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Supporting Information

Serine Hydroxymethyl Transferase from *Streptococcus thermophilus* and L-Threonine Aldolase from *E. coli* as Stereocomplementary Biocatalysts for the Synthesis of b-Hydroxy-a,w-diamino acid Derivatives

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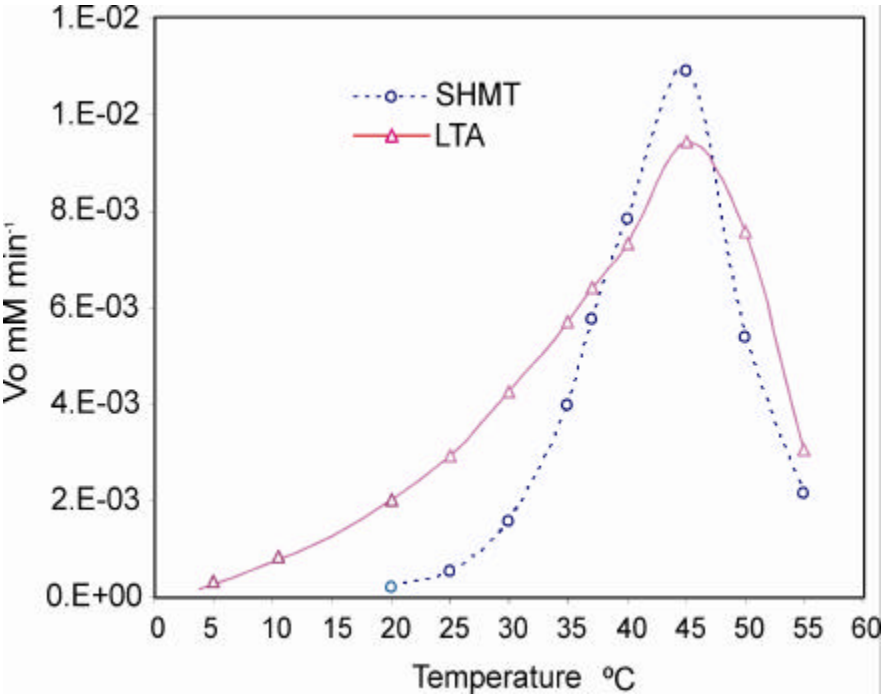


Figure 1. Temperature Profiles for SHMT and LTA. For assay conditions see L. Vidal, J. Calveras, P. Clapés, P. Ferrer and G. Caminal, *Appl. Microbiol. Biotechnol.* **2005**, *68*, 489-497.

Table 1. Kinetic Data for SHMT and LTA

	Sustrato	**K_m (mM)**	**V_{max} (mM min^{-1})**	**V_{max} (mmol min^{-1} mg-1)**	**V_{max}/K_m (U mg^{-1} mM^{-1})**
SHMT	L-treonine	24.6±5.4	13.4±1.4	1.49±0.13	0.061±0.03
	L-*allo* treonine	0.7±0.1	49.0±3.4	5.44±0.12	7.8±0.7
	D-treonine	nd	nd	nd	
LTA	L-treonine	3.3±1.2	8.22±0.56	4.94±0.20	1.5±0.6
	L-*allo* treonine	0.049±0.002	20.3±1.4	12.19±0.65	248±23
	D-treonine	nd	nd	nd	

Buffers used:for LTA: Tris.HCl 200 mM pH 8.0 and for SHMT: potasium phosphate 200 mM pH 6.5. The values of the kinetic constants are averages ±SD of three different determinations (Data from L. Vidal, J. Calveras, P. Clapés, P. Ferrer and G. Caminal, *Appl. Microbiol. Biotechnol.* **2005**, *68*, 489-497, and Vidal L: Producción de aldolasas recombinantes: de la biología molecular al desarrollo de procesos. PhD Thesis Barcelona: Universitat Autonoma de Barcelona: 2006.
For assay conditions see L. Vidal, J. Calveras, P. Clapés, P. Ferrer and G. Caminal, *Appl. Microbiol. Biotechnol.* **2005**, *68*, 489-497
nd: not detected

Figure 2. Reaction-time profile for the aldol addition of glycine to (*S*)-*N*-Cbz-alaninal under different reaction conditions at 25°C.

