

Electronic Supplementary Information

Synthesis of α -hydroxy ketones and vicinal (*R,R*)-diols by *Bacillus clausii*

DSM 8716^T butanediol dehydrogenase

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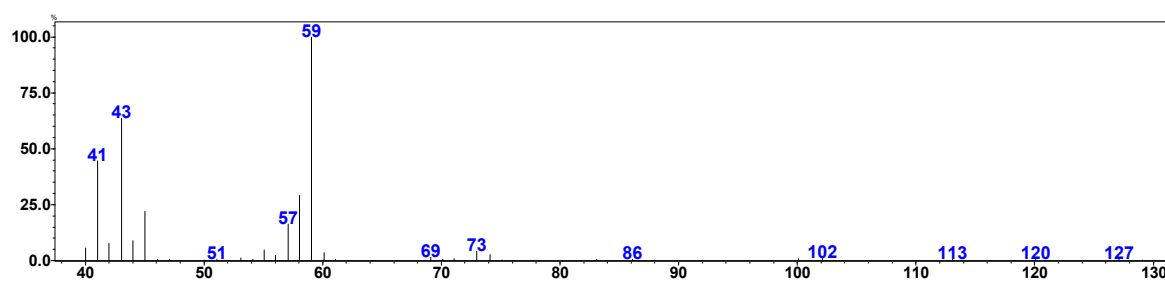
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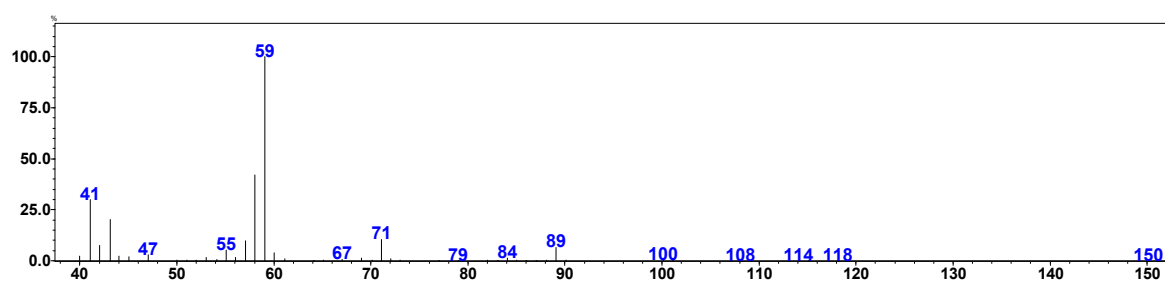
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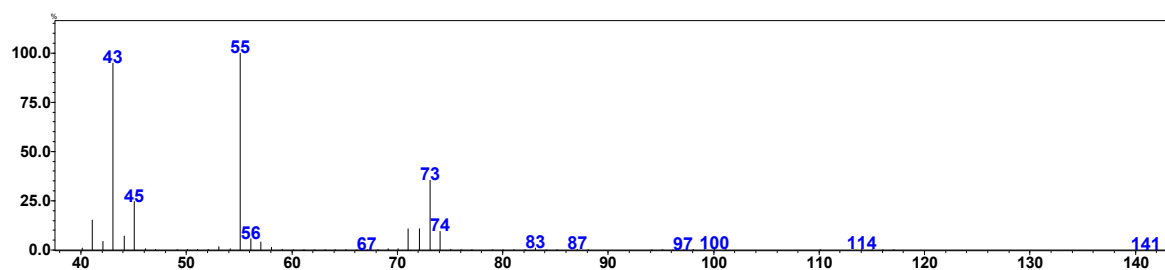
1 GC-MS spectra



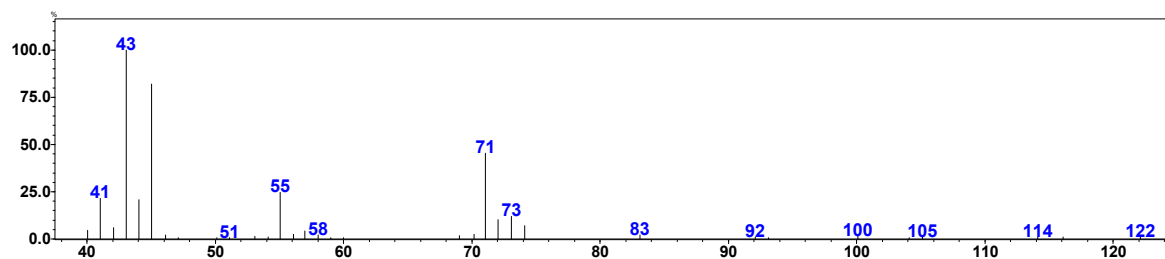
Supplementary Figure 1: Mass spectrum of 3-hydroxy-2-pentanone. Retention time: 16.4 min.



