

SUPPORTING INFORMATION

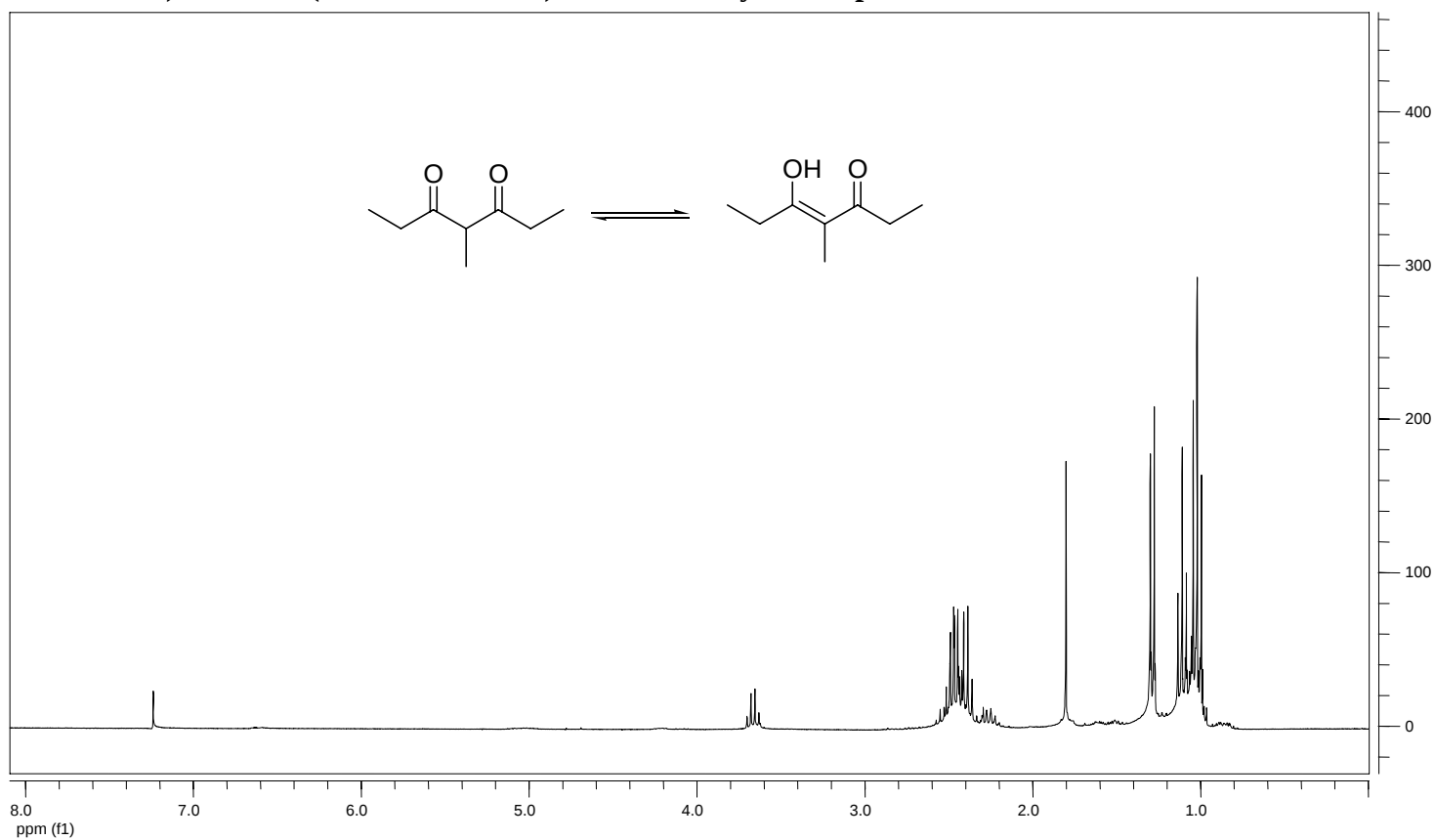
Title: A Two-Step Chemoenzymatic Synthesis of the Natural Pheromone (+)-Sitophilure Utilizing Isolated, NADPH-Dependent Ketoreductases

Author(s): Dimitris Kalaitzakis, J. David Rozzell, Spiros Kambourakis, Ioulia Smonou*

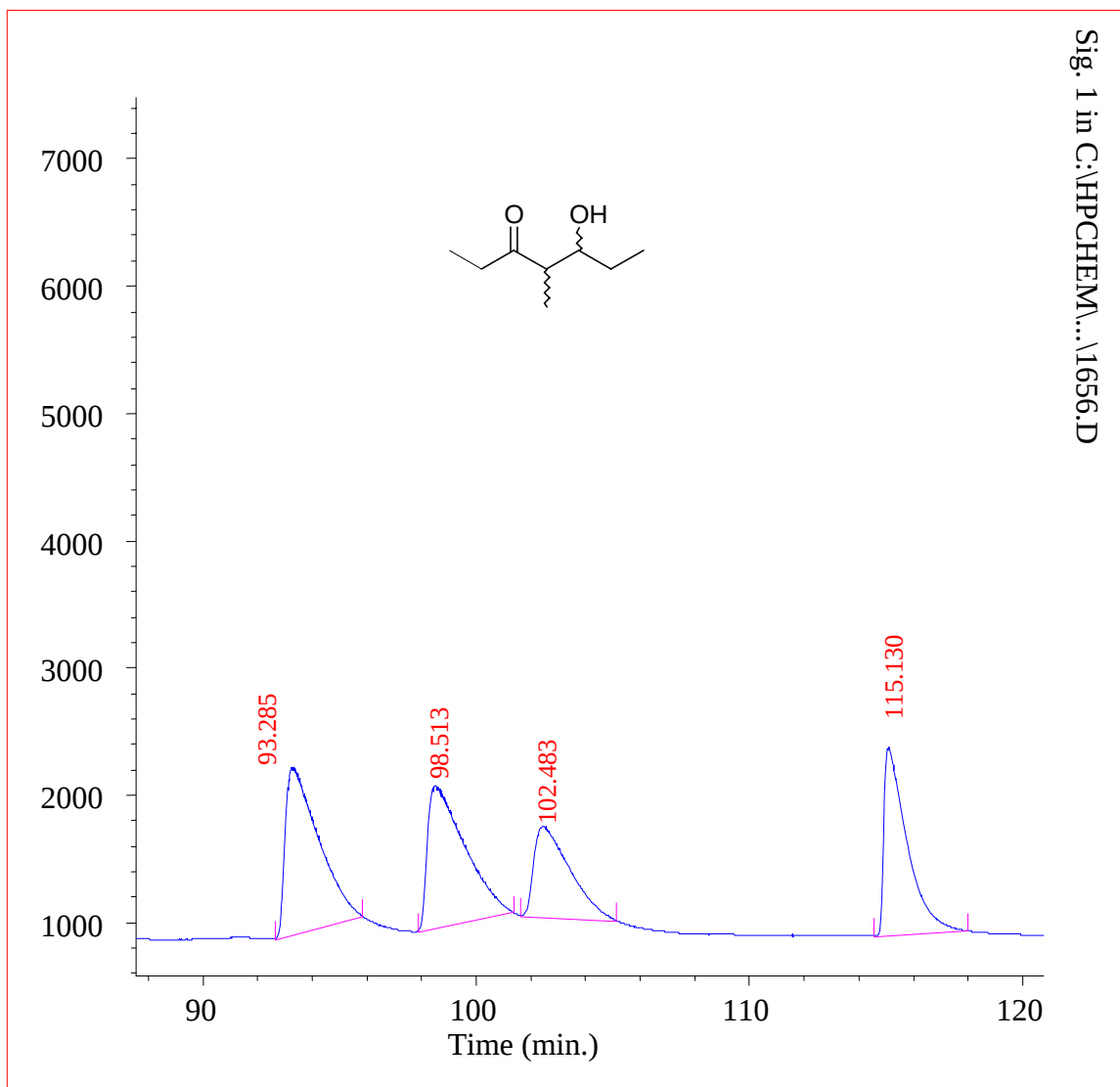
Ref. No.: O200500991

Analytical and Spectral Data

1) ^1H NMR (300 MHz, CDCl_3) of the 4-methyl-3,5-heptanedione

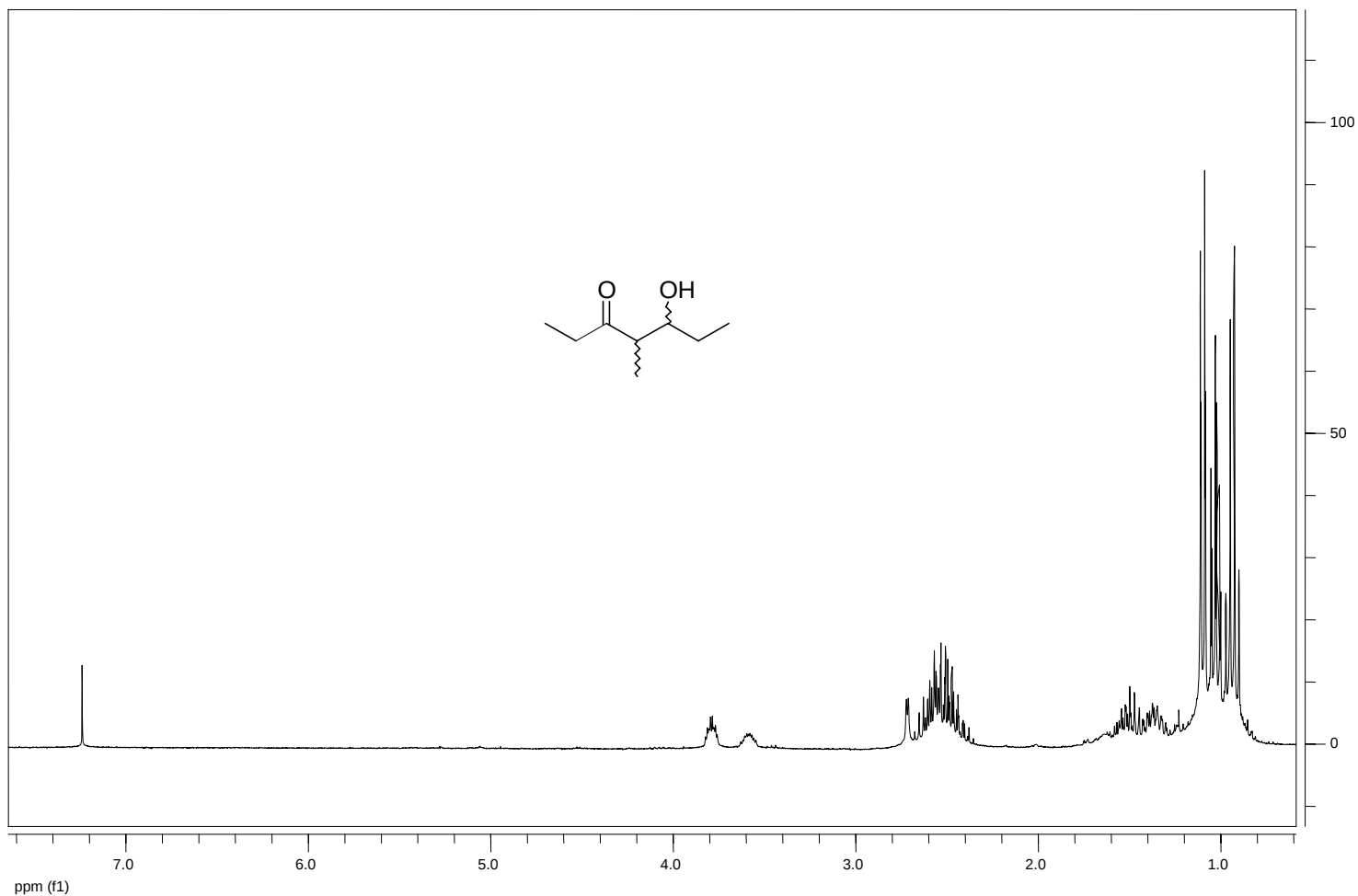


2) GC analysis of racemic keto alcohol-1 with chiral capillary column, 20% permethylated cyclodextrin 5-hydroxy-4-methyl-3-heptanone

