Supplementary Information

Enzyme-catalysed regio- and enantioselective preparative scale synthesis of (S)-2-hydroxy alkanones

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1. GC Methods

1.1. Method: 2,3-pentanedione reduction

For the 2,3-pentanedione reduction a temperature gradient from 95°C to 115°C was applied with a slope of 2°C min^{-1}.

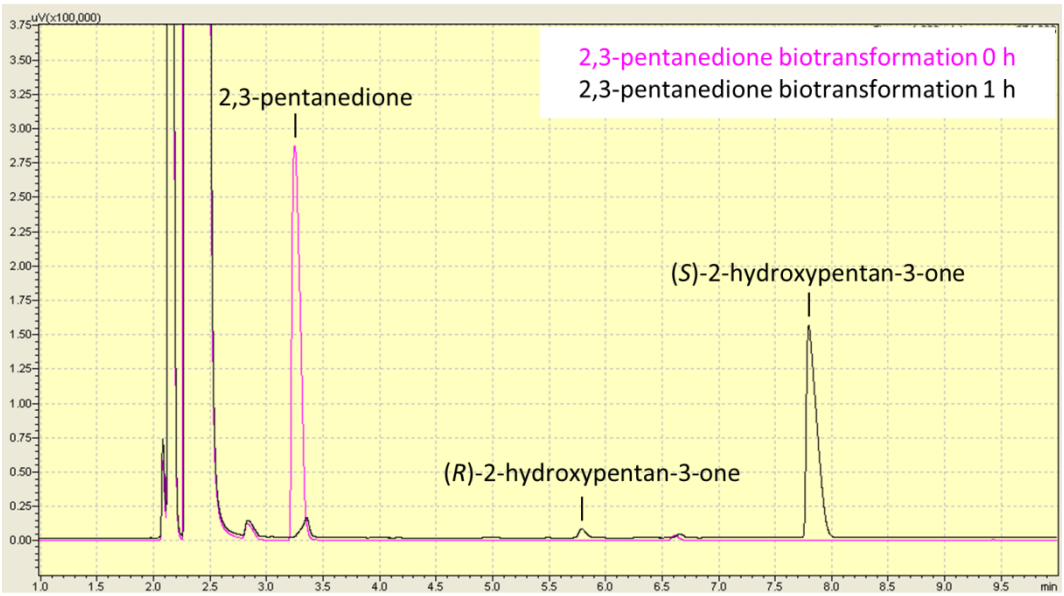


Figure S1. GC spectrum of the 2,3-pentanedione reduction by CPCR2 sampled at reaction start and after 1 h.

1.2. Method: 2,3-hexanedione reduction

For the 2,3-hexanedione reduction a temperature gradient from 98°C to 122°C was applied with a slope of 2°C min^{-1}.

