed at 210 and 214 nm wavelengths.

^b Major enantiomer of the enzymatic reactions appear in bold font.

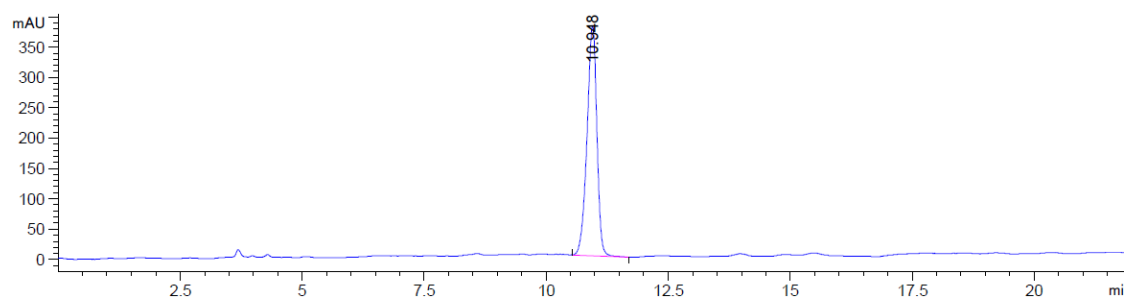
2. Chromatograms of *trans*-flavan-4-ols 2a-j in racemic and optically active form

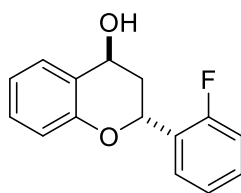


(2R*,4S*)-*trans*-2a

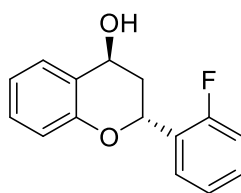
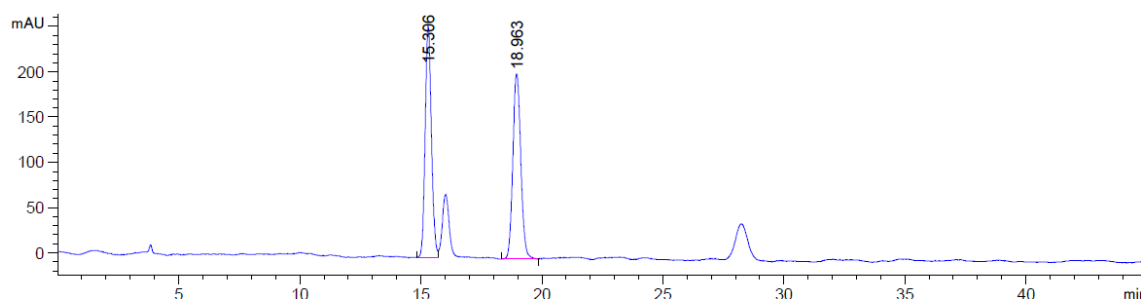


(2R,4S)-*trans*-2a

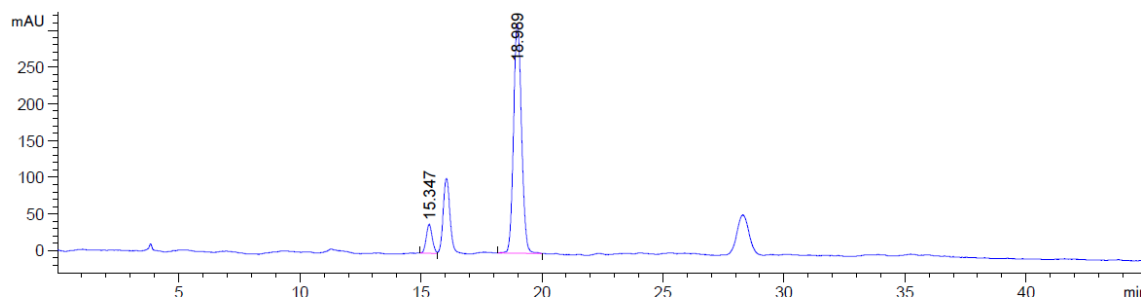


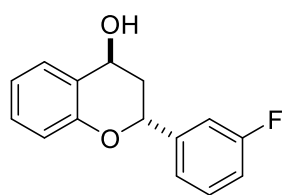


(2*R,4*S**)-trans-2b**

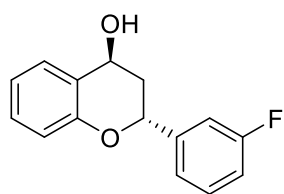
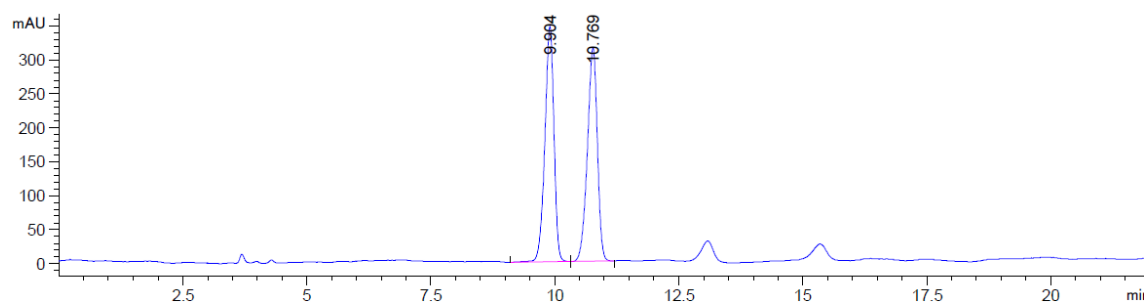