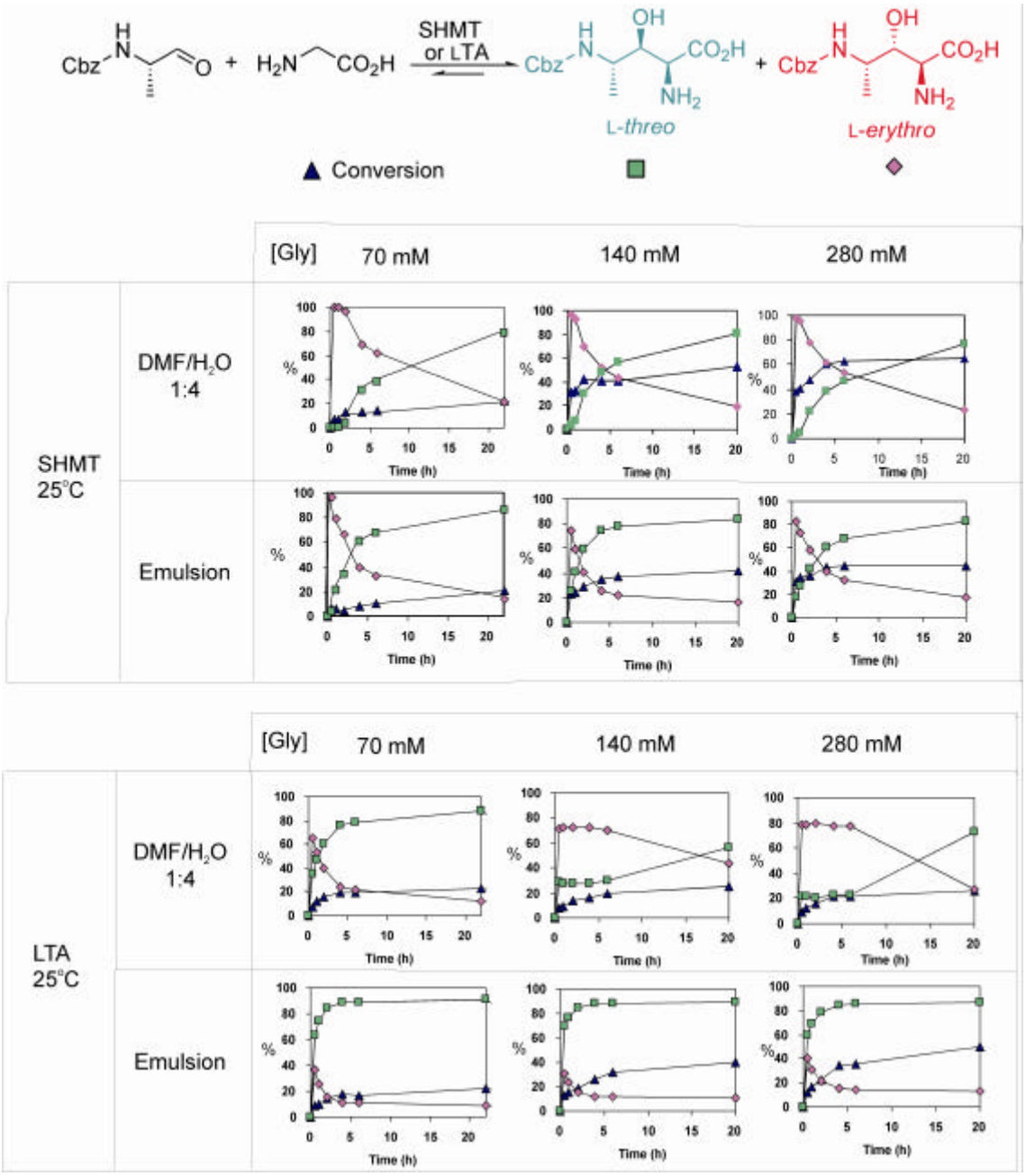


Figure 3. Reaction-time profile for the aldol addition of glycine to (*S*)-*N*-Cbz-alaninal under different reaction conditions at 4°C.