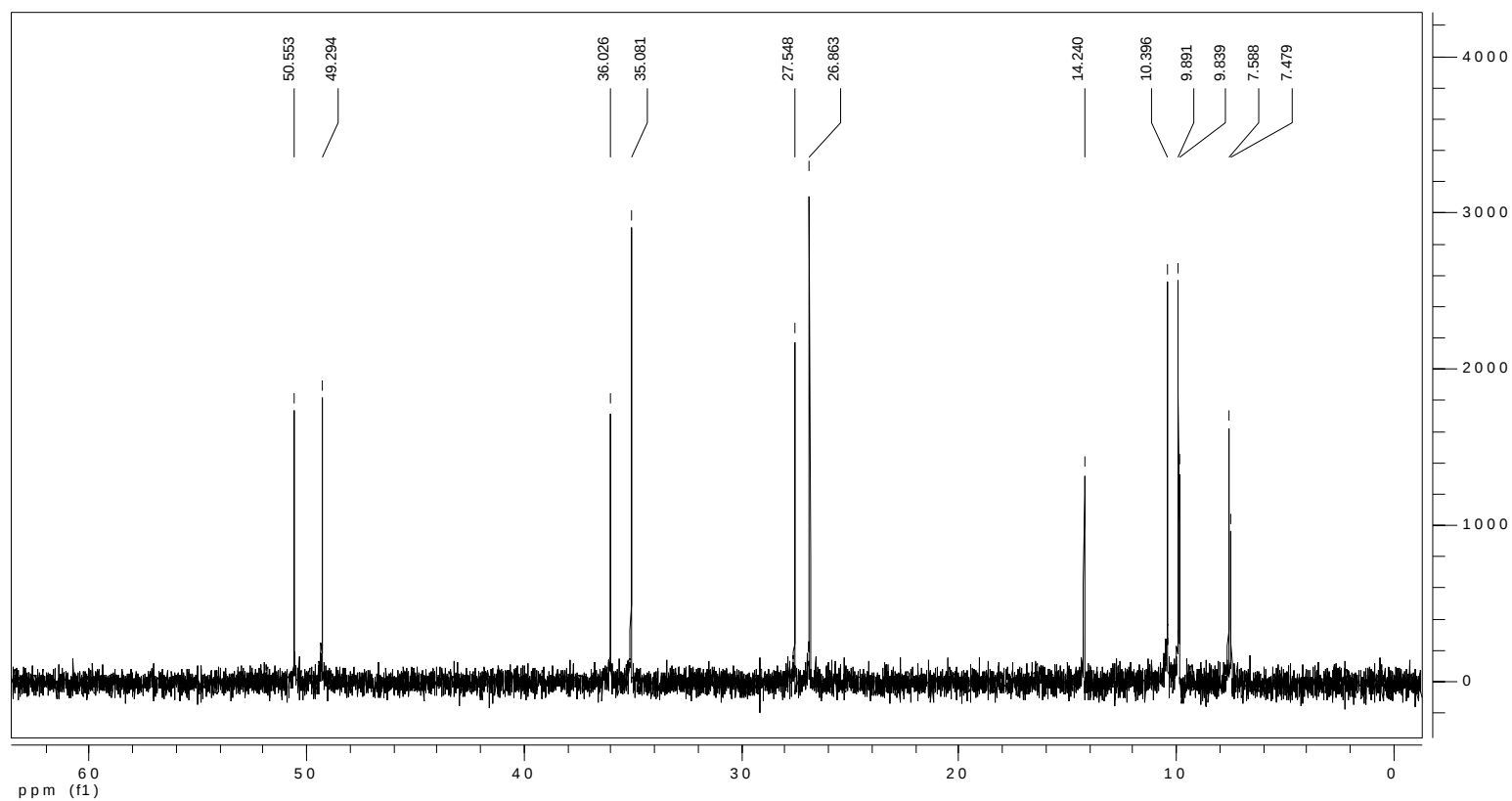
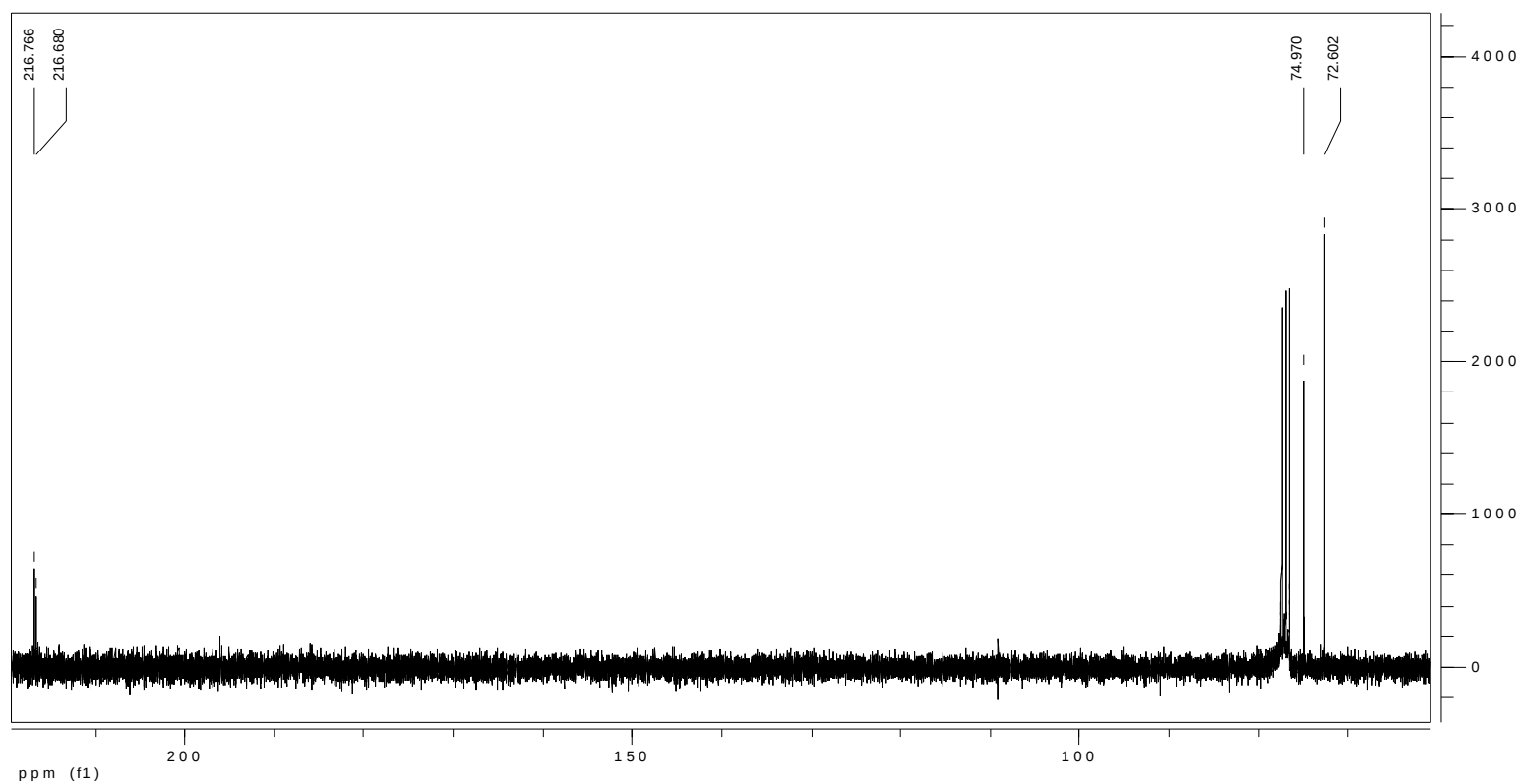