(2*R*,4*S*)-trans-2b

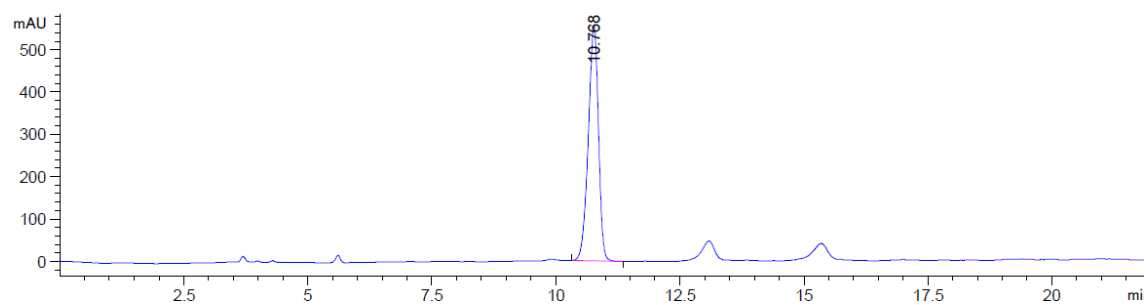


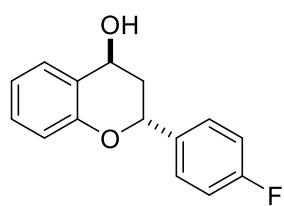


(2*R,4*S**)-trans-2c**

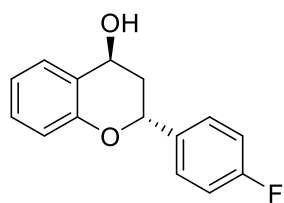
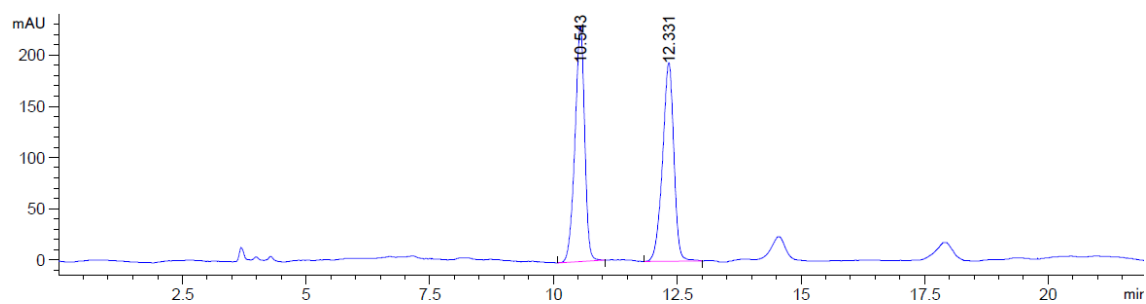


(2*R*,4*S*)-trans-2c

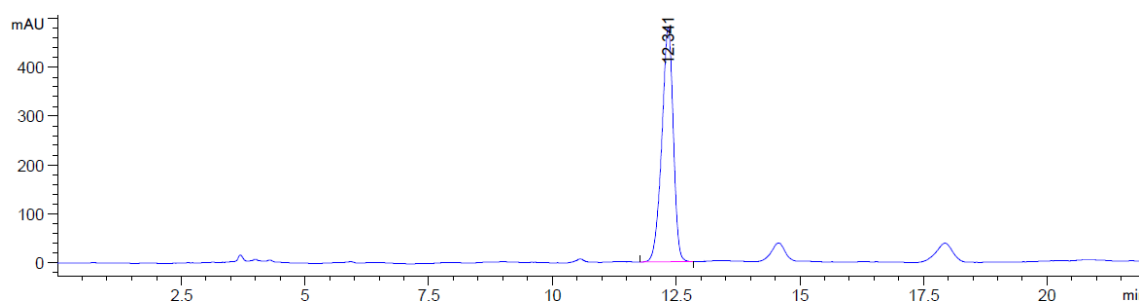


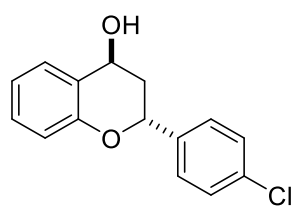


(2*R,4*S**)-trans-2d**

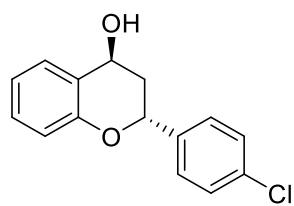
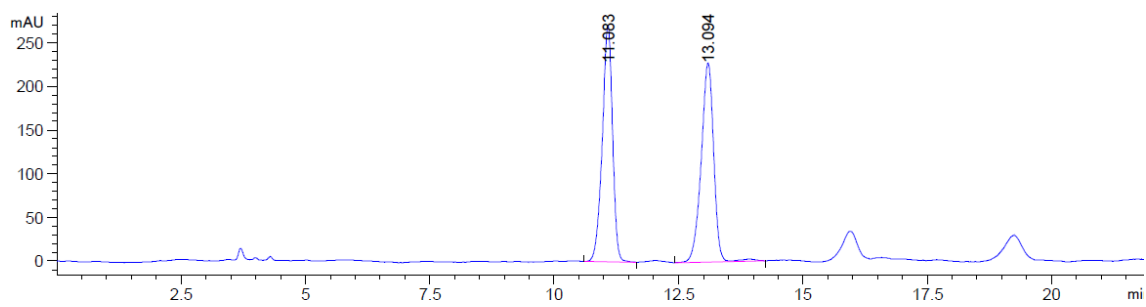