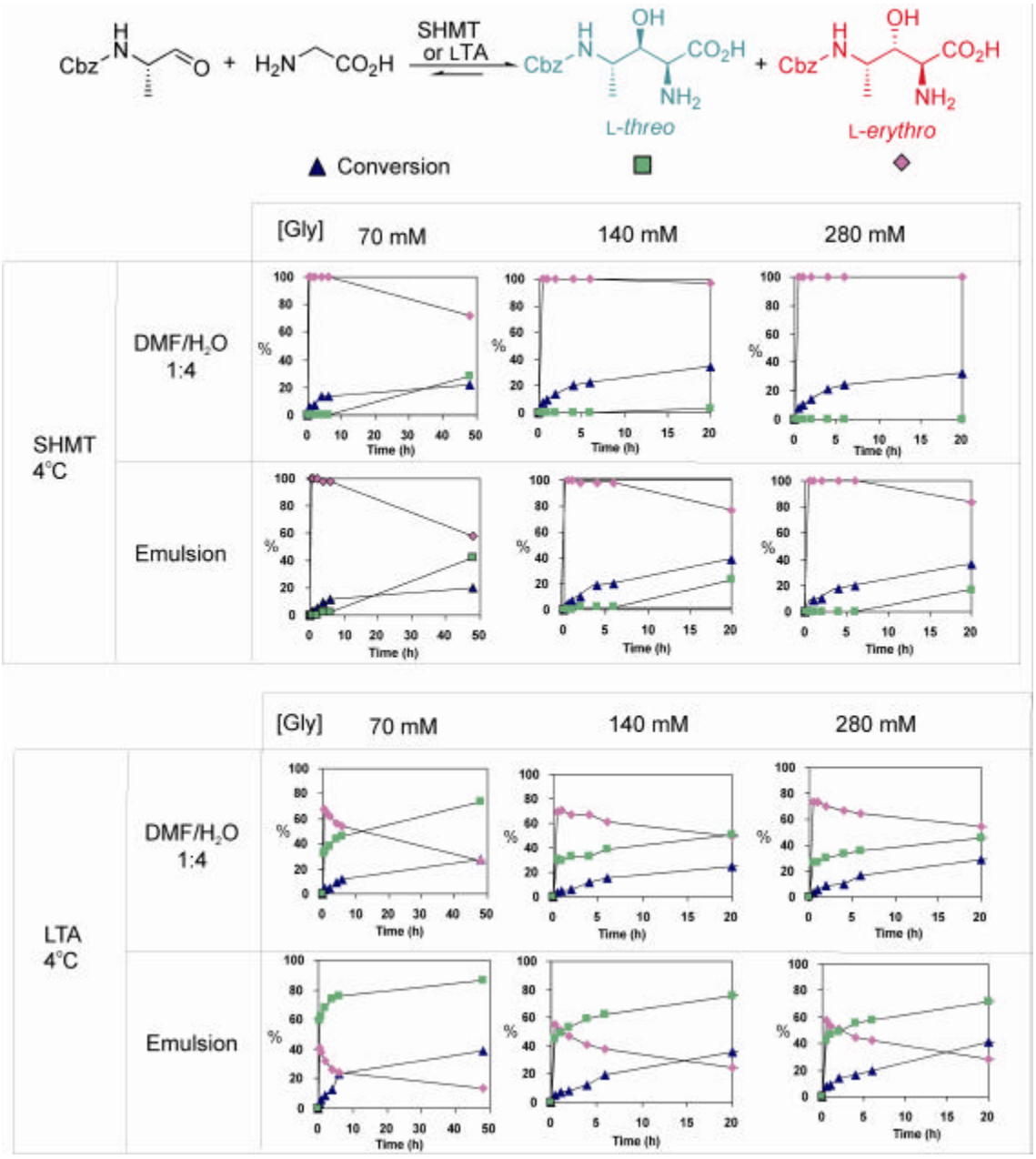


Figure 4. Reaction-time profile for the aldol addition of glycine to *N*-Cbz-glycinal under different reaction conditions at 25°C.