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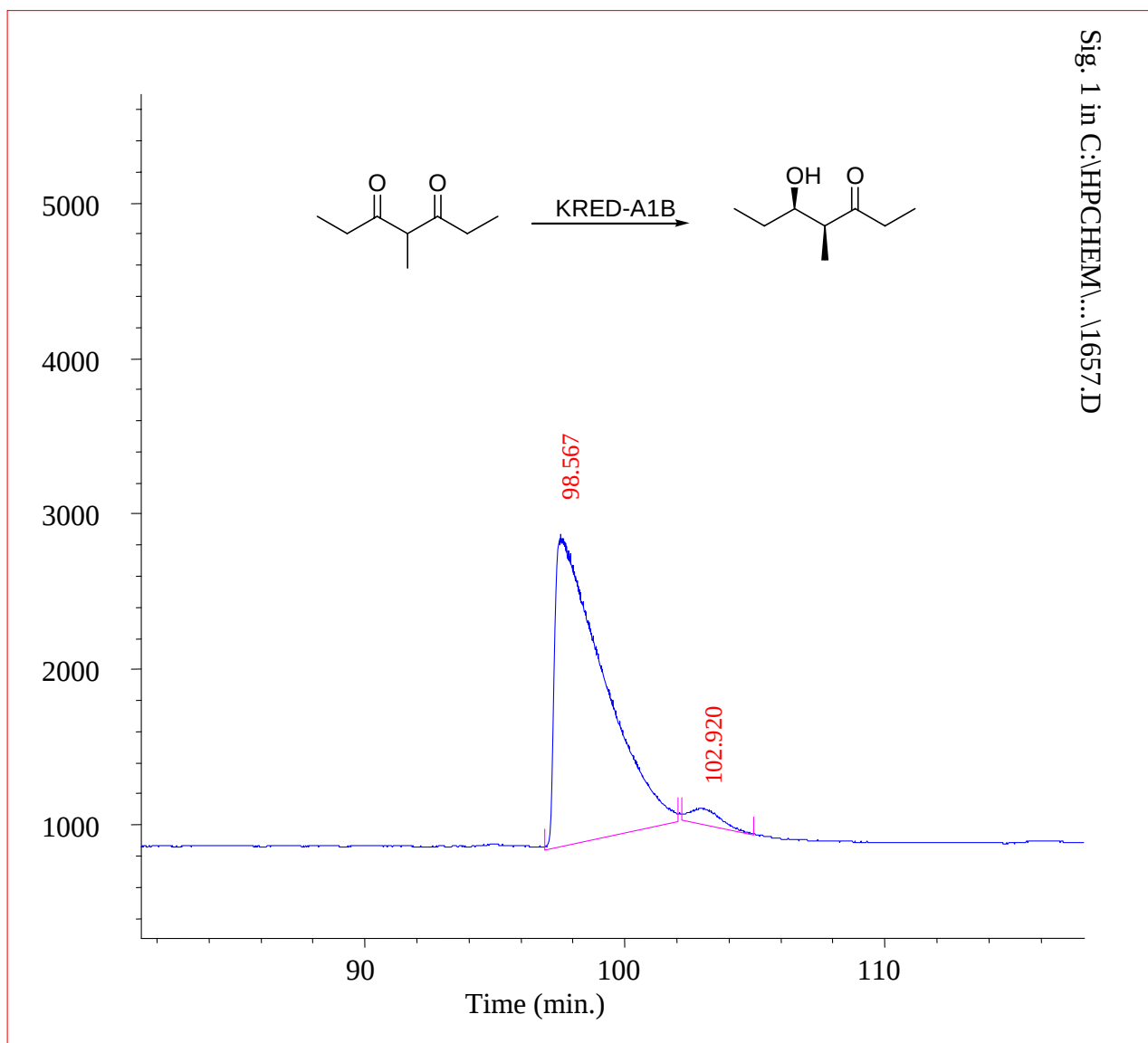
3) ^1H NMR (300 MHz, CDCl_3) of the racemic 5-hydroxy-4-methyl-3-heptanone



4) ^{13}C NMR (300 MHz, CDCl_3) of the racemic 5-hydroxy-4-methyl-3-heptanone

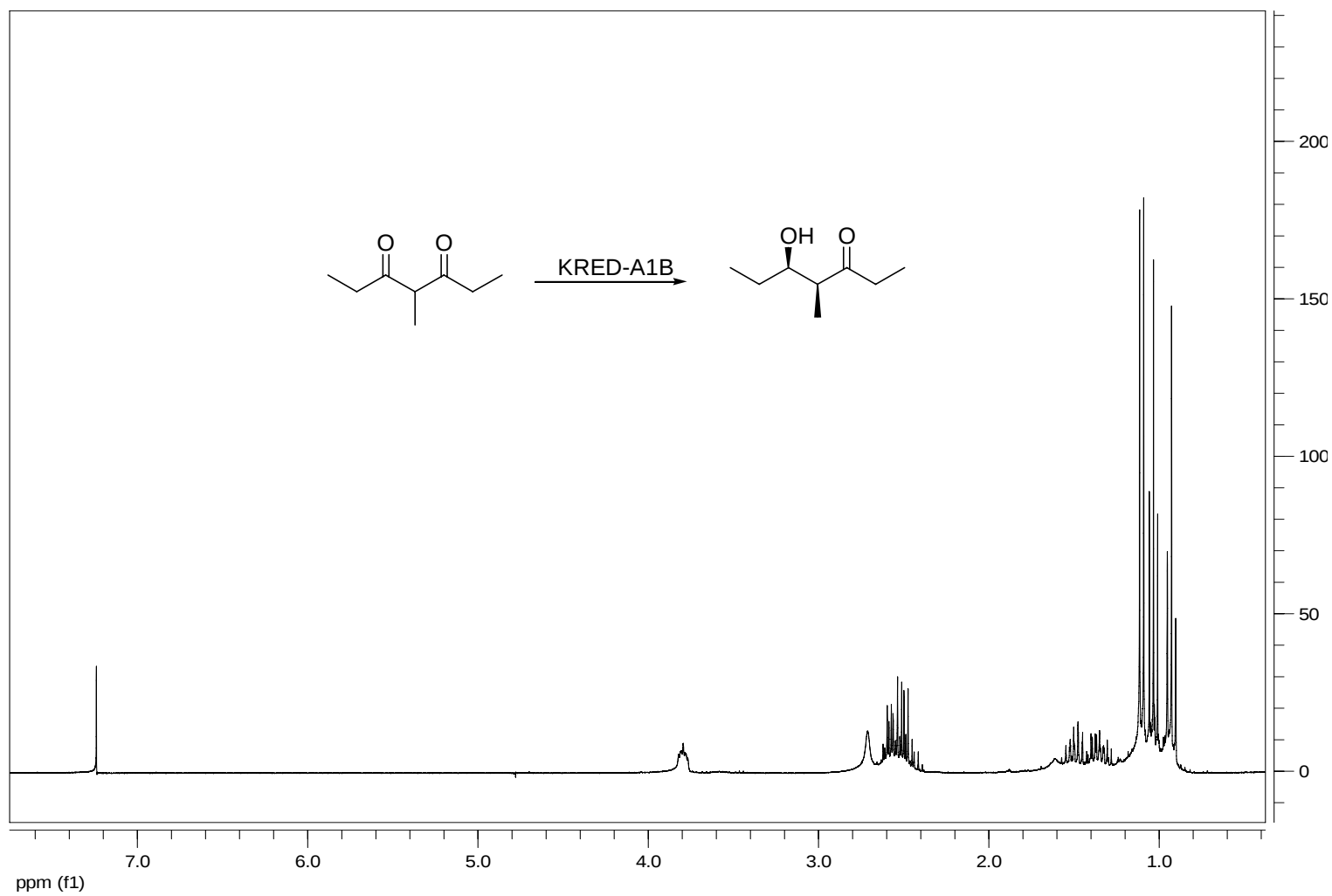


5) GC analysis of the product, after enzymatic reduction of 4-methyl-3,5-heptanedione with KRED-A1B (chiral capillary column, 20% permethylated cyclodextrin)