(2*R*,4*S*)-trans-2d

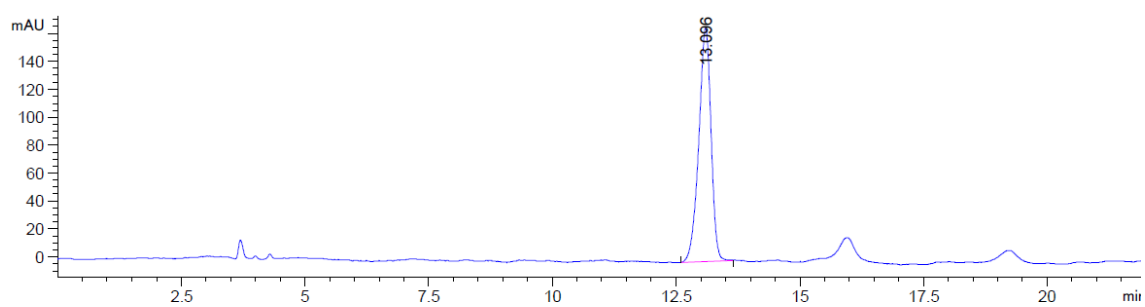


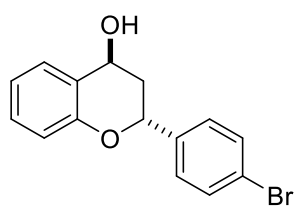


(2*R*^{*},4*S*^{*})-trans-2e

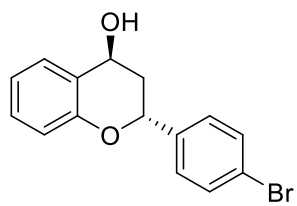
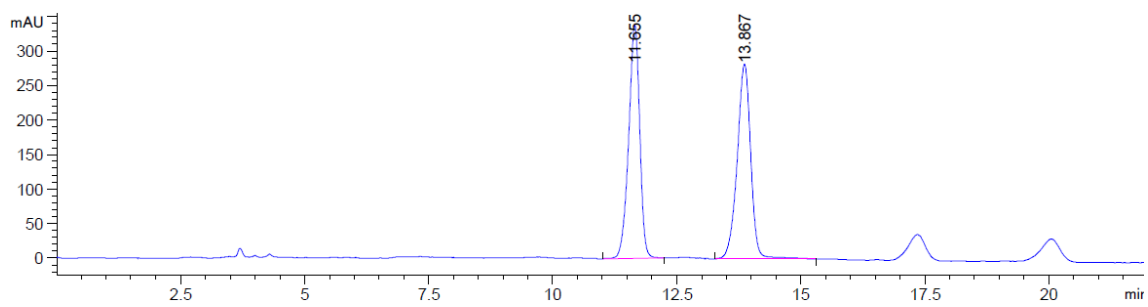


(2*R*,4*S*)-trans-2e

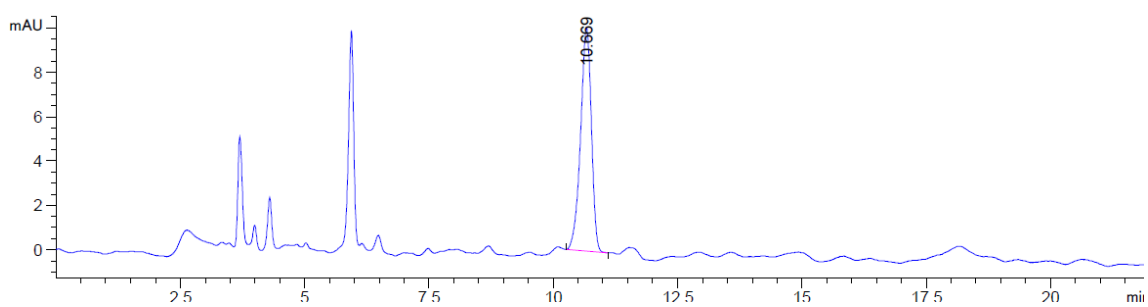


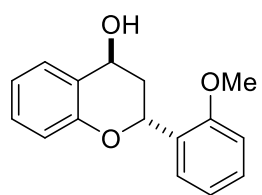


(2*R*^{*},4*S*^{*})-trans-2f

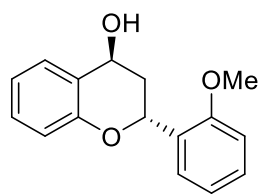
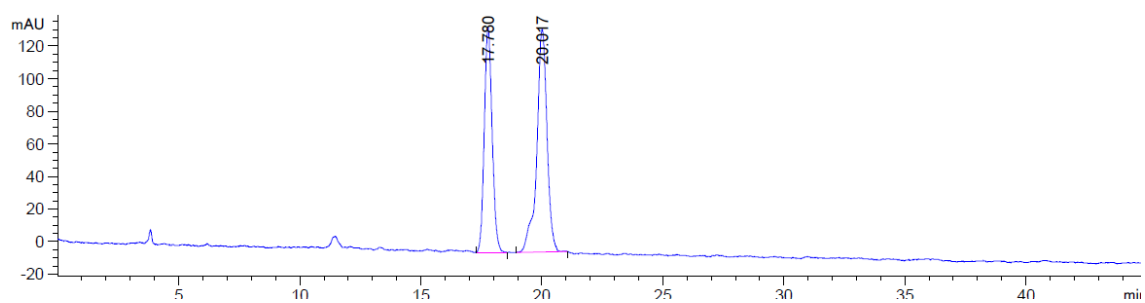