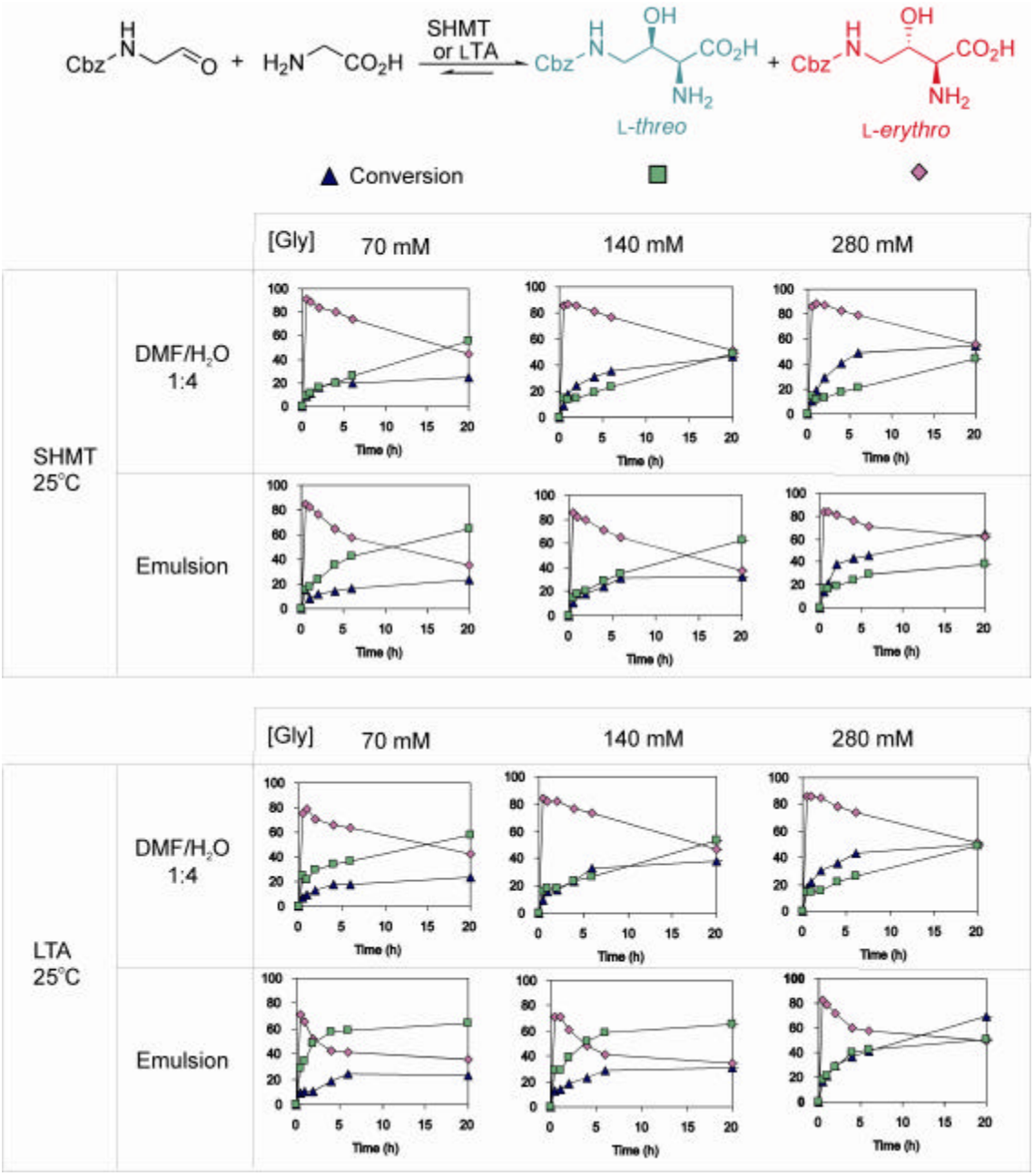


Figure 5. Reaction-time profile for the aldol addition of glycine to *N*-Cbz-glycinal under different reaction conditions at 4°C.