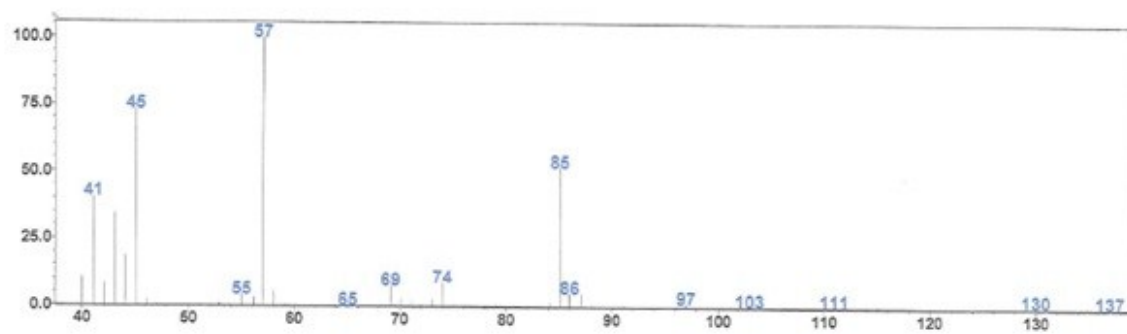
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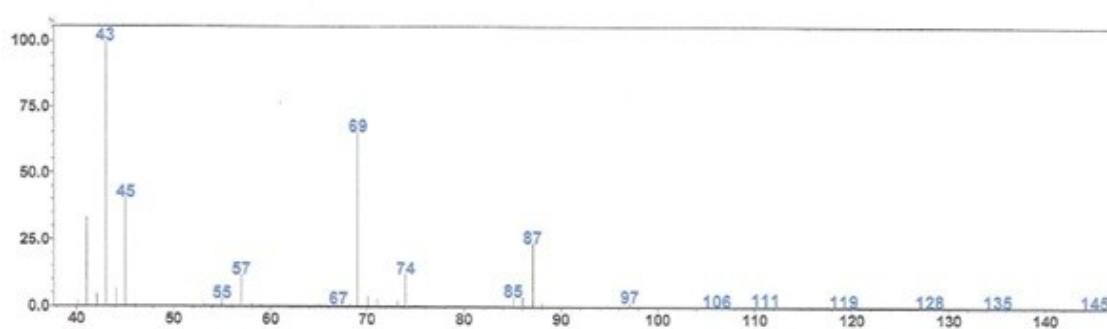
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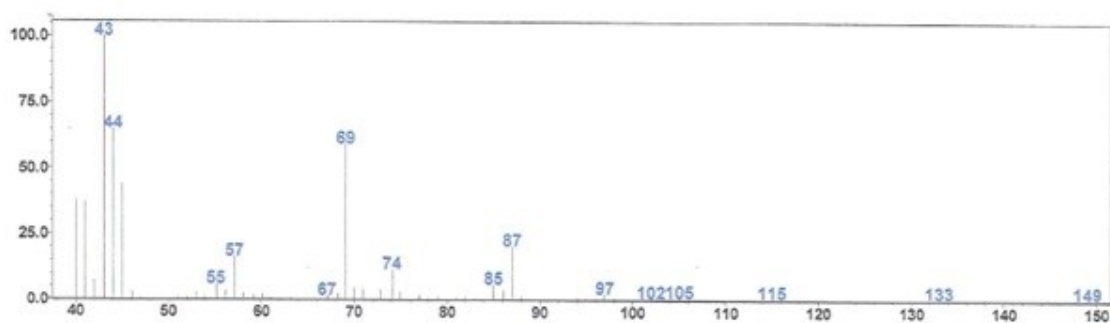
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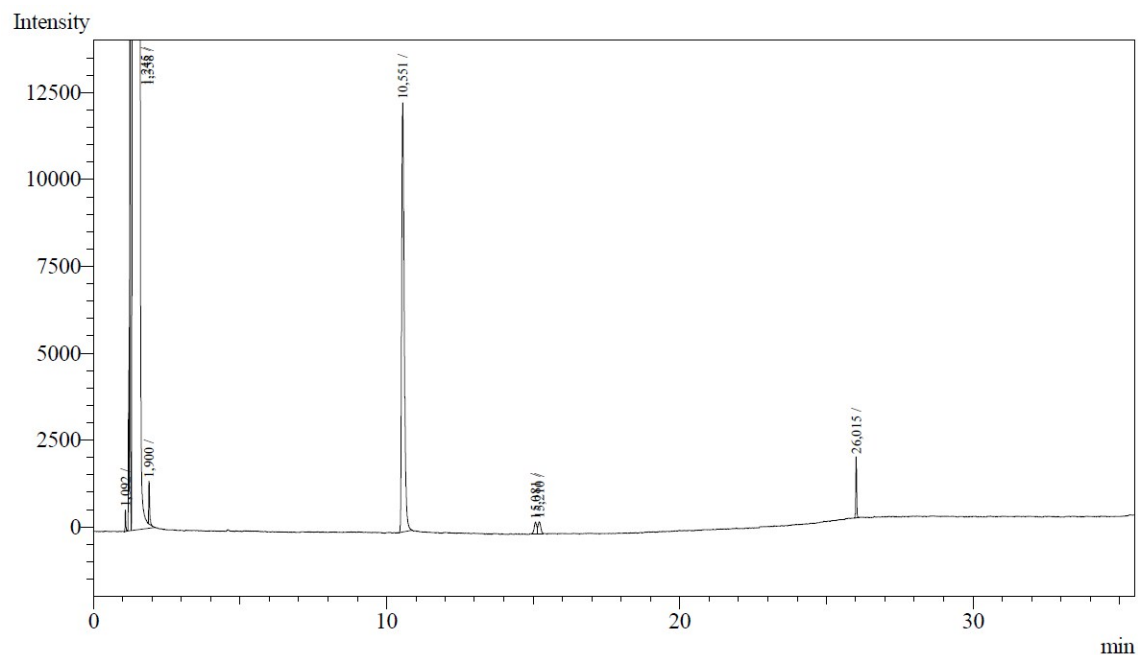