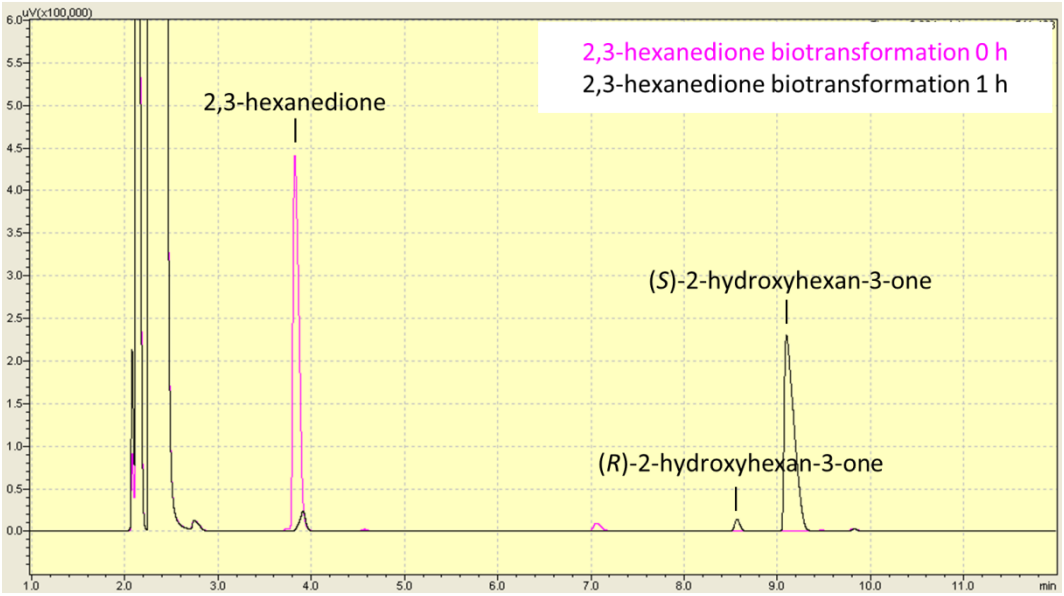


Figure S2. GC spectrum of the 2,3-hexanedione reduction by CPCR2 sampled at reaction start and after 1 h.

1.3. Method: 2,3-heptanedione reduction

For the 2,3-heptanedione reduction a temperature gradient from 105°C to 125°C was applied with a slope of 2°C min^{-1}.

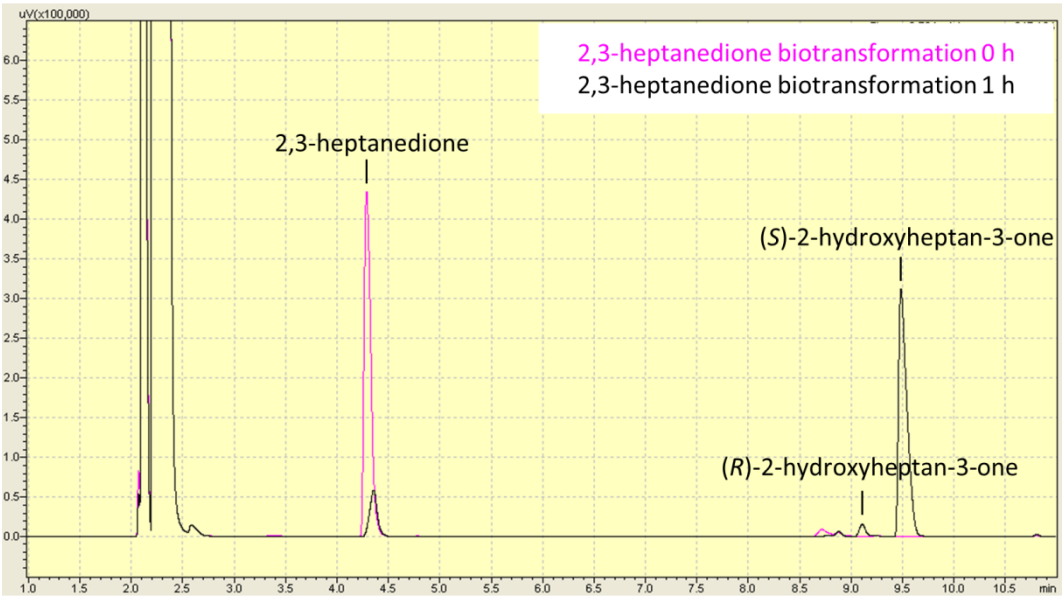


Figure S3. GC spectrum of the 2,3-heptanedione reduction by CPCR2 sampled at reaction start and after 1 h.