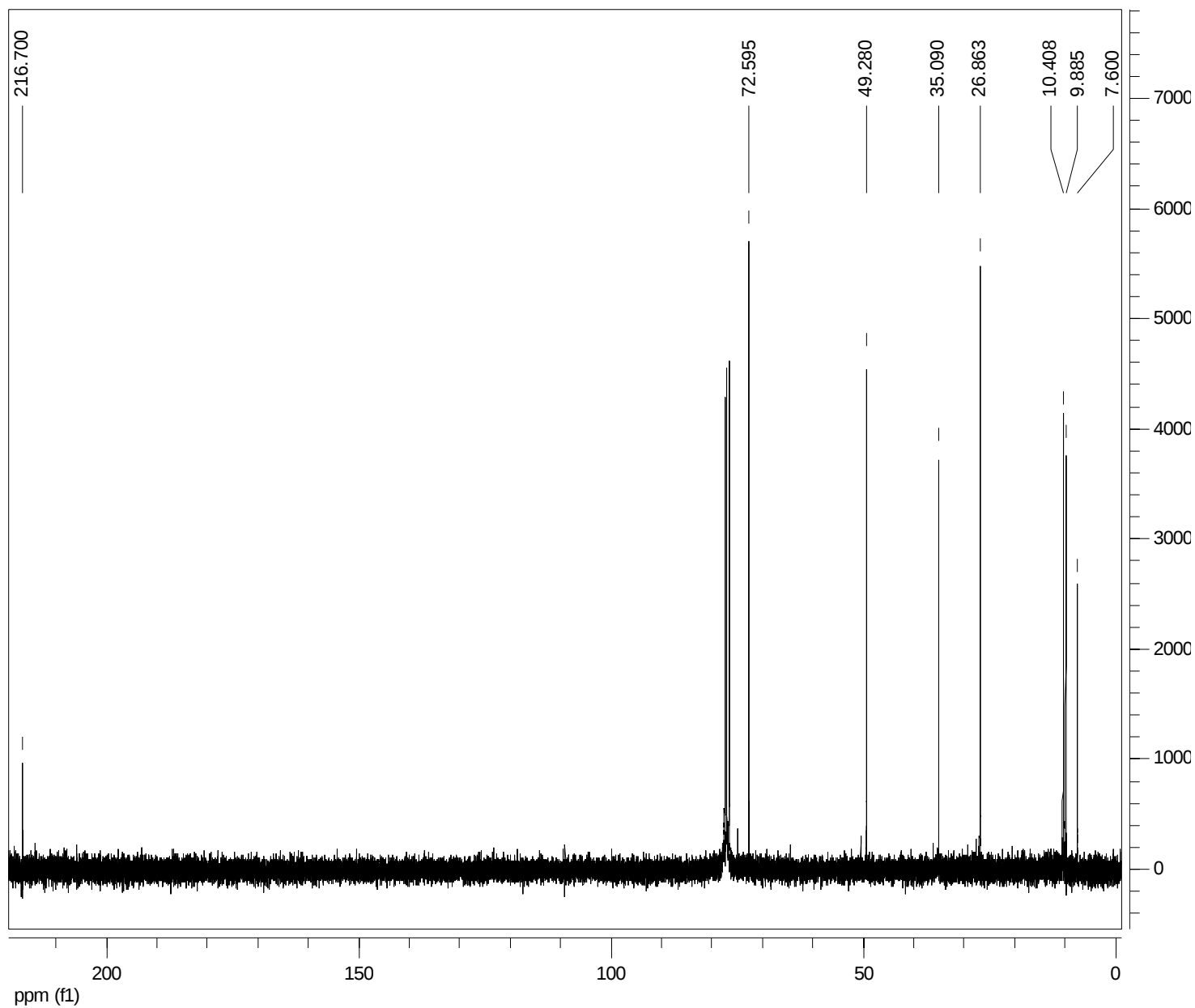


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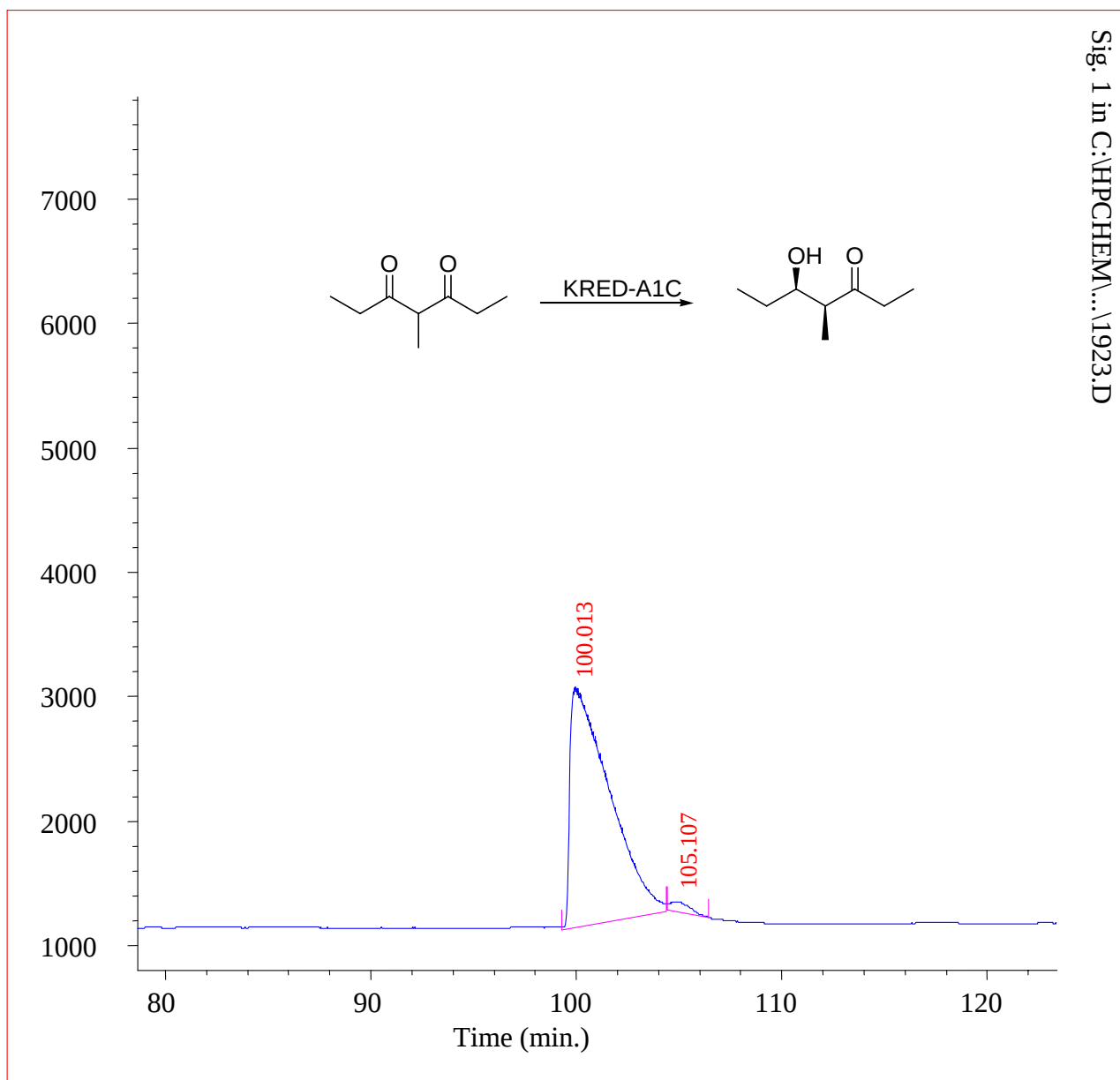
6) ^1H NMR (300 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone after enzymatic reduction with KRED-A1B



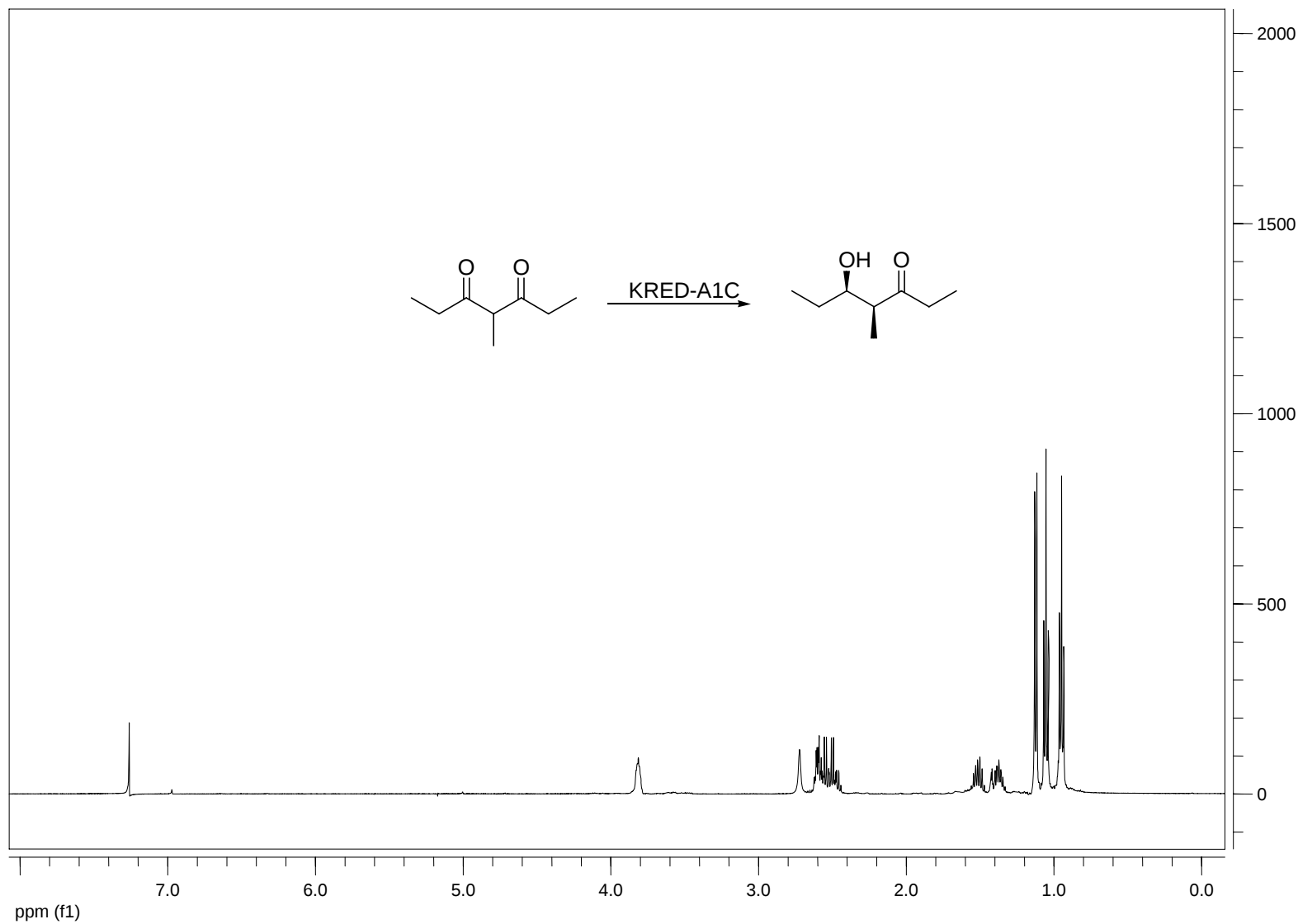
7) ^{13}C NMR (300 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone
after enzymatic reduction with KRED-A1B



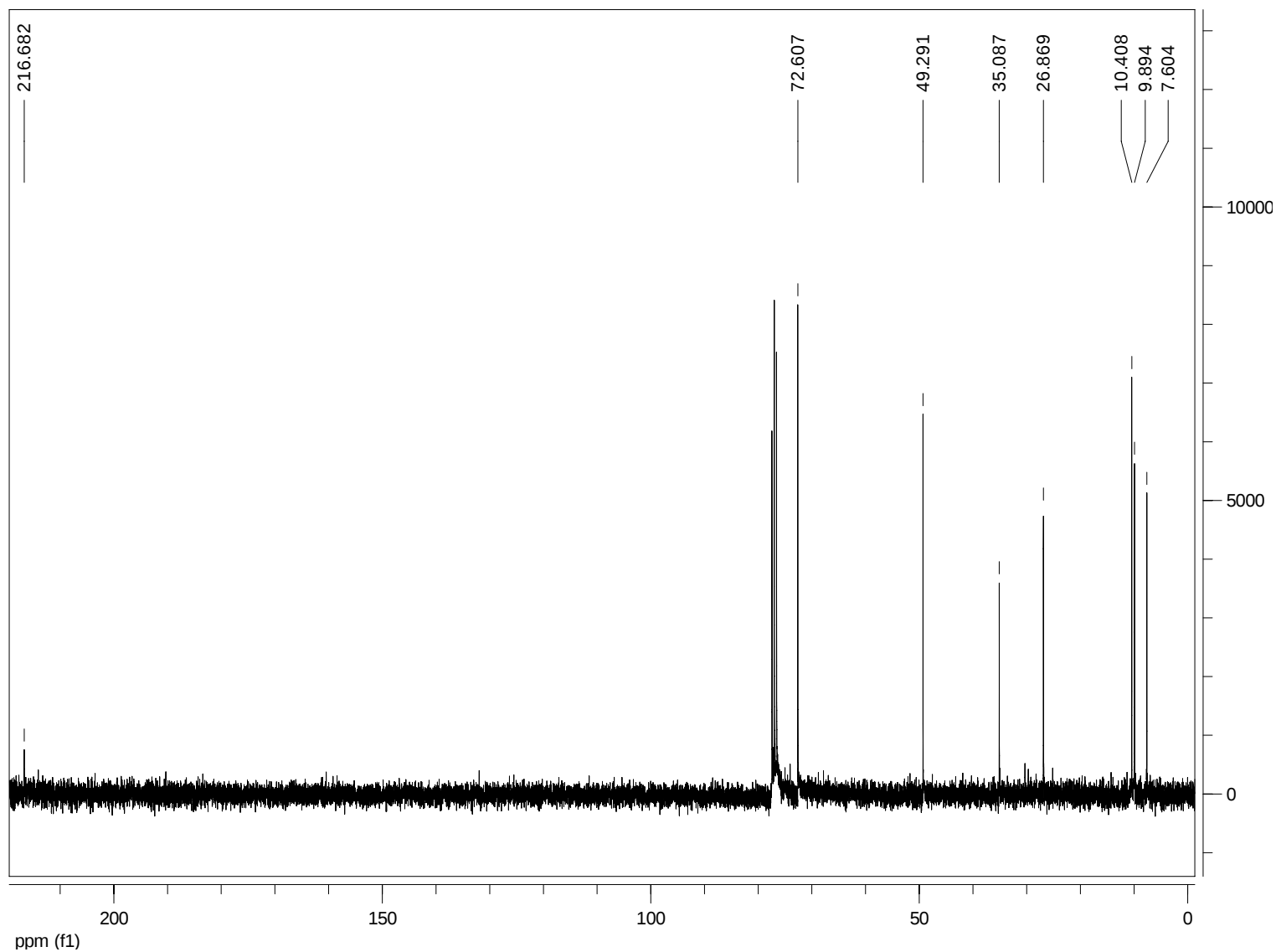
8) GC analysis of the product, after enzymatic reduction of 4-methyl-3,5-heptanedione with KRED-A1C (chiral capillary column, 20% permethylated cyclodextrin)