(2*R*,4*S*)-trans-2f

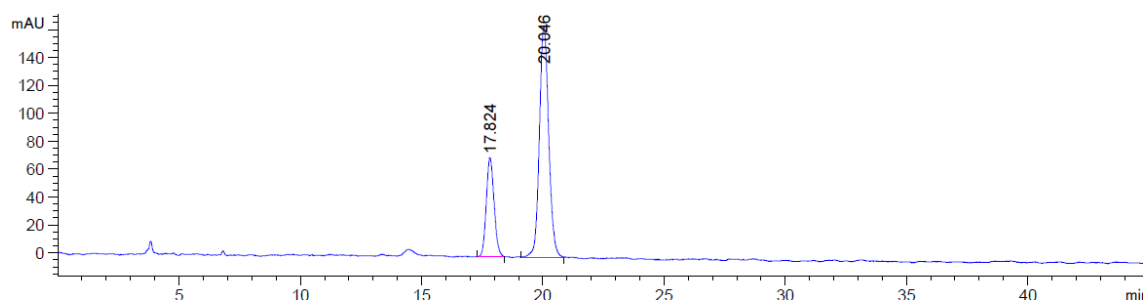


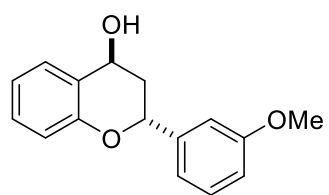


(2*R,4*S**)-trans-2g**

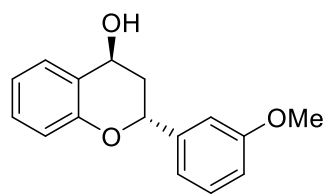
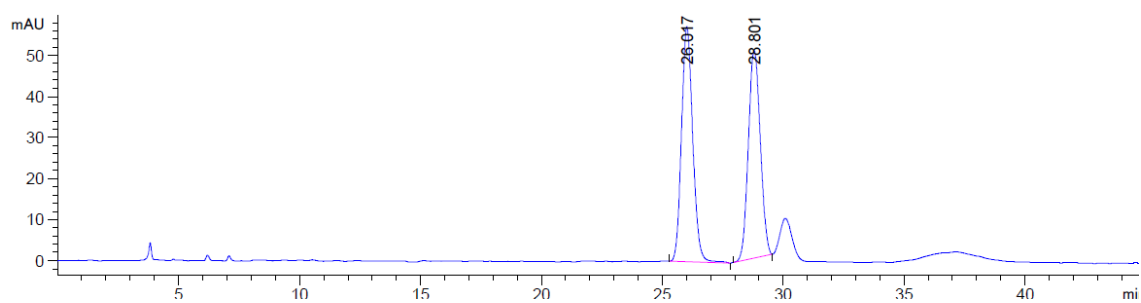


(2*R*,4*S*)-trans-2g

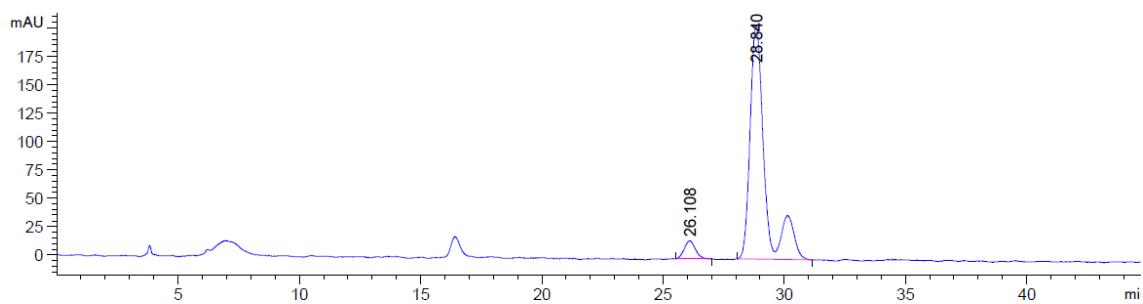


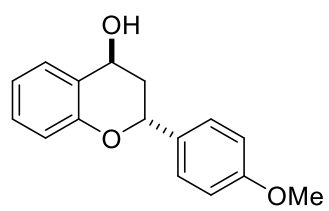


(2R,4S*)-trans-2h*

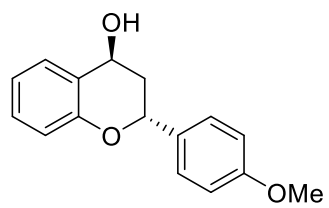
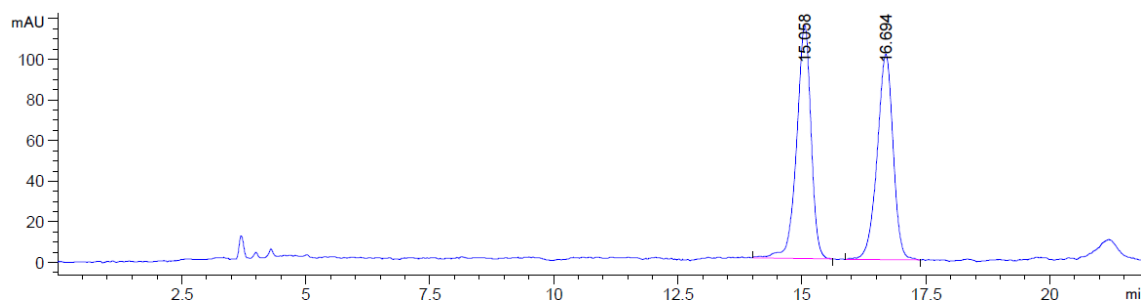