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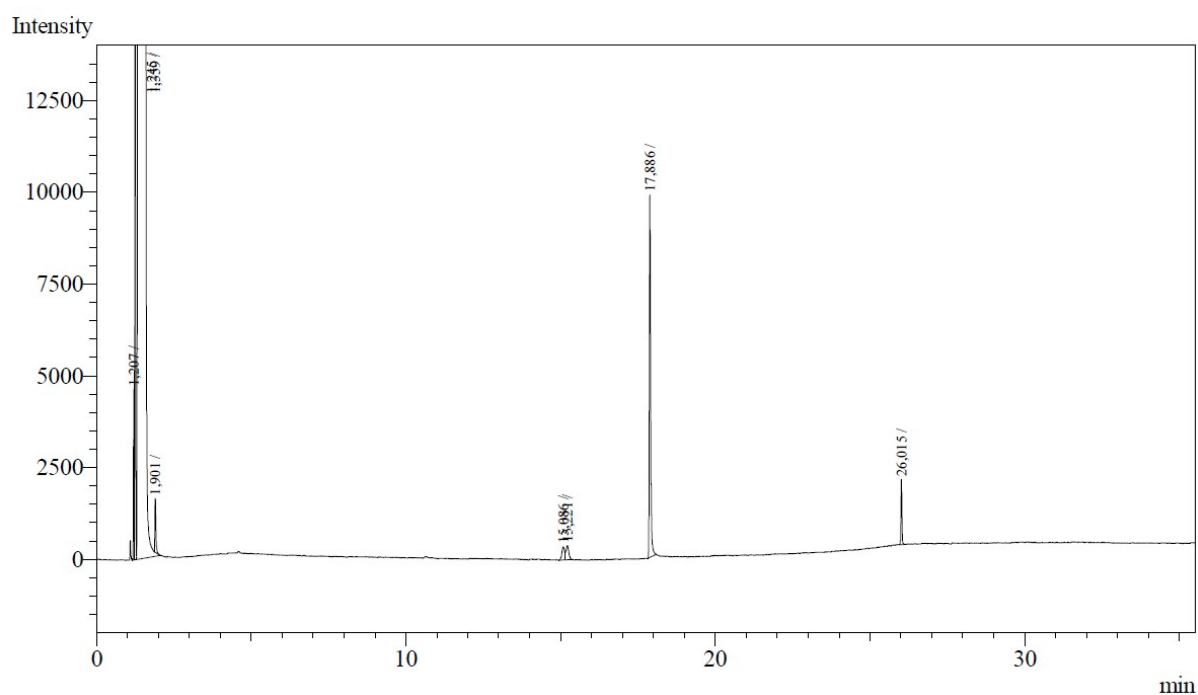


Supplementary Figure 7: Mass spectrum of (*S*)-3-hydroxy-2-hexanone. Retention time: 20.1 min.