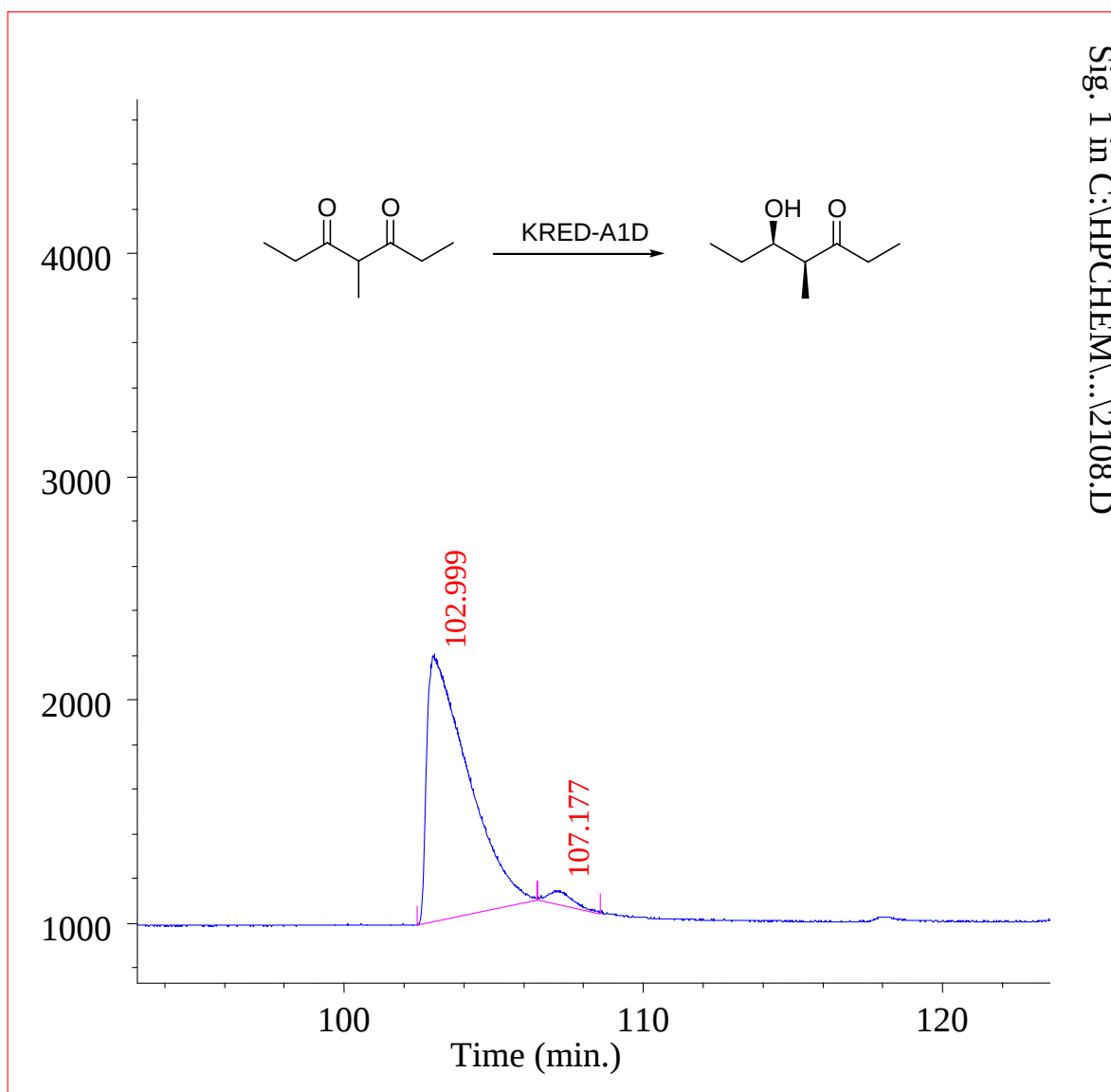
9) ^1H NMR (500 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone after enzymatic reduction with KRED-A1C



**10) ^{13}C NMR (300 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone
after enzymatic reduction with KRED-A1C**

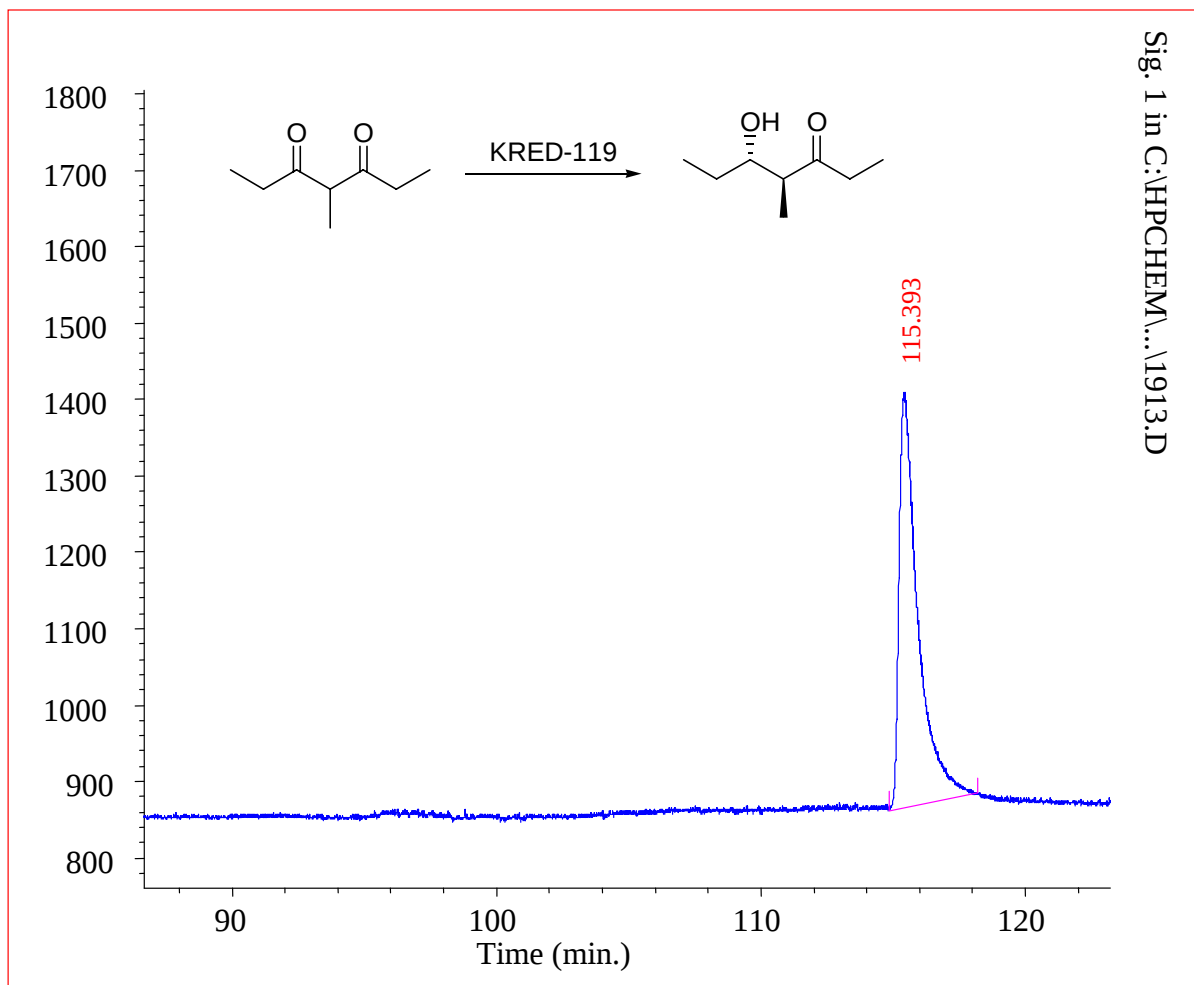


11) GC analysis of the product, after enzymatic reduction of 4-methyl-3,5-heptanedione with KRED-A1D (chiral capillary column, 20% permethylated cyclodextrin)