(2R,4S)-trans-2h

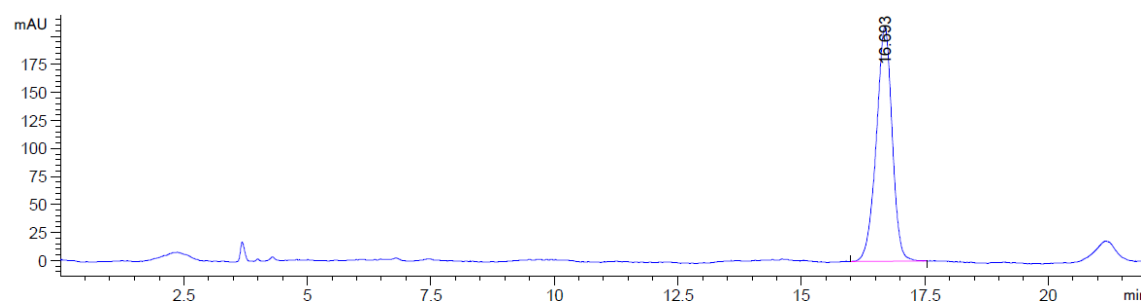


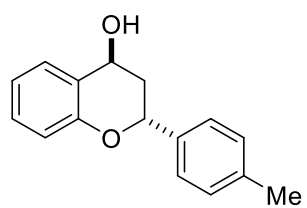


(2R,4S*)-trans-2i*

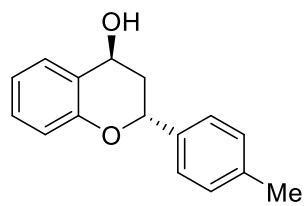
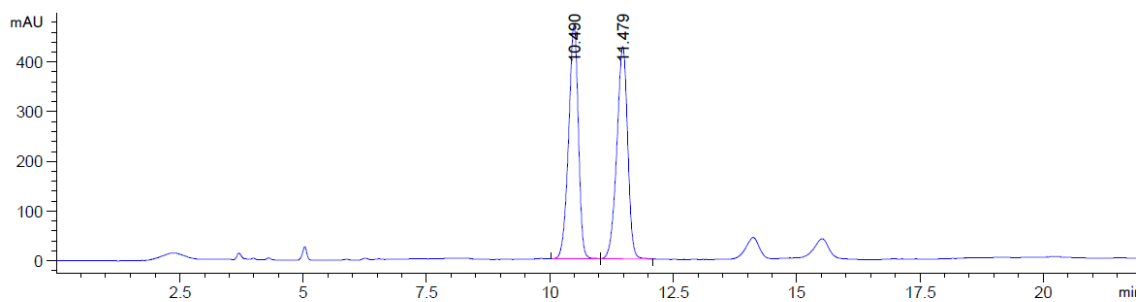


(2R,4S)-trans-2i

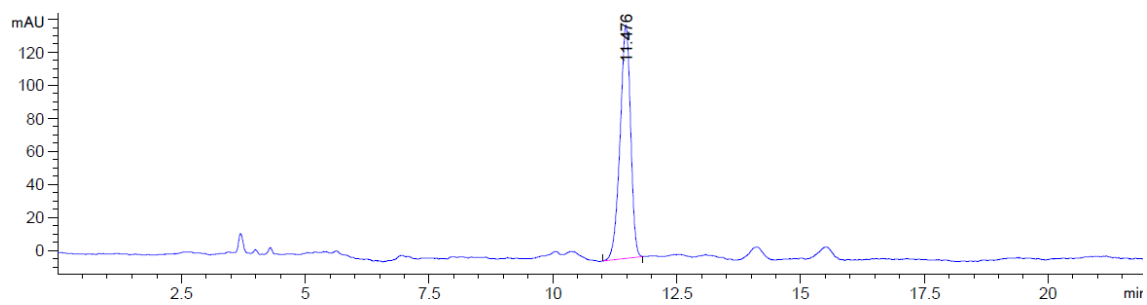




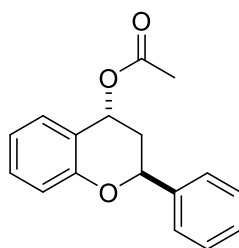
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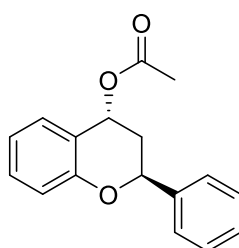
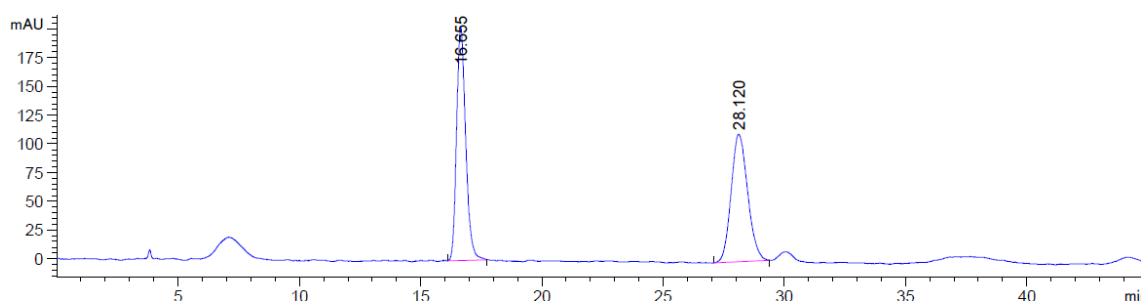
(2*R*,4*S*)-trans-2j



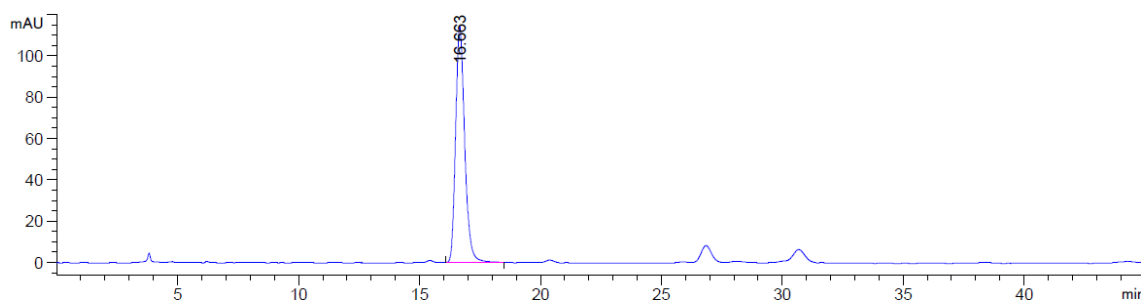
3. Chromatograms of *trans*-flavan-4-ol acetates 3a-j in racemic and optically active form

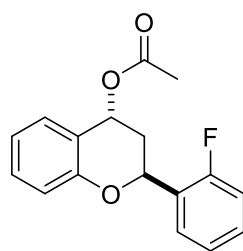


(2S*,4R*)-*trans*-3a

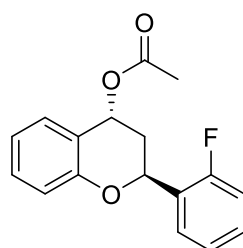
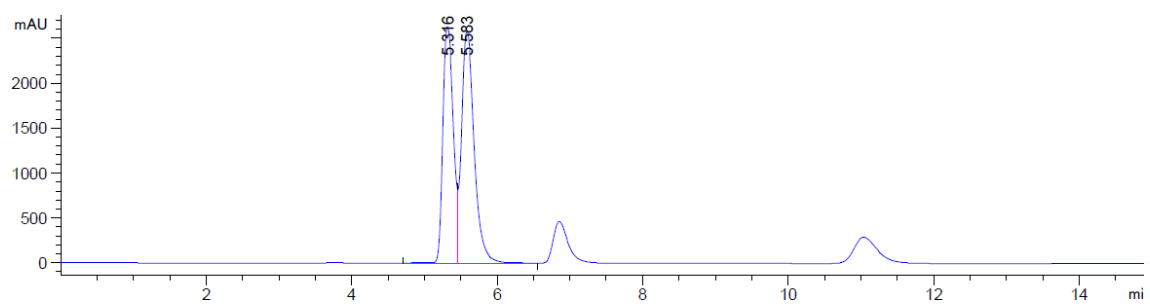