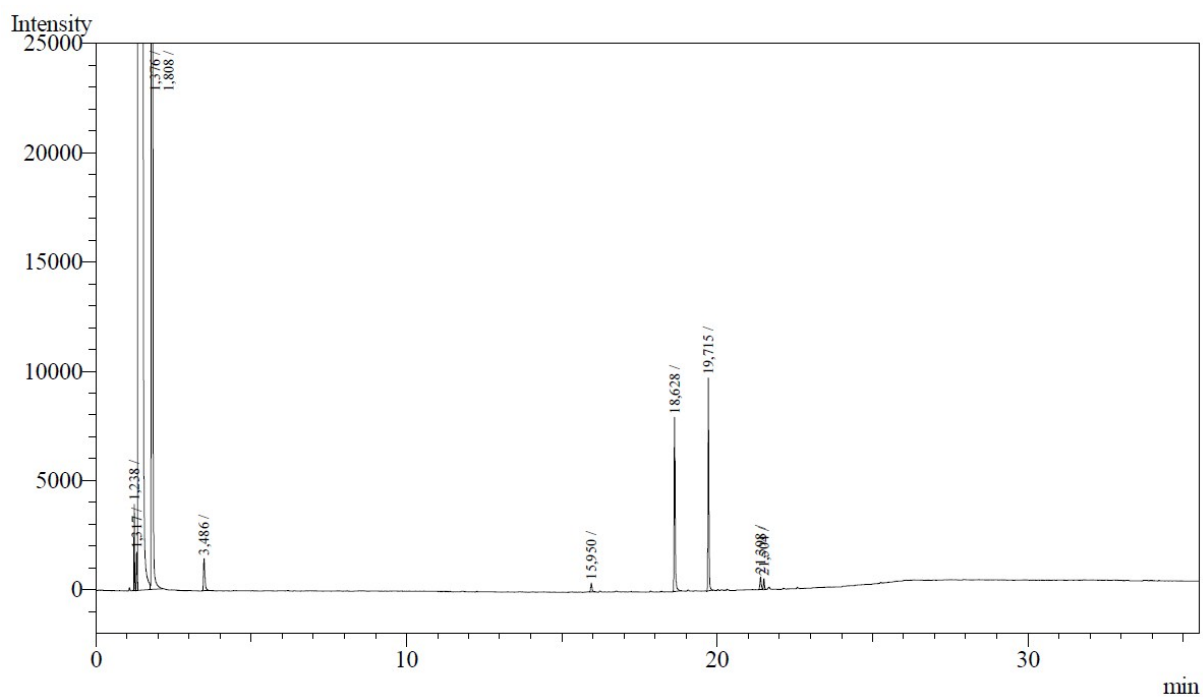
2 GC-Chromatogramms



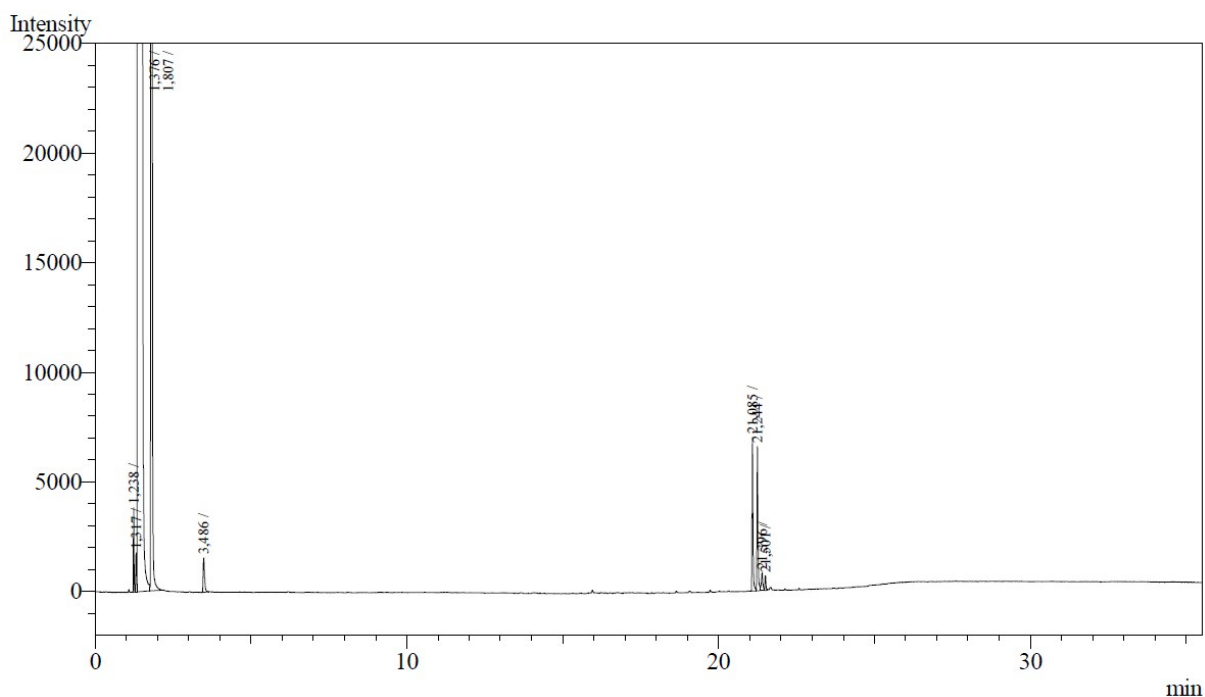
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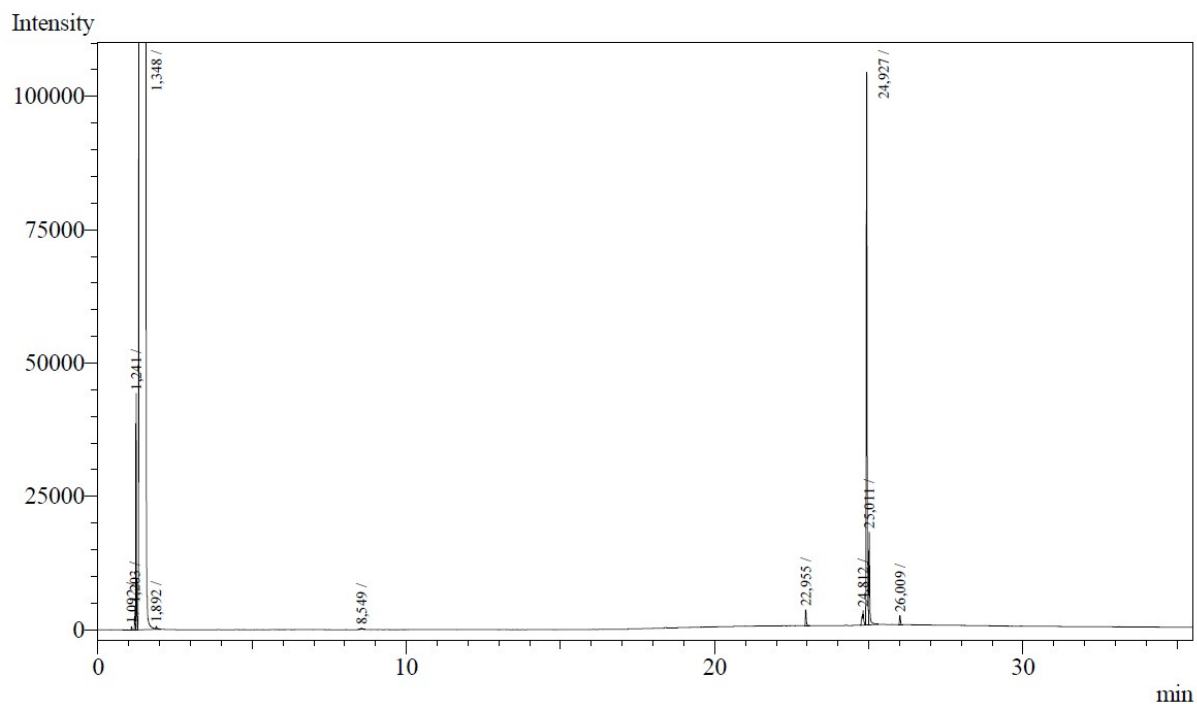
Supplementary Figure 9: Gas chromatogramm of the reduction of 3-hydroxy-3-methyl-2-butanone by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 60 min.