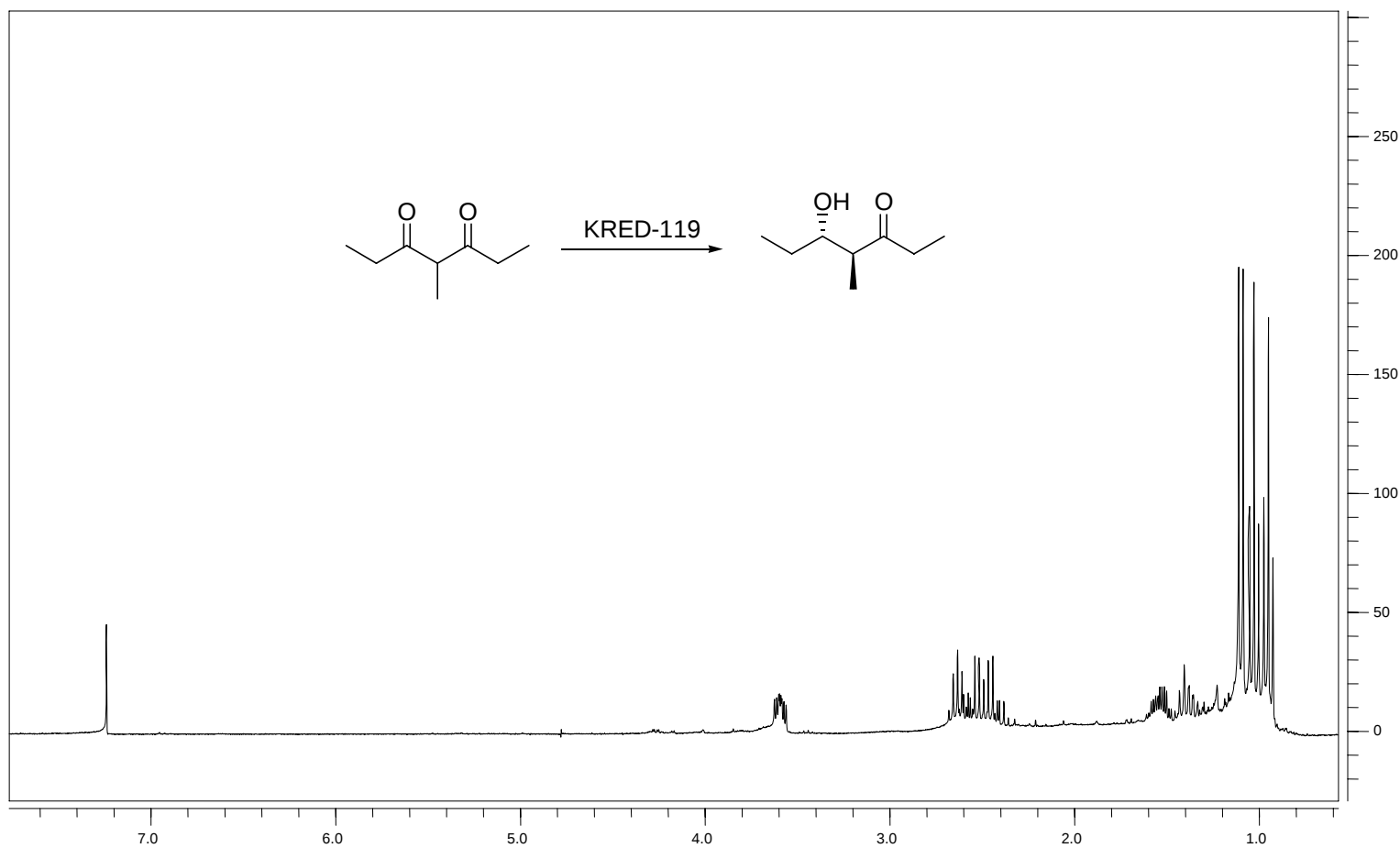


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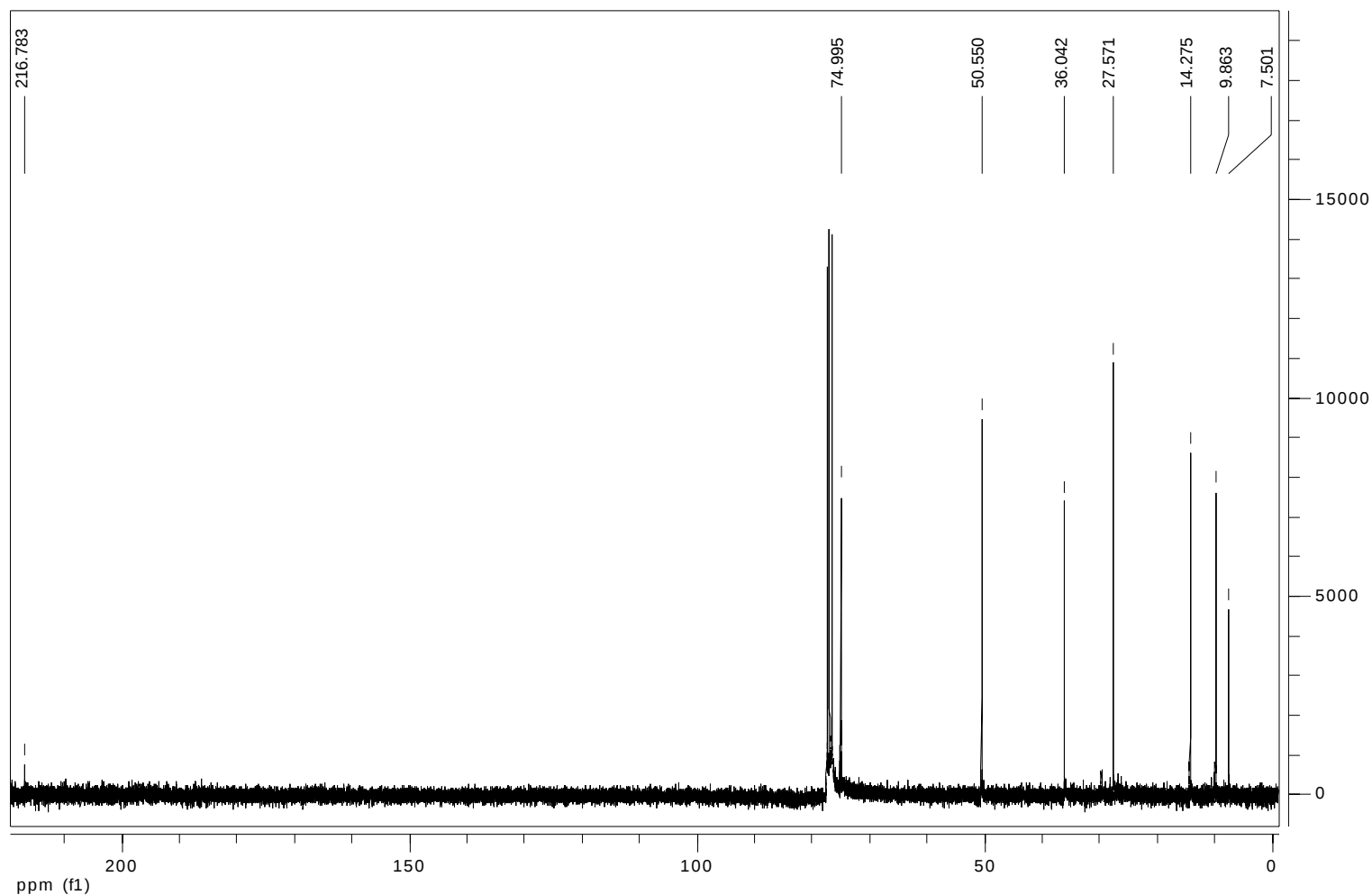
12) GC analysis of the product, after enzymatic reduction of 4-methyl-3,5-heptanedione with KRED-119 (chiral capillary column, 20% permethylated cyclodextrin)



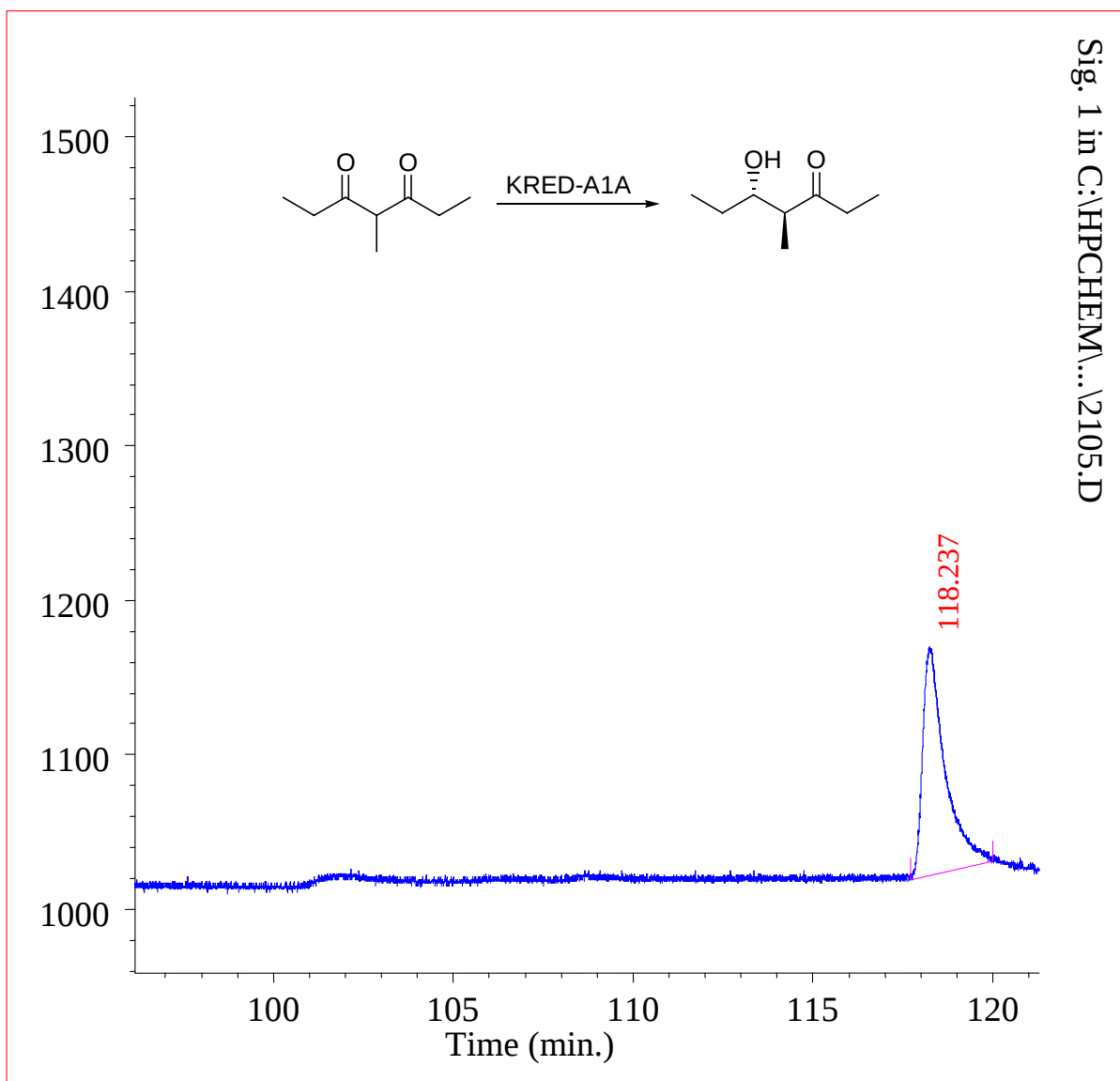
13) ^1H NMR (300 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone
after enzymatic reduction with KRED-119