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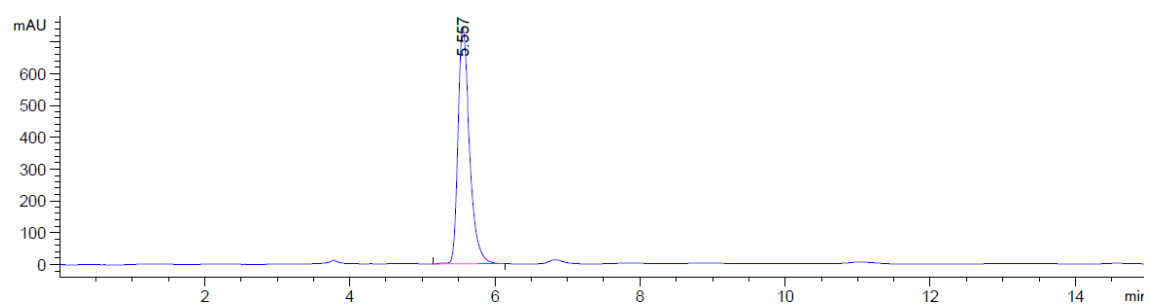


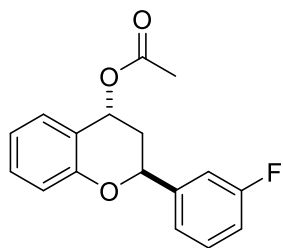


(2S*,4R*)-trans-3b

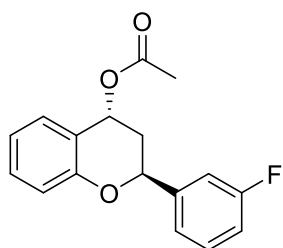
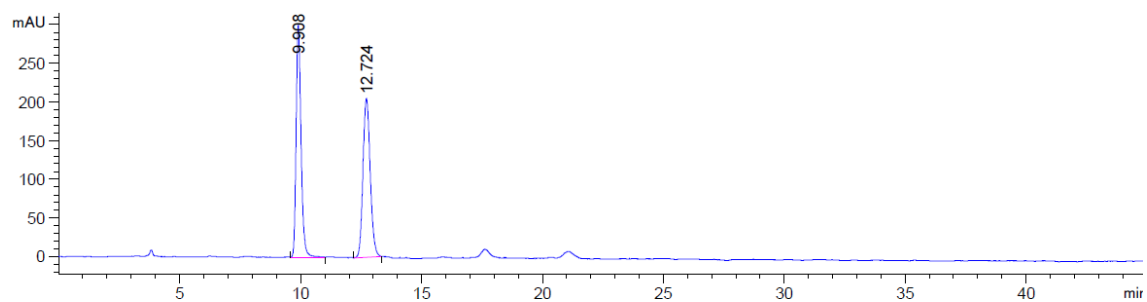


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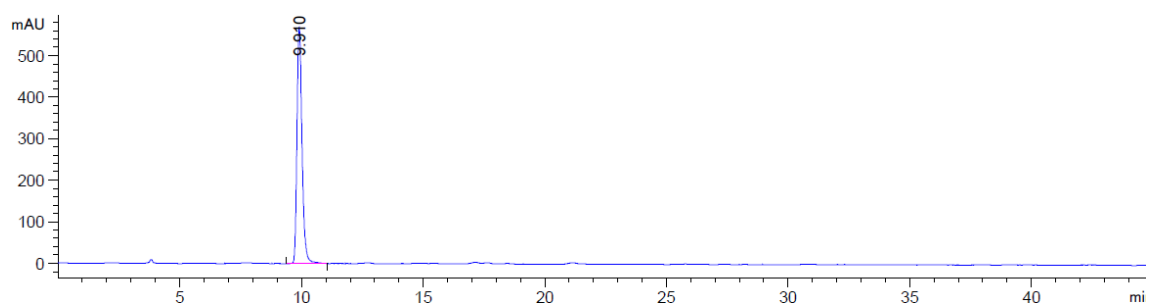