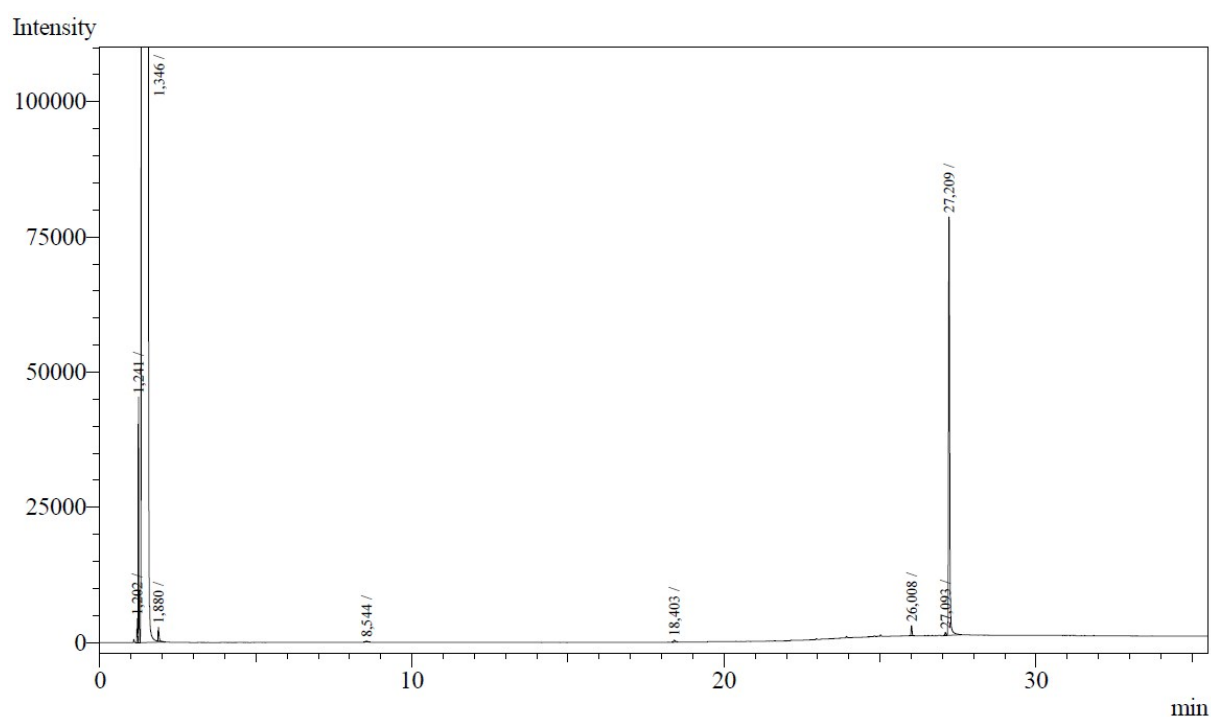
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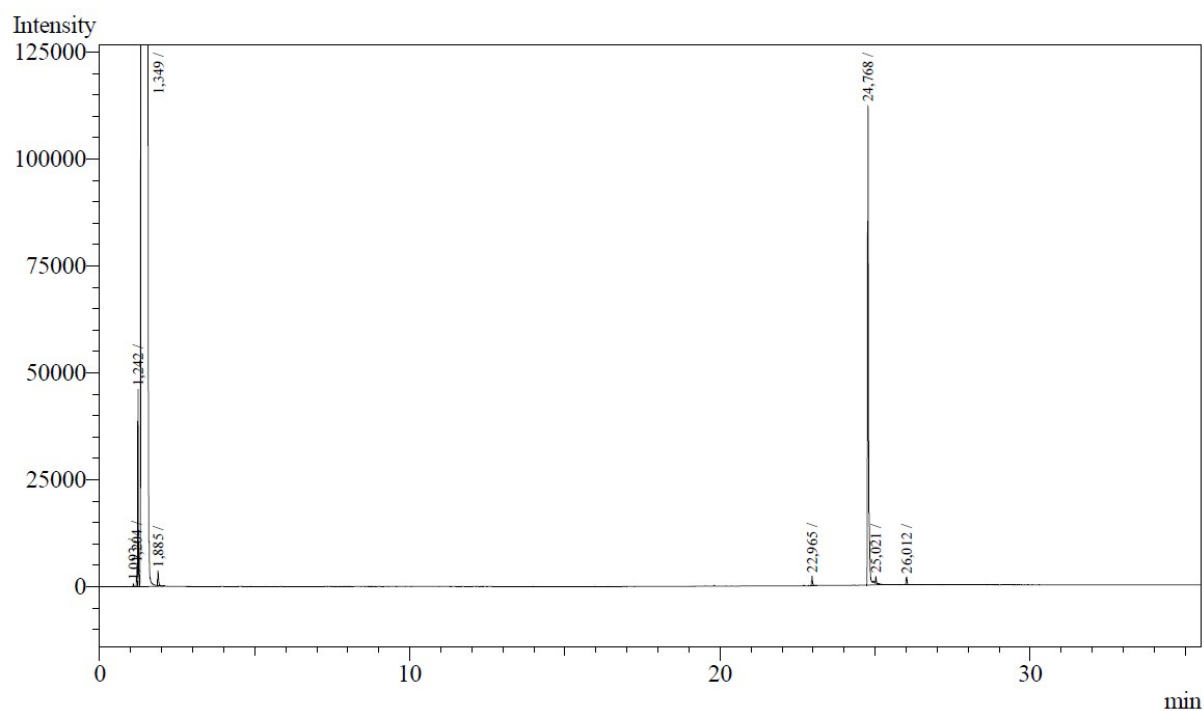
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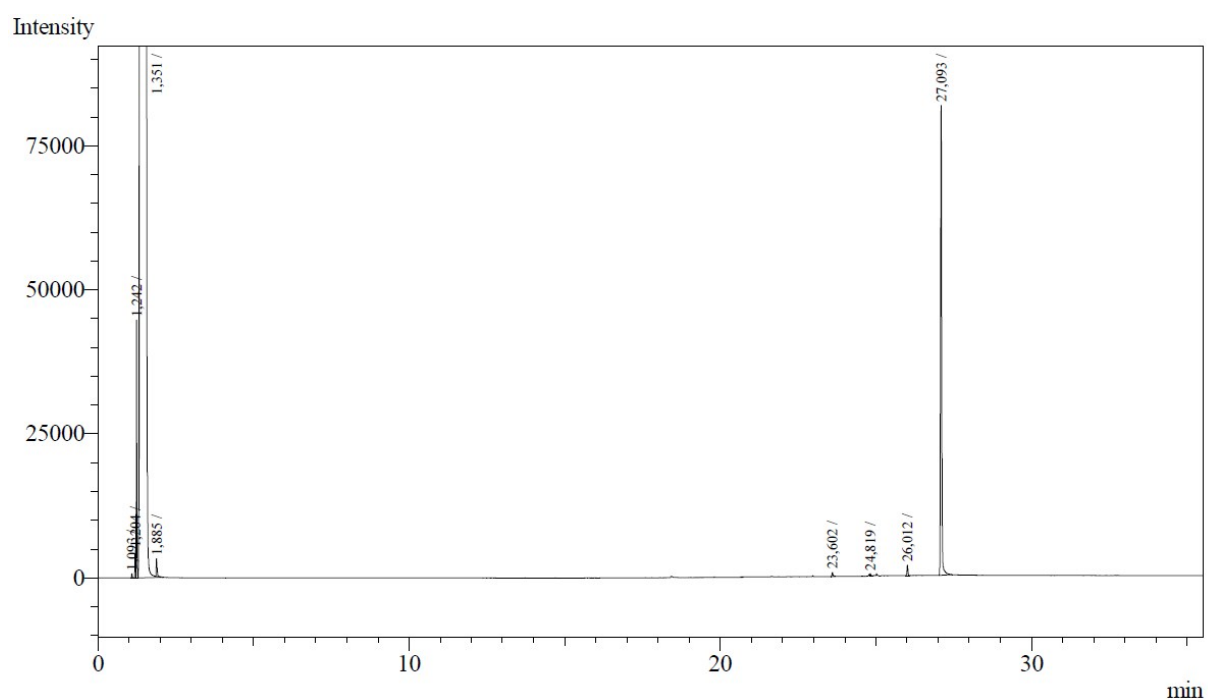
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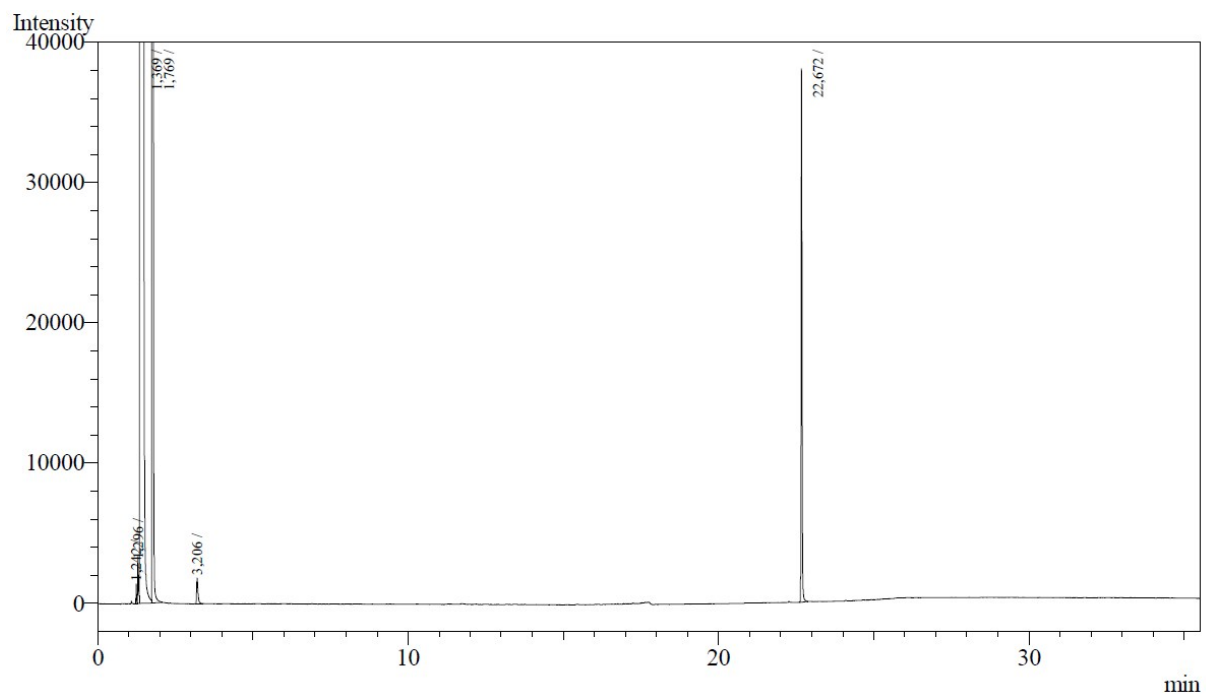
Supplementary Figure 13: Gas chromatogram of the reduction of (S)-HPP by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 60 min.