2. ^{1}H-NMR spectra – products

2.1. ^{1}H-NMR spectrum: (*S*)-2-hydroxypentan-3-one

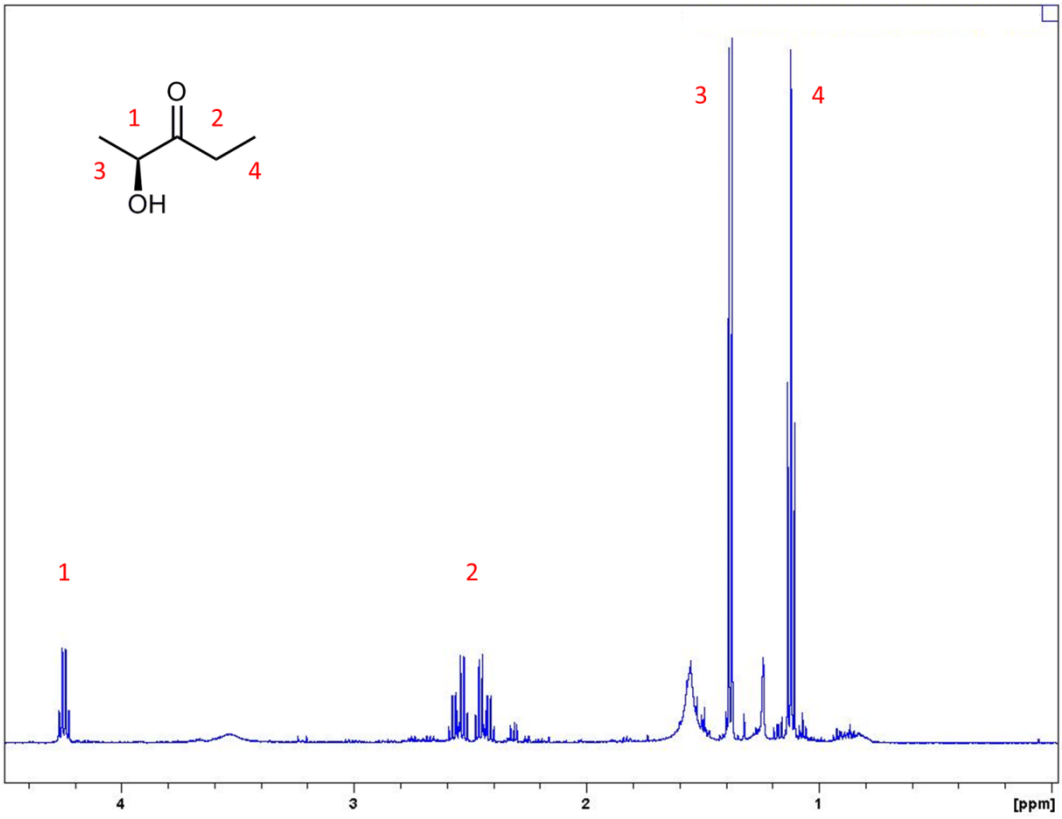


Figure S4. ^{1}H-NMR spectrum of (S)-2-hydroxypentan-3-one in d-Chloroform.

2.2. ^{1}H-NMR spectrum: (*S*)-2-hydroxyhexan-3-one

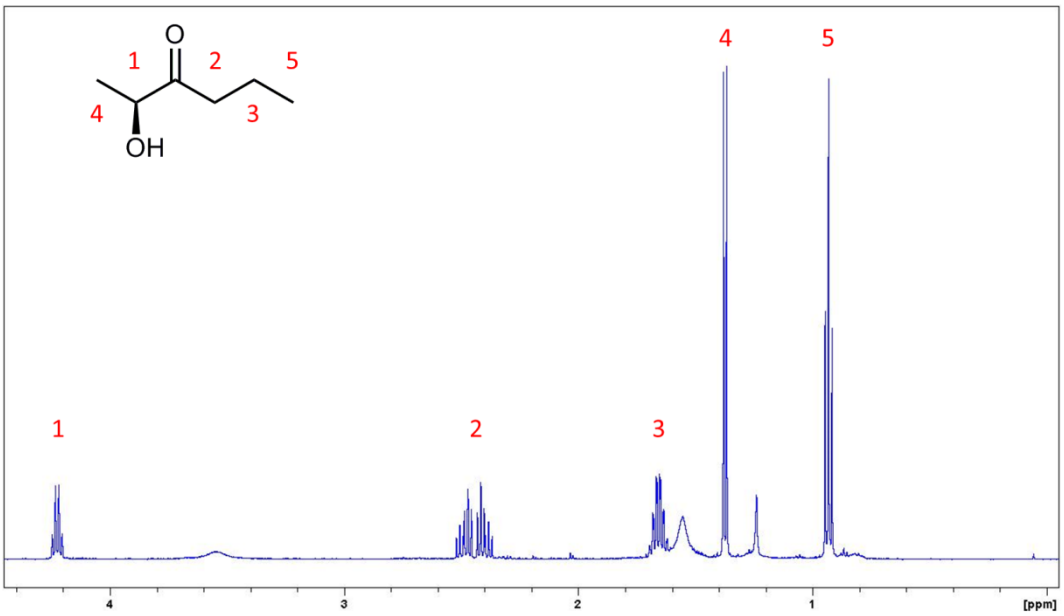


Figure S5. ^{1}H-NMR spectrum of (S)-2-hydroxyhexan-3-one in d-Chloroform.

