

Product name (S)-Roche ester, methyl (S) 3-hydroxy-2-methylpropionate
purity>99%, enantiomeric excess >99.5% (assay 99.6% e.e.)

Company

InCatT B.V.
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Product Characteristics

Product number RE0002(S)
Lot number IS20-63
CAS number 80657-57-4
Formula C₅H₁₀O₃
Molecular Weight 118.13

Tests report

Date 11-06-2020
Appearance (colour) COLOURLESS
Appearance (state) LIQUID
GC >99.0% purity
Optical purity assay 99.6%
¹H NMR According to literature. No aromatics detected.

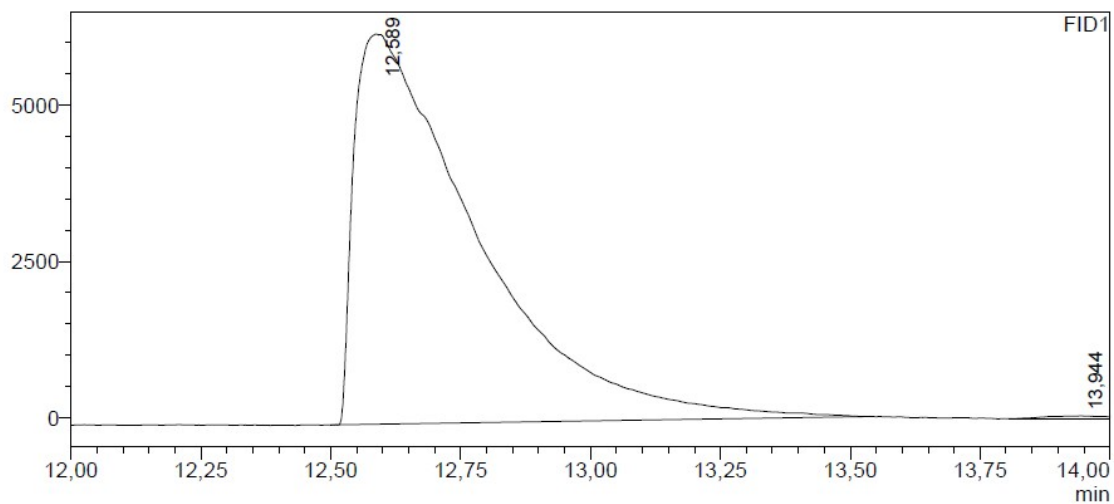
THIS CERTIFICATE GUARANTEES THE HIGH QUALITY OF THIS PRODUCT

Chiral GC spectrum

Batch IS20-63

<Chromatogram>

uV



<Peak Table>

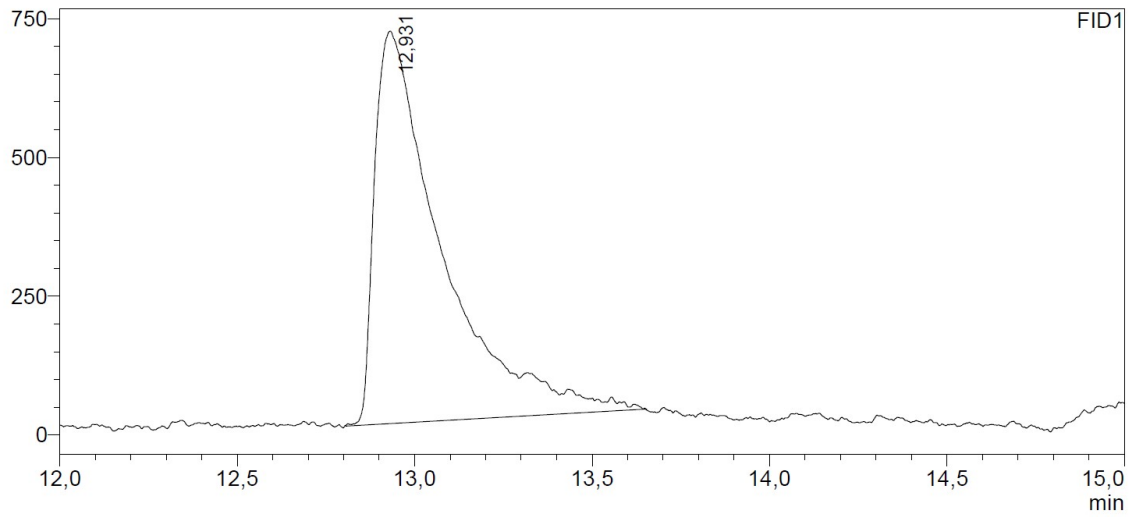
FID1

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12,589	102394	6226	0,000	ppm	M	(S)-Roche Ester
2	13,944	183	45	0,000	ppm	M	(R)-Roche Ester
Total		102577	6271				