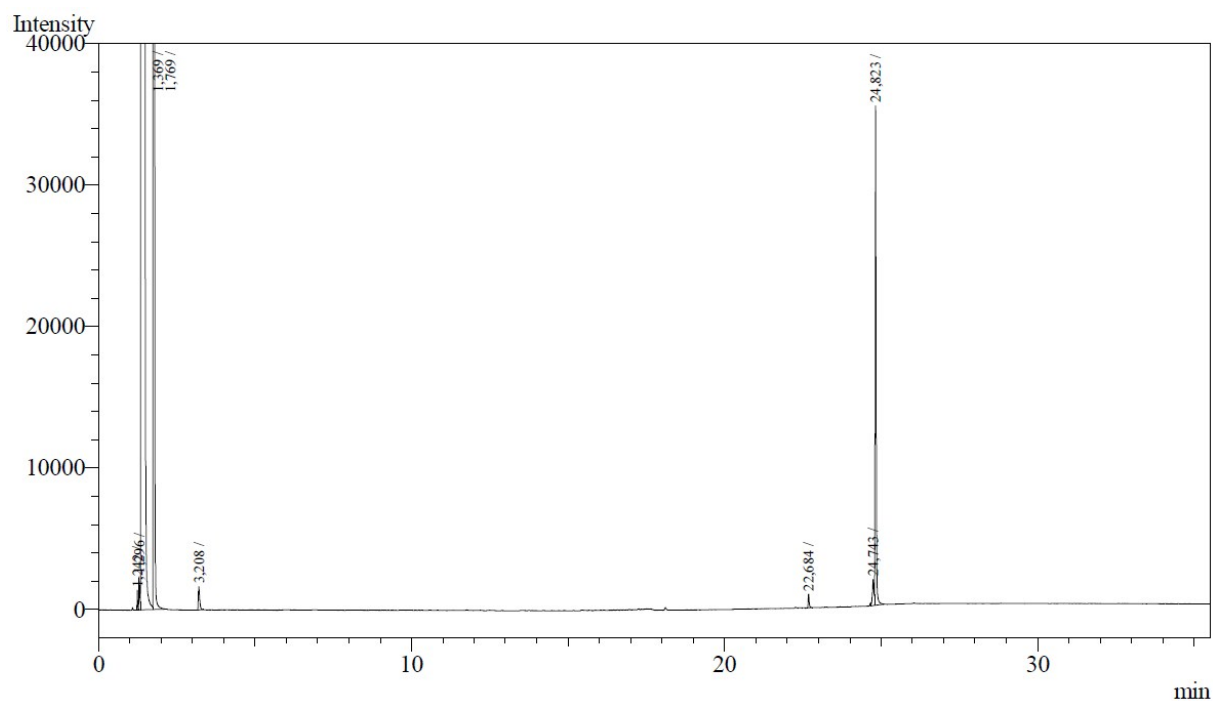
Supplementary Figure 14: Gas chromatogram of the reduction of (*R*)-HPP by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 0 min.