2.3. ^{1}H-NMR spectrum: (*S*)-2-hydroxyheptan-3-one

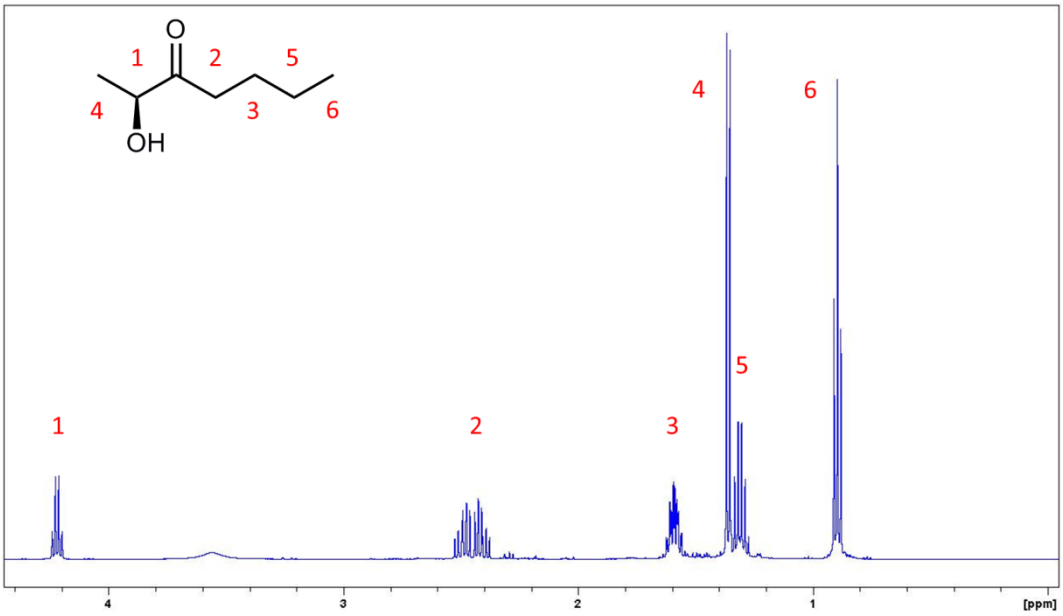
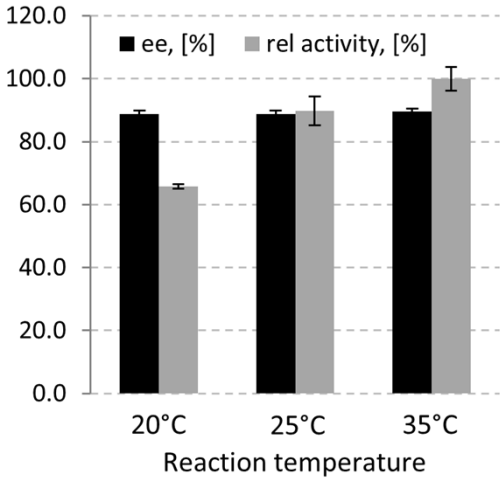
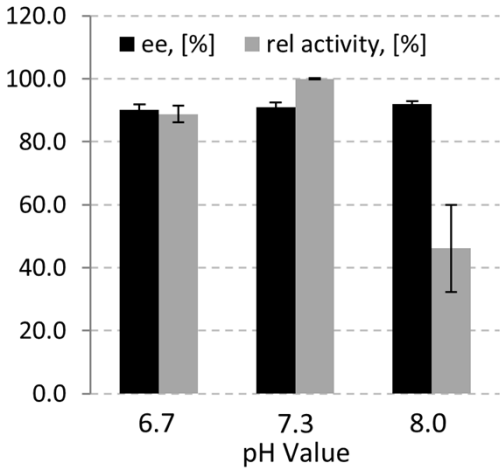


Figure S6. ^{1}H-NMR spectrum of (S)-2-hydroxyheptan-3-one in d-Chloroform.