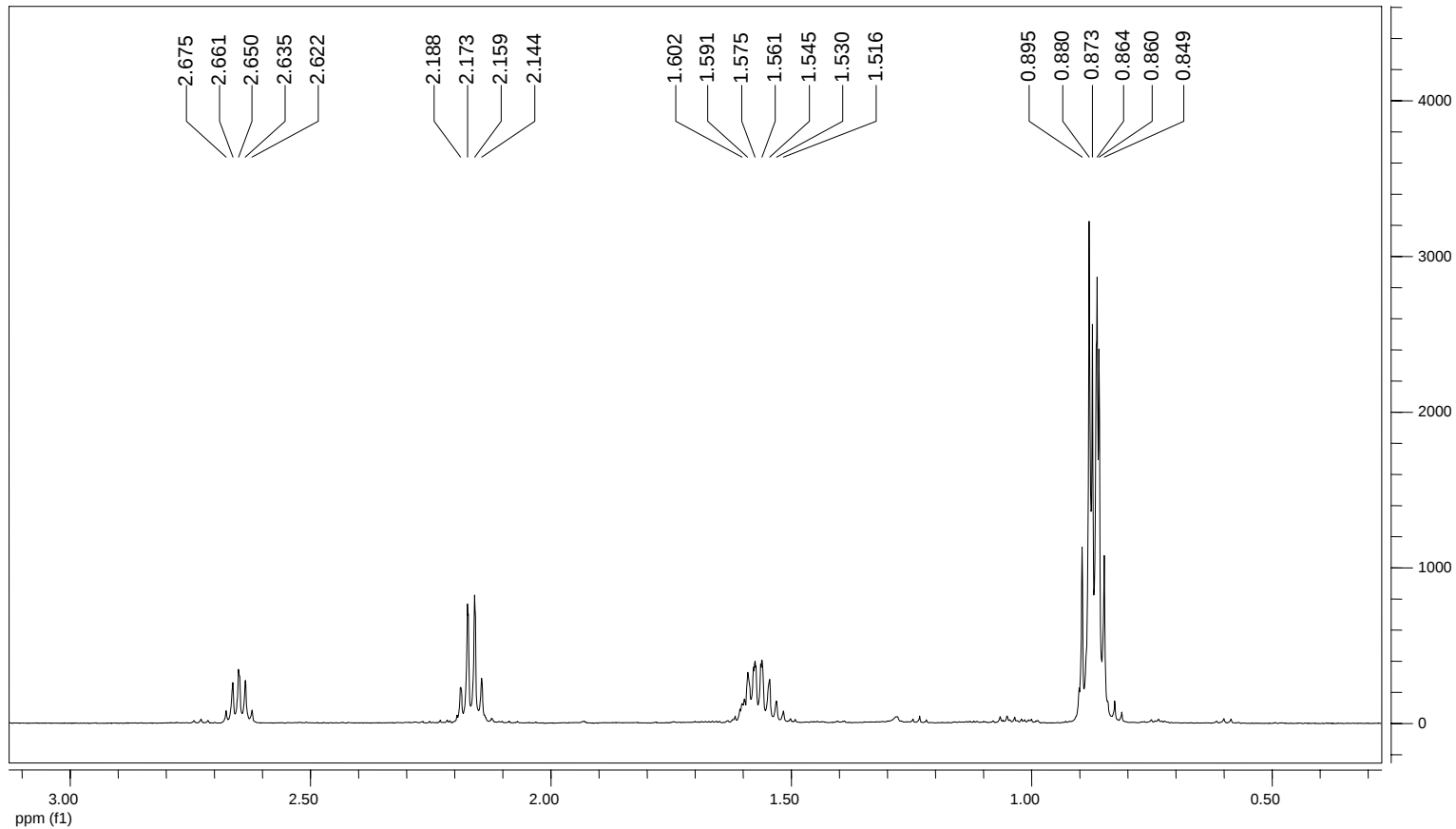
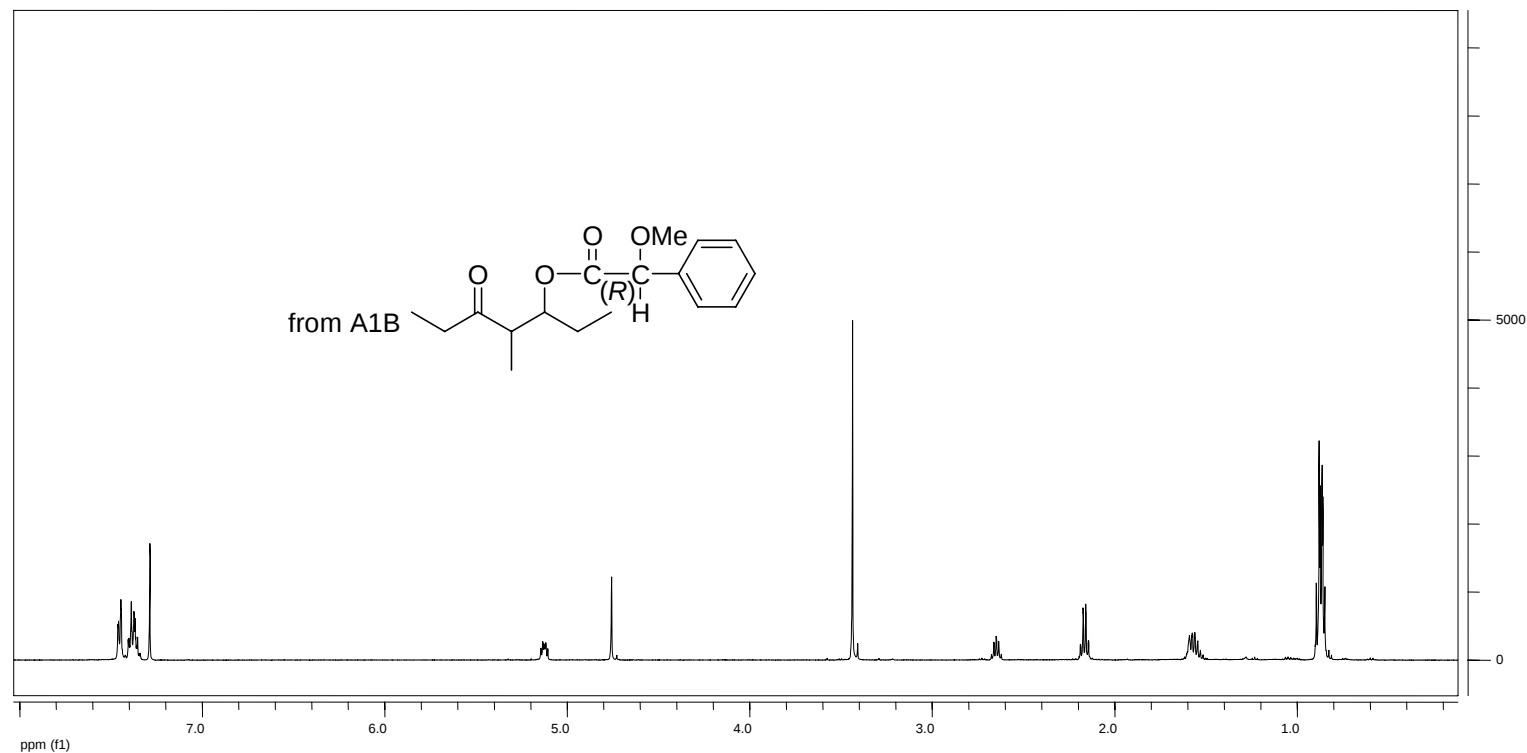
14) ^{13}C NMR (300 MHz, CDCl_3) of the produced 5-hydroxy-4-methyl-3-heptanone
after enzymatic reduction with KRED-119



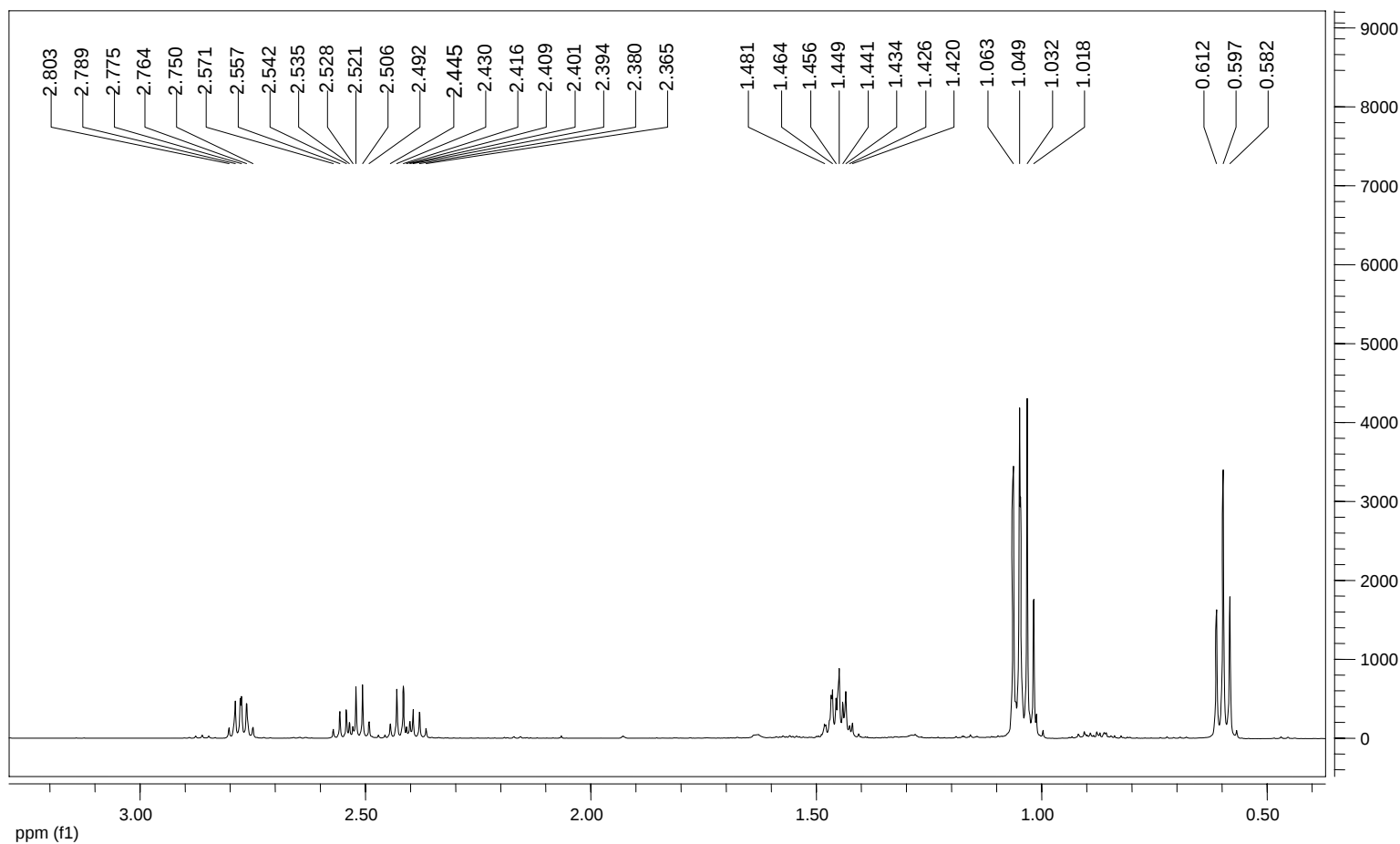
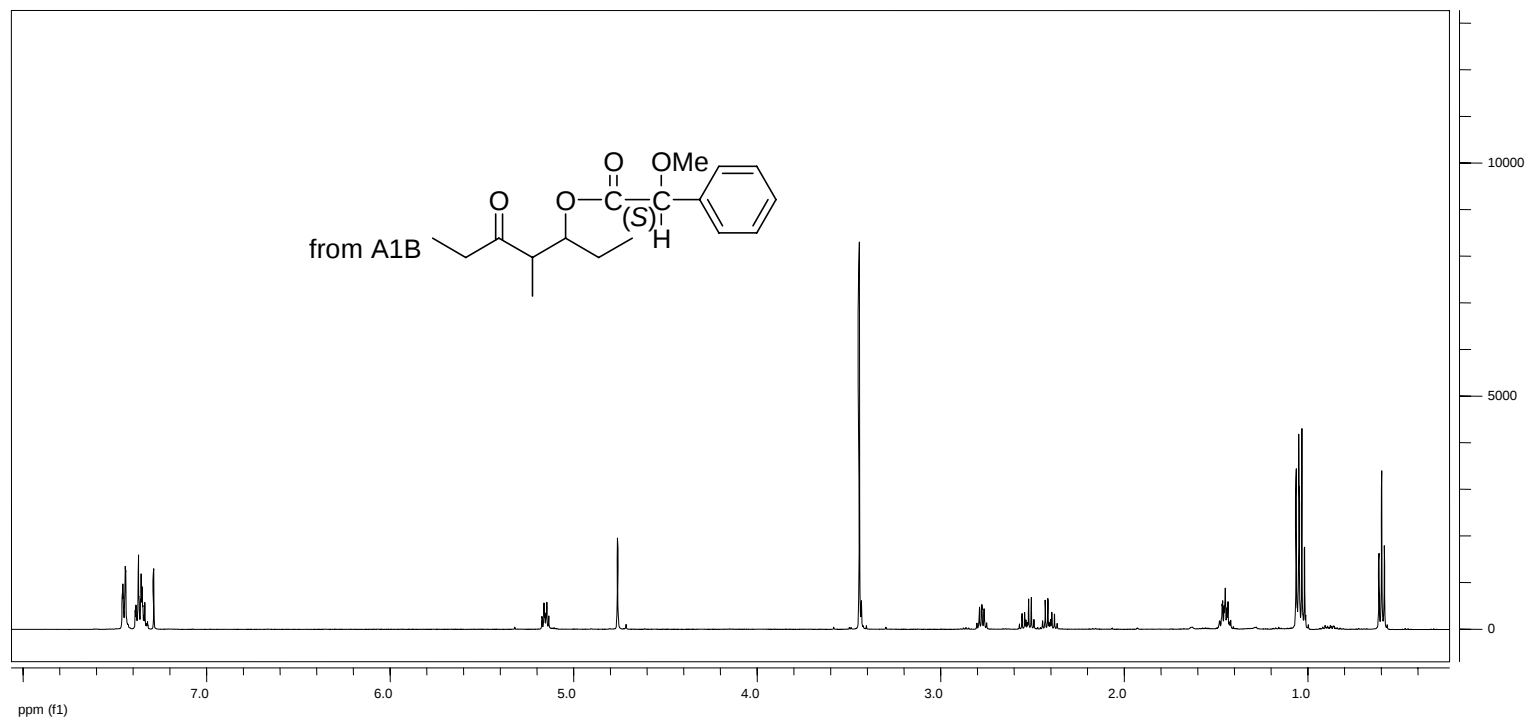
15) GC analysis of the product, after enzymatic reduction of 4-methyl-3,5-heptanedione with KRED-A1A (chiral capillary column, 20% permethylated cyclodextrin)