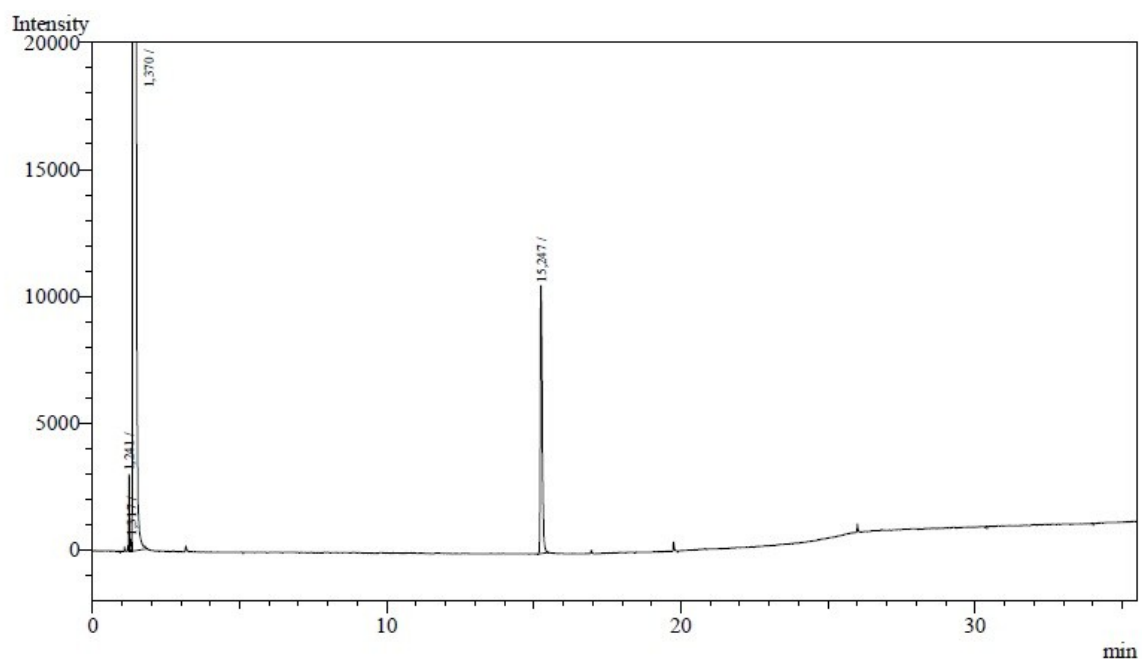
Supplementary Figure 15: Gas chromatogram of the reduction of (*R*)-HPP by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 60 min.



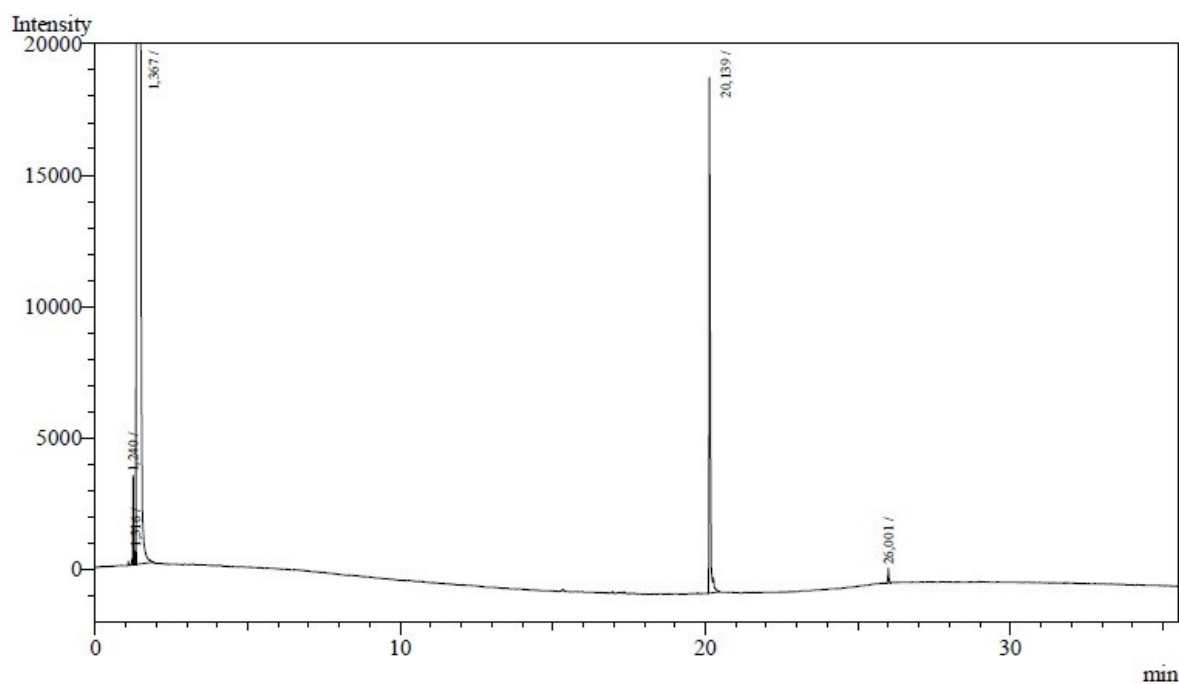
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Supplementary Figure 17: Gas chromatogramm of the reduction of 1-phenyl-1,2-propanedione by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 60 min.