3. Process optimization





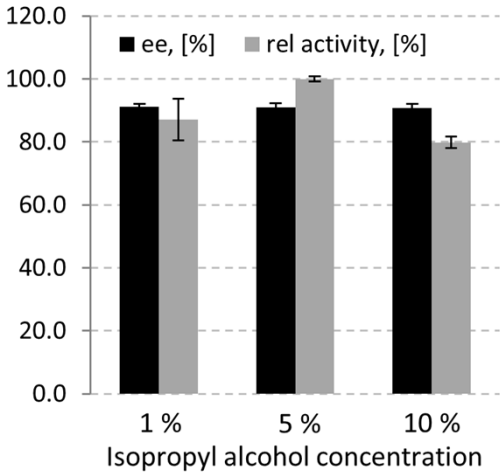


Figure S7. Influence of the different reaction parameters on the activity and stereospecificity of the CPCR2 catalyzed reduction of 2,3-pentanedione.

4. H-NMR spectra – Mosher´s esters

4.1. Mosher´s ester: (*S*)-2-hydroxypentan-3-one

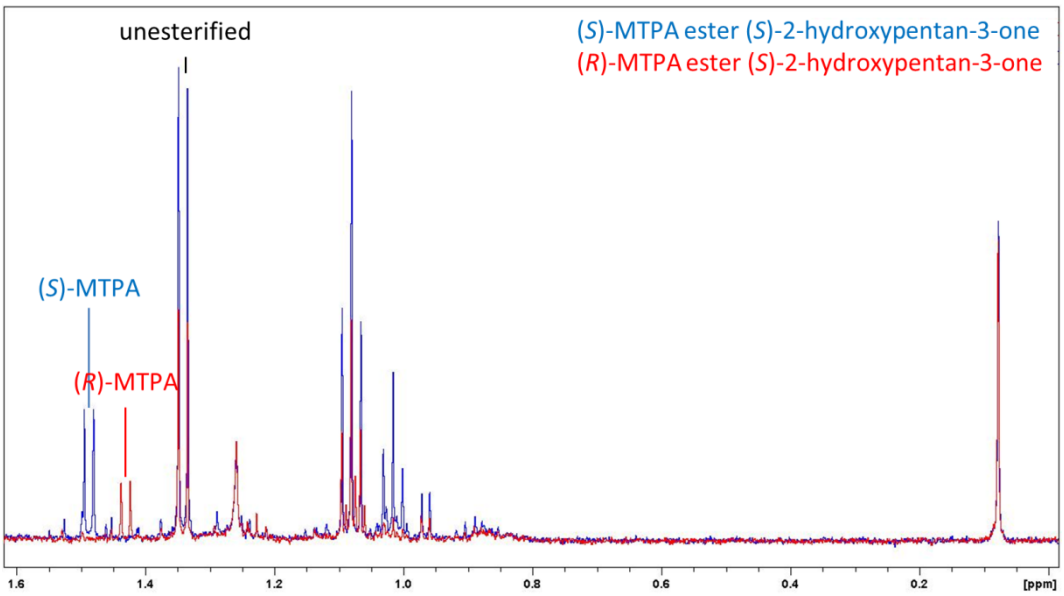


Figure S8. ^{1}H-NMR spectrum of the Mosher's esters of (S)-2-hydroxypentan-3-one with (*S*)-MTPA and (*R*)-MTPA in d-dichloromethane.