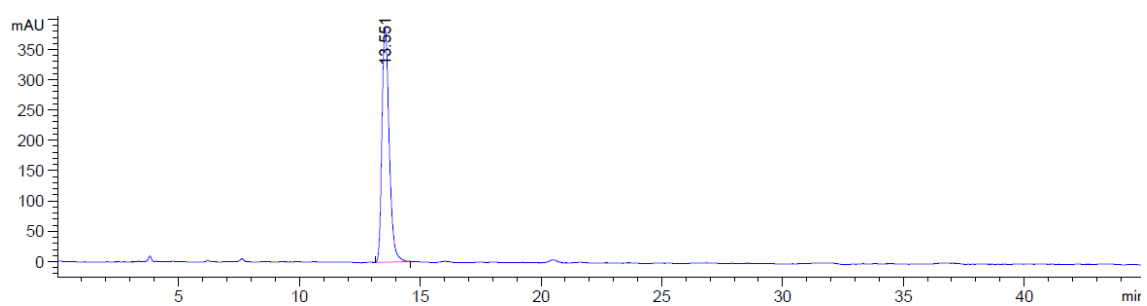
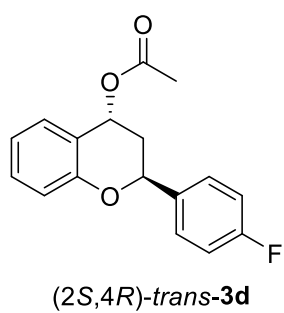
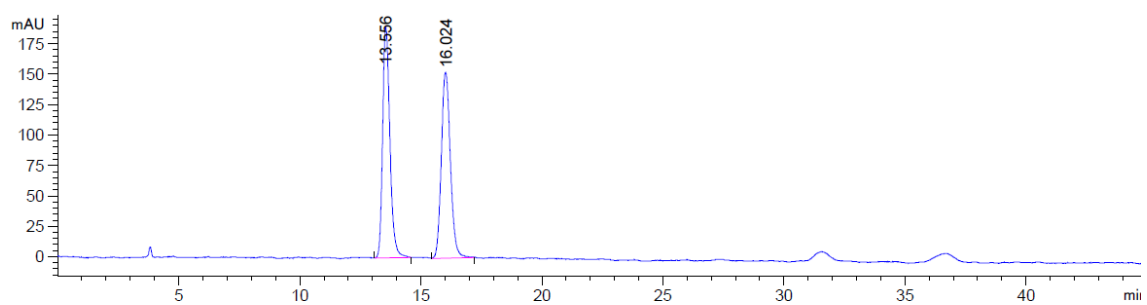
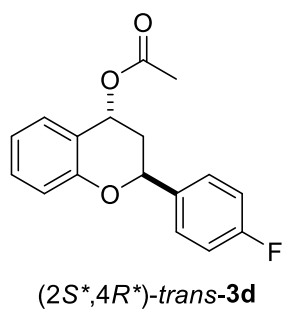


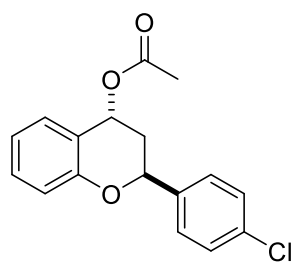
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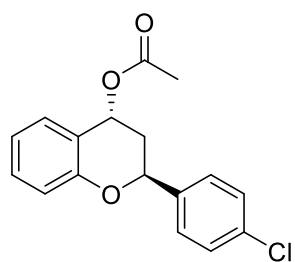
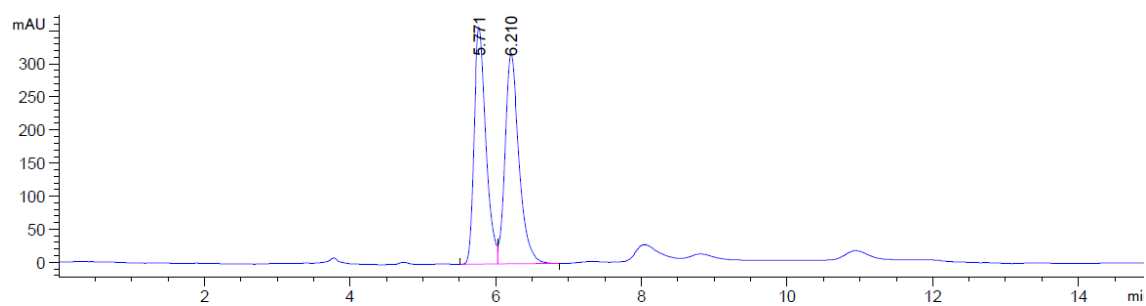
(2S,4R)-trans-3c



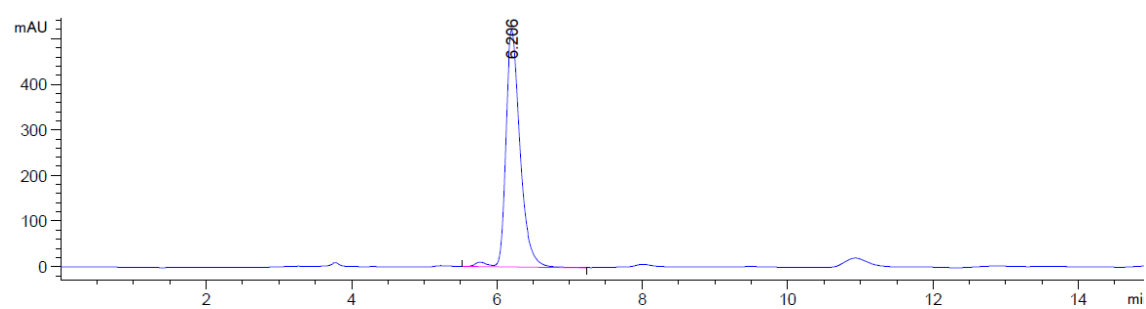


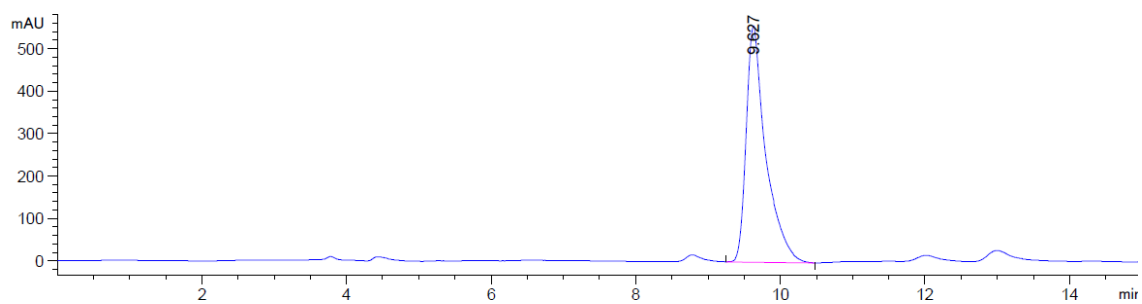
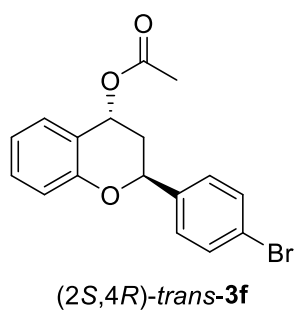
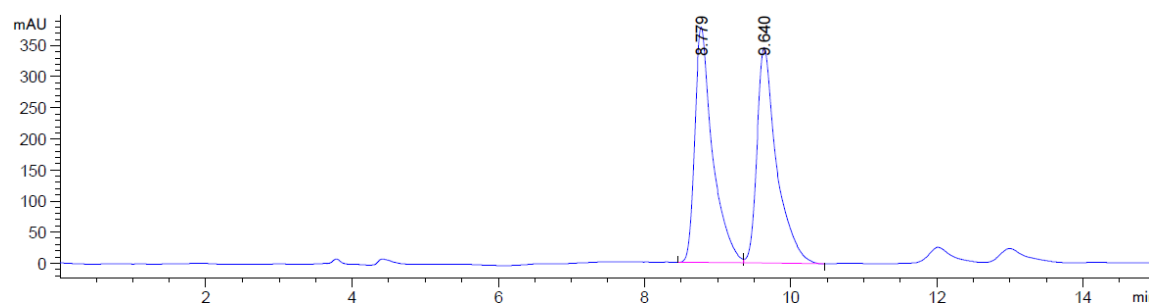
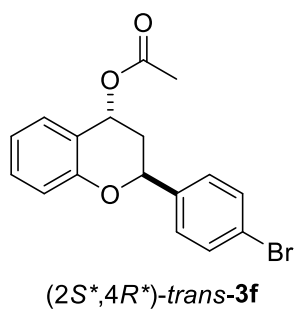