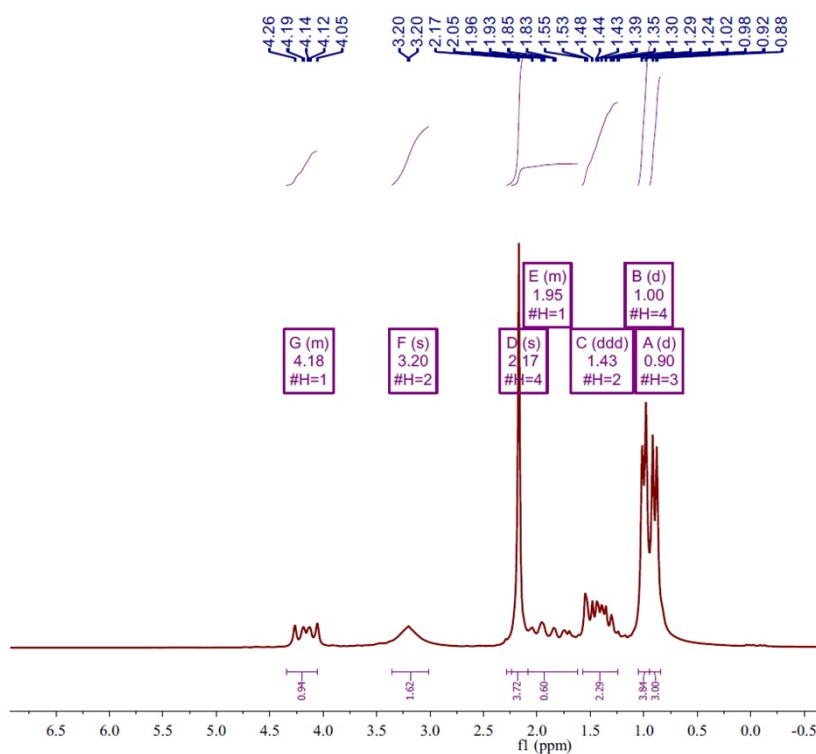


Supplementary Figure 18: Gas chromatogramm of the reduction of 2,3-heptanedione by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 0 min.

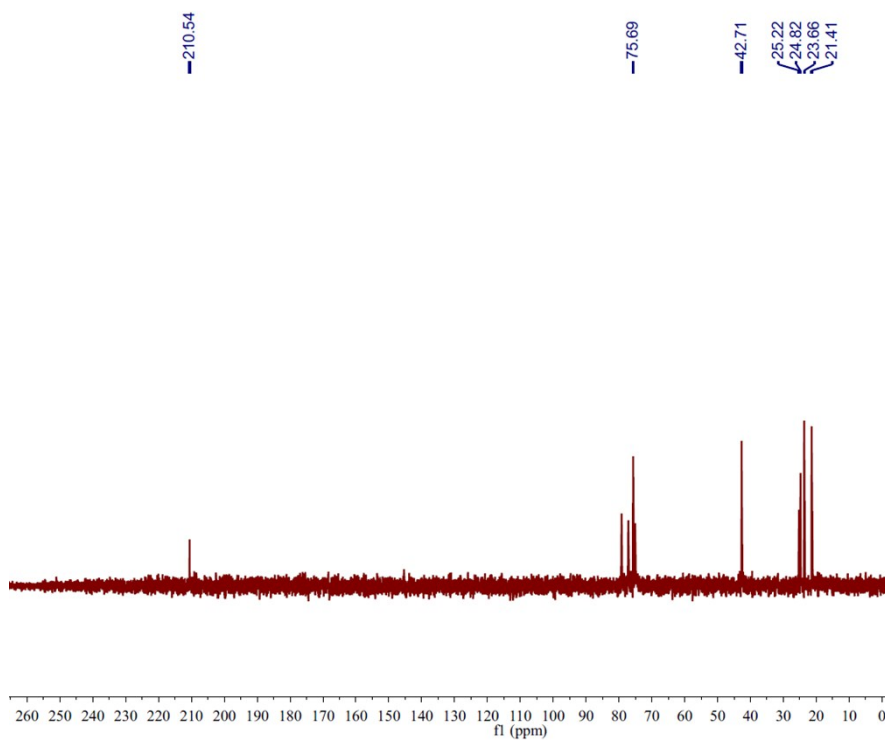


Supplementary Figure 19: Gas chromatogramm of the reduction of 2,3-heptanedione by BcBDH. Substrate (10 mM each) was reduced by 1 U BDH using formate (30 mM) and formate dehydrogenase (5 U) to regenerate NADH (0.3 mM) at 30 °C in MES-NaOH buffer (50 mM, pH 6.8; 1 ml). Reaction time 60 min.

3 NMR



Supplementary Figure 20: ^1H -NMR of biocatalytic product (*R*)-5-methyl-3-hydroxy-2-hexanone, containing small amounts of 5-methyl-2-hydroxy-3-hexanone. (CDCl_3) σ 0.90 (d, 3H), 1.00 (d, 4H), 1.43 (ddd, 2H), 1.95 (m, 1H), 2.17 (s, 4H), 3.20 (s, 2H) 4.18 (m, 1H). s = singlet; d = doublet; ddd = doublet of doublet of doublet; m = multiplet.



Supplementary Figure 21: ^{13}C -NMR of biocatalytic product (*R*)-5-methyl-3-hydroxy-2-hexanone, containing small amounts of 5-methyl-2-hydroxy-3-hexanone. (CDCl_3) σ 21.41; 23.66; 24.82; 25.22; 42.71; 75.69; 210.54.