4.2. Mosher´s ester: (*S*)-2-hydroxyhexan-3-one

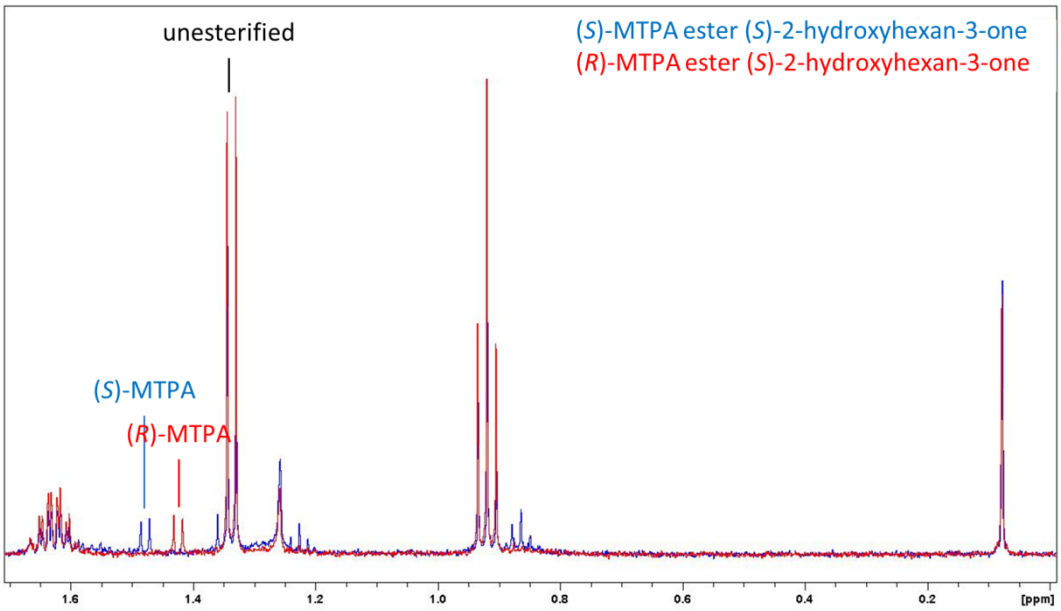


Figure S9. ^{1}H-NMR spectrum of the Mosher´s esters of (S)-2-hydroxyhexan-3-one with (*S*)-MTPA and (*R*)-MTPA in d-dichloromethane.

4.3. Mosher´s ester: (*S*)-2-hydroxyheptan-3-one

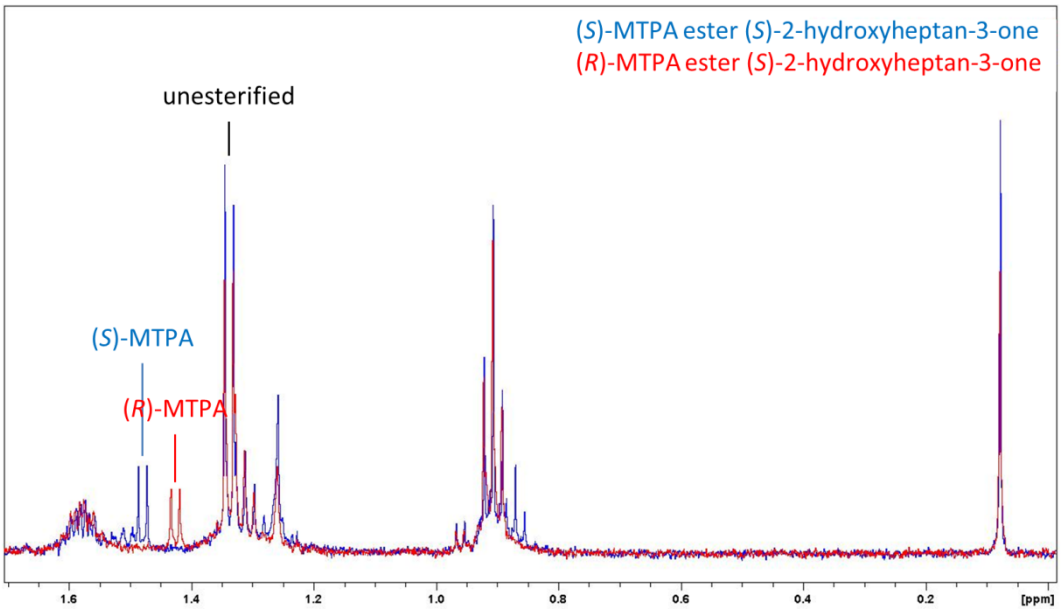


Figure S10. ^{1}H-NMR spectrum of the Mosher's esters of (S)-2-hydroxyheptan-3-one with (*S*)-MTPA and (*R*)-MTPA in d-dichloromethane.