Supplementary Material

Synthesis and structure determination of diastereomeric carbapenems in the Ad₇E-reaction of (±)-4,4-dimethyl-3-mercaptodihydrofuran-2(3H)-one with chiral carbapenem enol phosphate

Zuleykha Valiullina,* Adeliya Galeeva,a Alexander Lobov,a Leonard Khalilov,b and Mansur Miftakhov*a

a Ufa Institute of Chemistry, Ufa Federal Research Centre of the Russian Academy of Sciences, 450054 Ufa, Russian Federation
b Institute of Petrochemistry and Catalysis, Ufa Federal Research Centre of the Russian Academy of Sciences, 450071 Ufa, Russian Federation
E-mail: bioreg@anrb.ru

Table of Contents

1. Copies of 1H and 13C NMR spectra of compound 5 S2
2. Copies of 1H and 13C NMR spectra of compound 6 S4
3. Copies of 1H and 13C NMR spectra of compound 3 S6
4. Copies of 1H and 13C NMR spectra of compound 7 S8
5. Copies of 1H and 13C NMR spectra of compound 8 S10
6. Copies of 1H and 13C NMR spectra of compound 1a S12
7. Copies of 1H and 13C NMR spectra of compound 1b S17
8. Copies of 1H and 13C NMR spectra of compound 11a S22
9. Copies of 1H and 13C NMR spectra of compound 11b S27
10. Copies of 1H NMR spectra of (±)-3 and spectra (±)-3 after each addition of (-)-Eu (hfc)₃ S32
11. Copies of 1H NMR spectra mixture of diastereomers 1a and 1b for determination of their ratio S35
NMR data

Figure S1. Complete $^1$H NMR spectrum of compound 5 in CDCl$_3$, 500 MHz.

Figure S2. Expanded $^1$H NMR spectrum of compound 5 in CDCl$_3$, 500 MHz.
Figure S3. Complete $^{13}$C{$^{1}$H} spectrum of compound 5 in CDCl$_3$, 125 MHz.

Figure S4. DEPT-135 editing $^{13}$C{$^{1}$H} NMR spectrum of compound 5 in CDCl$_3$, 125 MHz: a) $^{13}$C{$^{1}$H} spectrum; b) DEPT-135.
Figure S5. Complete $^1$H NMR spectrum of compound 6 in CDCl₃, 500 MHz.

Figure S6. Expanded $^1$H NMR spectrum of compound 6 in CDCl₃, 500 MHz.
Figure S7. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound 6 in CDCl$_3$, 125 MHz.

Figure S8. DEPT-135 editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 6 in CDCl$_3$, 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135.
Figure S9. Complete $^1$H NMR spectrum of compound 3 in CDCl$_3$, 500 MHz.

Figure S10. Expanded $^1$H NMR spectrum of compound 3 in CDCl$_3$, 500 MHz.
Figure S11. Complete $^{13}$C-{$^1$H} spectrum of compound 3 in CDCl$_3$, 125 MHz.

Figure S12. DEPT-135 editing $^{13}$C-{$^1$H} NMR spectrum of compound 3 in CDCl$_3$, 125 MHz: a) $^{13}$C-{$^1$H} spectrum; b) DEPT-135.
Figure S13. Complete $^1$H NMR spectrum of compound 7 in Acetone-$d_6$, 500 MHz.

Figure S14. Expanded $^1$H NMR spectrum of compound 7 in Acetone-$d_6$, 500 MHz.
Figure S15. Complete $^{13}$C-$^1$H spectrum of compound 7 in Acetone-$d_6$, 125 MHz.

Figure S16. DEPT-135 editing $^{13}$C-$^1$H NMR spectrum of compound 7 in Acetone-$d_6$, 125 MHz: a) $^{13}$C-$^1$H spectrum; b) DEPT-135.
Figure S17. Complete $^1$H NMR spectrum of compound 8 in Acetone-$d_6$, 500 MHz.

Figure S18. Expanded $^1$H NMR spectrum of compound 8 in Acetone-$d_6$, 500 MHz.
**Figure S19.** Complete $^{13}$C{[^1]H} spectrum of compound 8 in Acetone-$d_6$, 125 MHz.

**Figure S20.** DEPT-135 editing $^{13}$C{[^1]H} NMR spectrum of compound 8 in Acetone-$d_6$, 125 MHz: a) $^{13}$C{[^1]H} spectrum; b) DEPT-135.
Figure S21. Complete $^1$H NMR spectrum of compound 1a in CDCl$_3$, 500 MHz.

Figure S22. Expanded $^1$H NMR spectrum of compound 1a in CDCl$_3$, 500 MHz.
Figure S23. Complete $^{13}$C{¹H} spectrum of compound 1a in CDCl₃, 125 MHz.

Figure S24. DEPT editing $^{13}$C{¹H} NMR spectrum of compound 1a in CDCl₃, 125 MHz: a) $^{13}$C{¹H} spectrum; b) DEPT-135; c) DEPT-90.
Figure S25. $^{1}H, ^{13}C$ HSQC NMR spectrum of compound 1a in CDCl$_3$, 500 MHz.