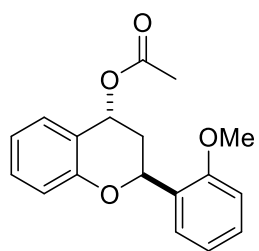
(2*S,4*R**)-trans-3e**



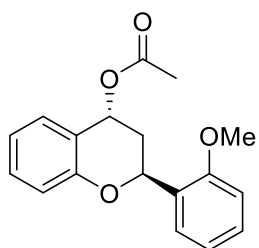
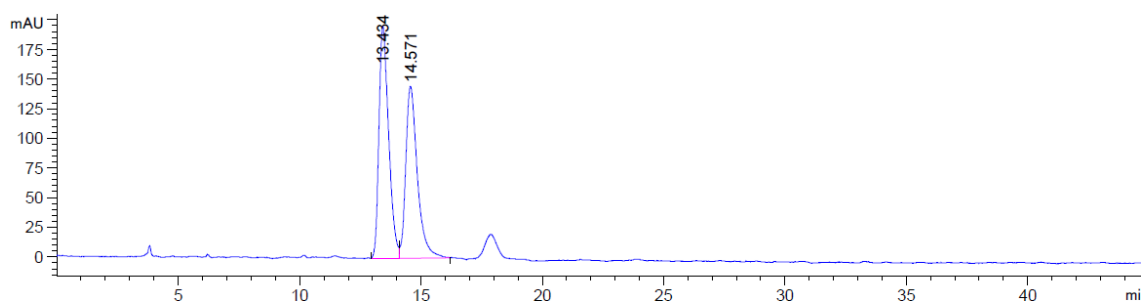
(2*S*,4*R*)-trans-3e



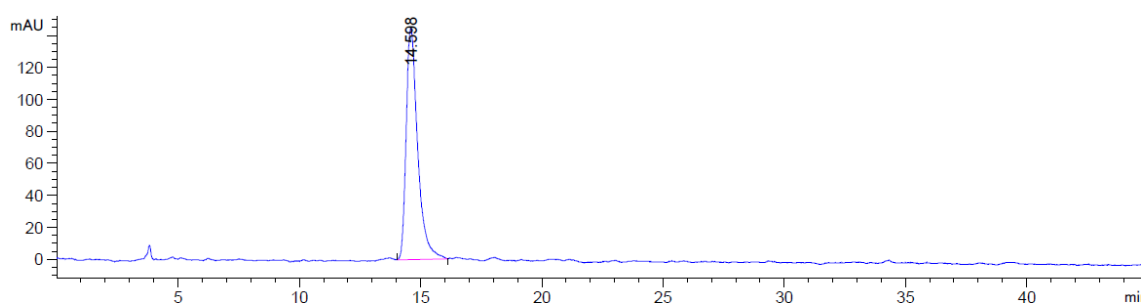


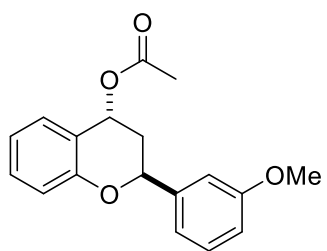


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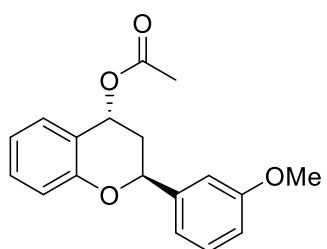
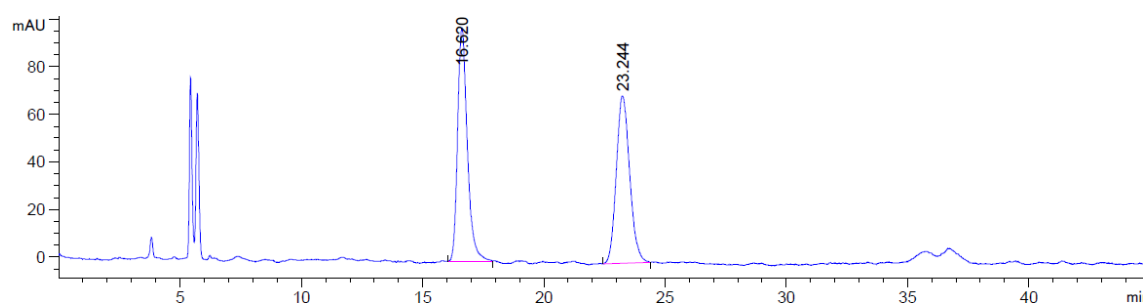


(2*S*,4*R*)-trans-3g





(2S,4R*)-trans-3h*



(2S,4R)-trans-3h