Calculated enantiomeric excess: 99.63%

Diluted sample
<Chromatogram>

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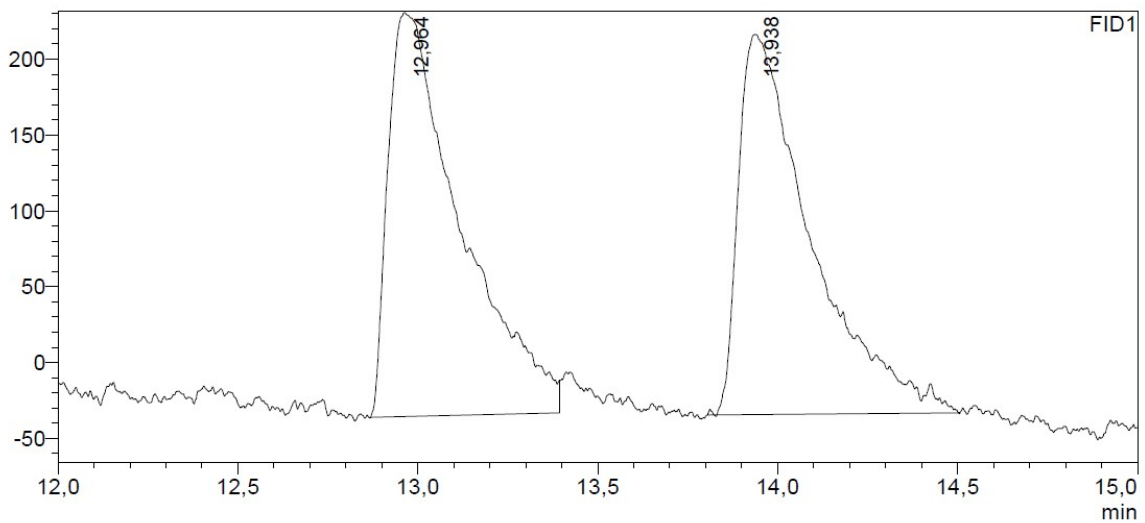
<Peak Table>

FID1							
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12,931	9285	706	0,000	ppm	M	(S)-Roche Ester
Total		9285	706				

Racemic: roches ester

<Chromatogram>

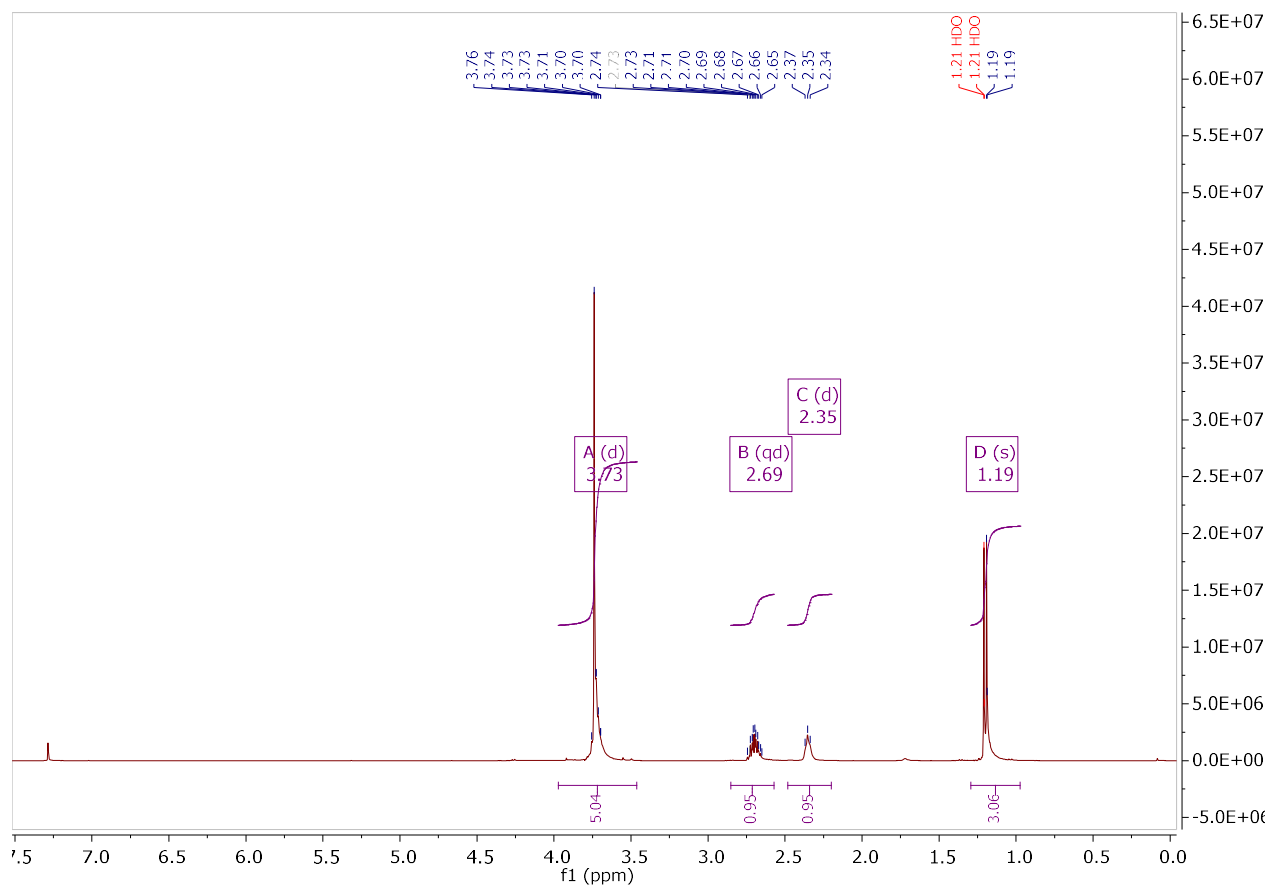
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<Peak Table>