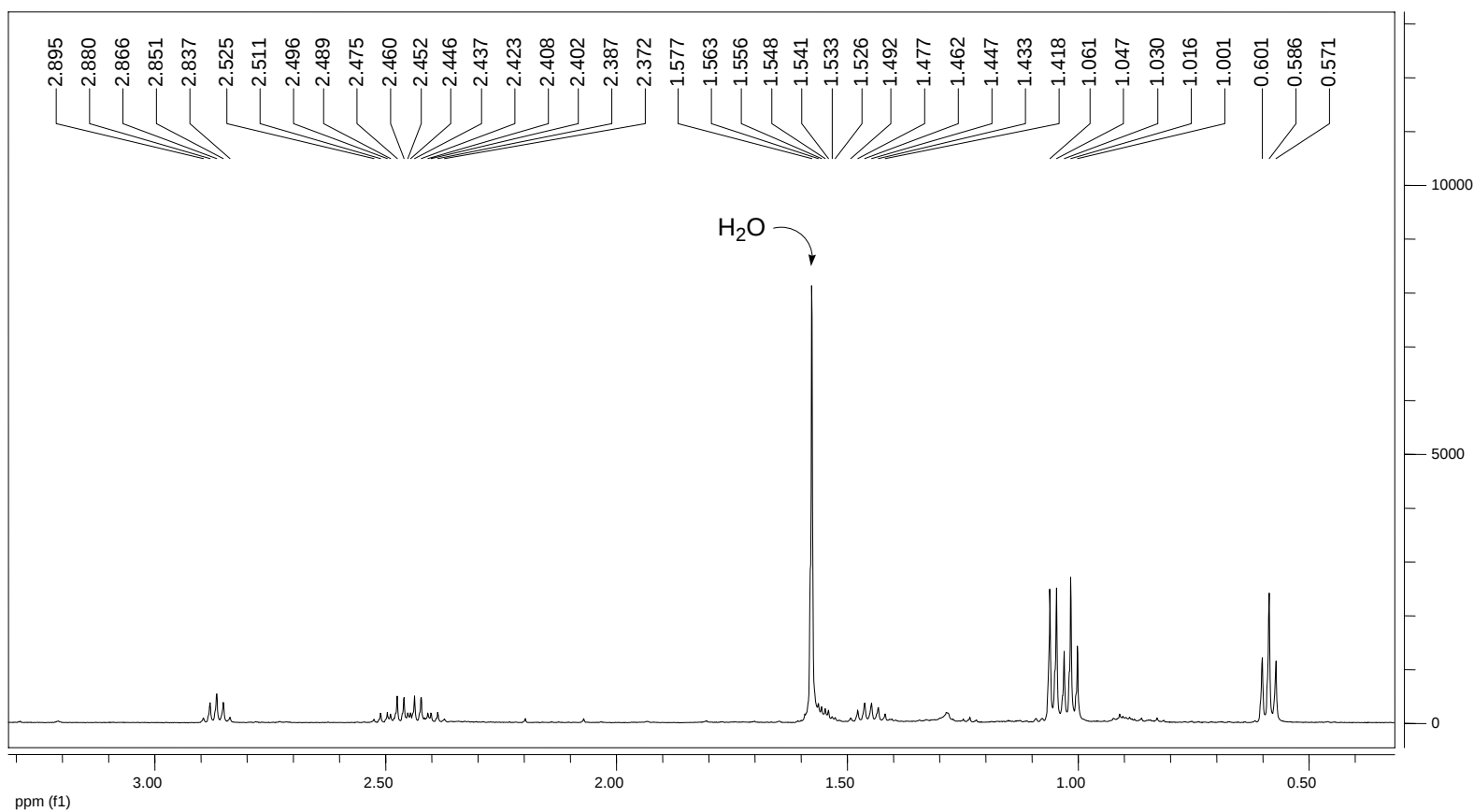
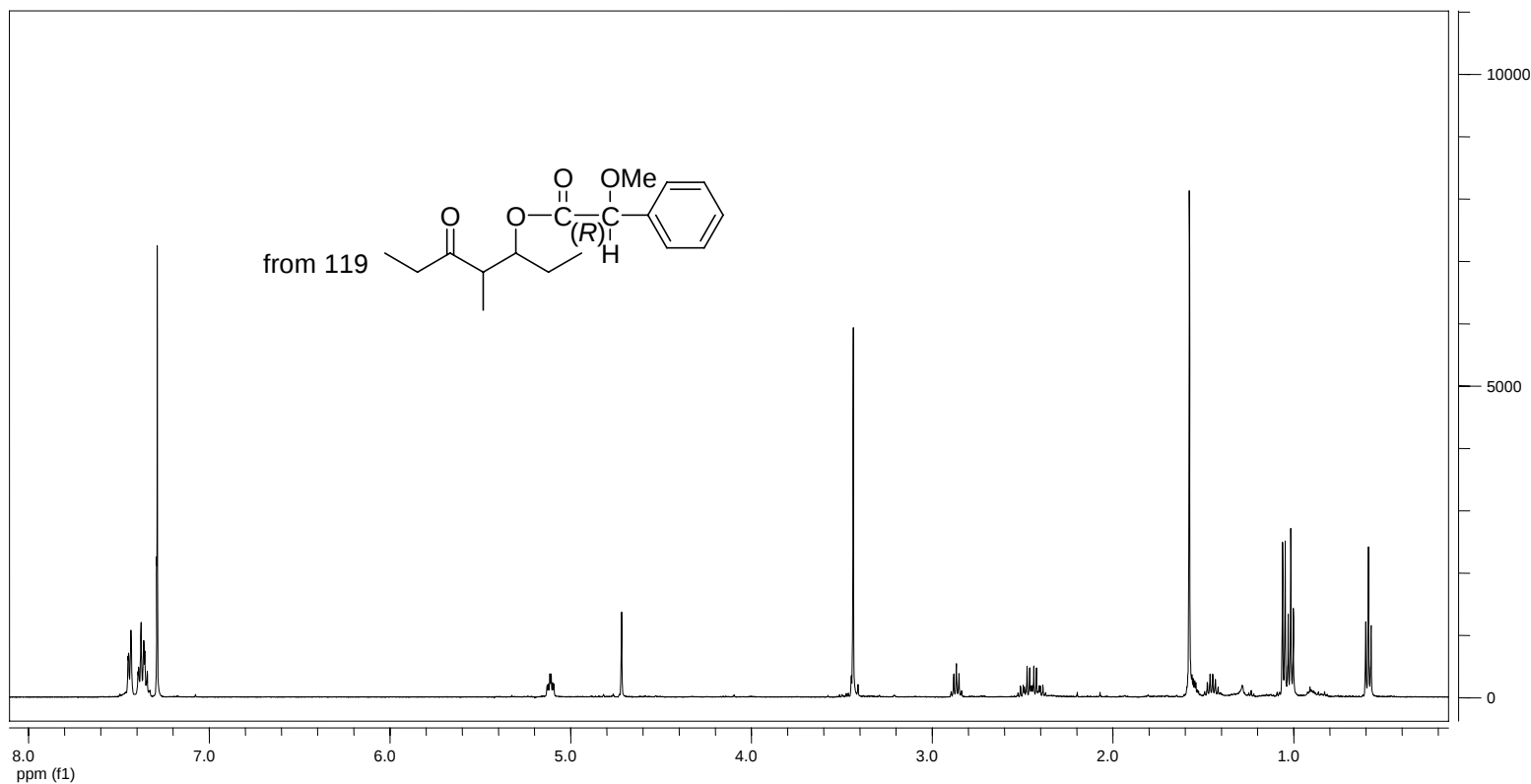
16) ^1H NMR (500 MHz, CDCl_3) of the (*R*)-MPA ester of 5-hydroxy-4-methyl-3-heptanone produced after enzymatic reduction with KRED-A1B



17) ^1H NMR (500 MHz, CDCl_3) of the (S)-MPA ester of 5-hydroxy-4-methyl-3-heptanone produced after enzymatic reduction with KRED-A1B



18) ^1H NMR (500 MHz, CDCl_3) of the (*R*)-MPA ester of 5-hydroxy-4-methyl-3-heptanone produced after enzymatic reduction with KRED-119



19) ^1H NMR (500 MHz, CDCl_3) of the (S)-MPA ester of 5-hydroxy-4-methyl-3-heptanone produced after enzymatic reduction with KRED-119