Figure S26. $^{1}H, ^{13}C$ HMBC NMR spectrum of compound 1a in CDCl$_3$, 500 MHz.
Figure S27. \([\text{H}, \text{H}]\) COSY NMR spectrum of compound 1a in CDCl$_3$, 500 MHz.
Figure S28. \(^{1}H, ^{1}H\) NOESY NMR spectrum of compound 1a in CDCl\(_3\), 500 MHz.
Figure S29. Complete $^1$H NMR spectrum of compound 1b in CDCl$_3$, 500 MHz.

Figure S30. Expanded $^1$H NMR spectrum of compound 1b in CDCl$_3$, 500 MHz.
Figure S31. Complete $^{13}$C{\(^1\)H} spectrum of compound 1b in CDCl\(_3\), 125 MHz.

Figure S32. DEPT editing $^{13}$C{\(^1\)H} NMR spectrum of compound 1b in CDCl\(_3\), 125 MHz: a) $^{13}$C{\(^1\)H} spectrum; b) DEPT-135; c) DEPT-90.
Figure S33. $\{^1\text{H}, ^{13}\text{C}\}$ HSQC NMR spectrum of compound 1b in CDCl$_3$, 500 MHz.

Figure S34. $\{^1\text{H}, ^{13}\text{C}\}$ HMBC NMR spectrum of compound 1b in CDCl$_3$, 500 MHz.
Figure S35. $^{1}H, ^{1}H$ COSY NMR spectrum of compound 1b in CDCl$_3$, 500 MHz.
Figure S36. \(^{1}H, ^{1}H\) NOESY NMR spectrum of compound 1b in CDCl\(_3\), 500 MHz.
Figure S37. Complete $^1$H NMR spectrum of compound 11a in CDCl$_3$, 500 MHz.

Figure S38. Expanded $^1$H NMR spectrum of compound 11a in CDCl$_3$, 500 MHz.
Figure S39. Complete $^{13}$C{$^1$H} spectrum of compound 11a in CDCl$_3$, 125 MHz.

Figure S40. DEPT editing $^{13}$C{$^1$H} NMR spectrum of compound 11a in CDCl$_3$, 125 MHz: a) $^{13}$C{$^1$H} spectrum; b) DEPT-135; c) DEPT-90.
Figure S41. \( ^1\text{H}, ^{13}\text{C} \) HSQC NMR spectrum of compound 11a in CDCl\(_3\), 500 MHz.

Figure S42. \( ^1\text{H}, ^{13}\text{C} \) HMBC NMR spectrum of compound 11a in CDCl\(_3\), 500 MHz.
Figure S43. $^{1}{\text{H, }^{1}{\text{H}}}$ COSY NMR spectrum of compound 11a in CDCl$_3$, 500 MHz.
Figure S44. $^{1}H, ^{1}H$ NOESY NMR spectrum of compound 11a in CDCl$_3$, 500 MHz.
Figure S45. Complete $^1$H NMR spectrum of compound 11b in CDCl$_3$, 500 MHz.

Figure S46. Expanded $^1$H NMR spectrum of compound 11b in CDCl$_3$, 500 MHz.
Figure S47. Complete $^{13}\text{C}\{^1\text{H}\}$ spectrum of compound 11b in CDCl$_3$, 125 MHz.

Figure S48. DEPT editing $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound 11b in CDCl$_3$, 125 MHz: a) $^{13}\text{C}\{^1\text{H}\}$ spectrum; b) DEPT-135; c) DEPT-90.
Figure S49. $^{1}H$, $^{13}C$ HSQC NMR spectrum of compound 11b in CDCl$_3$, 500 MHz.

Figure S50. $^{1}H$, $^{13}C$ HMBC NMR spectrum of compound 11b in CDCl$_3$, 500 MHz.
Figure S51. $^{1}{H}, ^{1}{H}$ COSY NMR spectrum of compound 11b in CDCl$_3$, 500 MHz.
Figure S52. \( ^1 \text{H}, ^1 \text{H} \) NOESY NMR spectrum of compound 11b in CDCl\(_3\), 500 MHz.
Figure S53. Spectrum (±)-3 (a) and spectra (±)-3 after each addition of (-)-Eu (hfc)$_3$ (b-g).
**Figure S54.** Spectrum S-3 (a) and spectra S-3 after each addition of (-)-Eu (hfc)$_3$ (b-g).
**Figure S55.** SH signal in the spectrum of S-3 (a) and spectra of S-3 (b-f) after each addition of (-)-Eu (hfc)₃.

**Figure S56.** SH signal in the spectrum of (±)-3 (a) and spectra of (±)-3 after each addition of (-)-Eu (hfc)₃ (b-f).
Figure S57. Part of $^1$H NMR spectrum of reaction mixture after reaction 2 and 3, before column chromatography ($1a$:$1b$ = 2:1, by integrated intensity of signals H-6)
**Figure S58.** Part of $^1$H NMR spectrum of mixture 1a, 1b after column chromatography on SiO$_2$ with CHCl$_3$-MeOH-Et$_3$N (1a:1b = 1:3.3).
Figure S59. Part of $^1$H NMR spectrum of mixture 1a, 1b after column chromatography 1a on SiO$_2$ with CHCl$_3$-MeOH-Et$_3$N (1a:1b = 1:5).