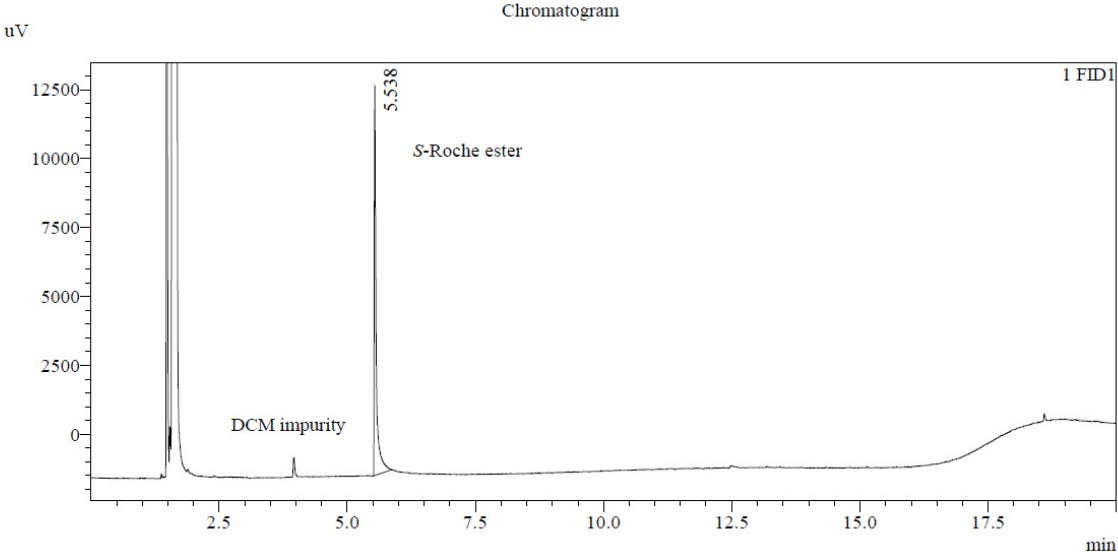
FID1							
Peak#	Ret. Time	Area	Height	Area%	Name		
1	12,964	3710	266	51,644	(S)-Roche Ester		
2	13,938	3474	250	48,356	(R)-Roche Ester		
Total		7184	516	100,000			

^1H NMR in CDCl_3



^1H NMR (400 MHz, Chloroform-*d*) δ 3.73 (d, $J = 4.8$ Hz, 5H), 2.69 (qd, $J = 7.2, 4.7$ Hz, 1H), 2.35 (d, $J = 6.6$ Hz, 1H), 1.19 (s, 3H).

GC-analysis



Peak Table

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.538	37554	14083	100.000			
Total		37554	14083				

Peak at 3.9 stems from dichloromethane (used to dilute teh sample).