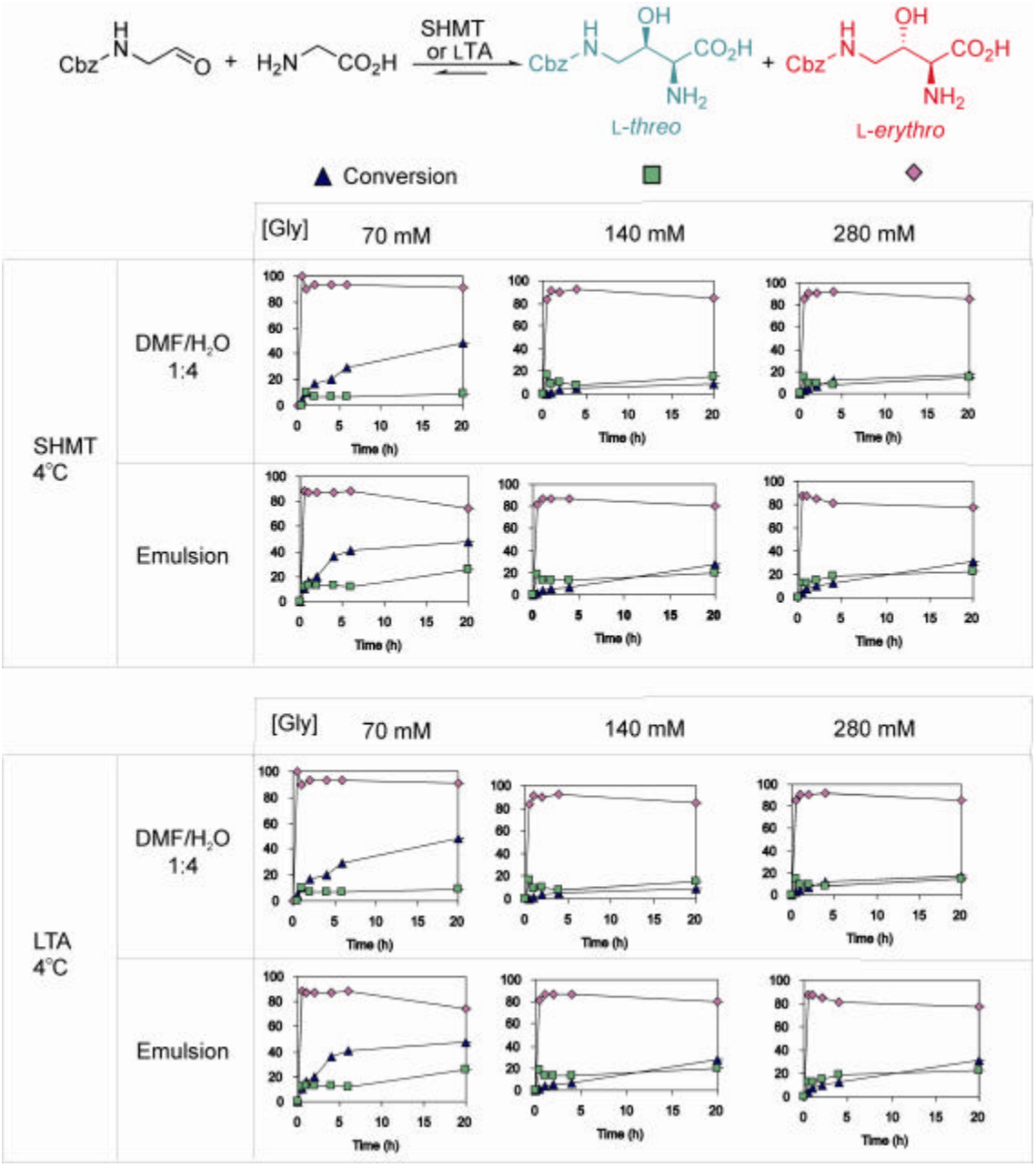


Figure 6. Reaction-time profile for the aldol addition of glycine to benzyloxyacetaldehyde under different reaction conditions at 25°C.

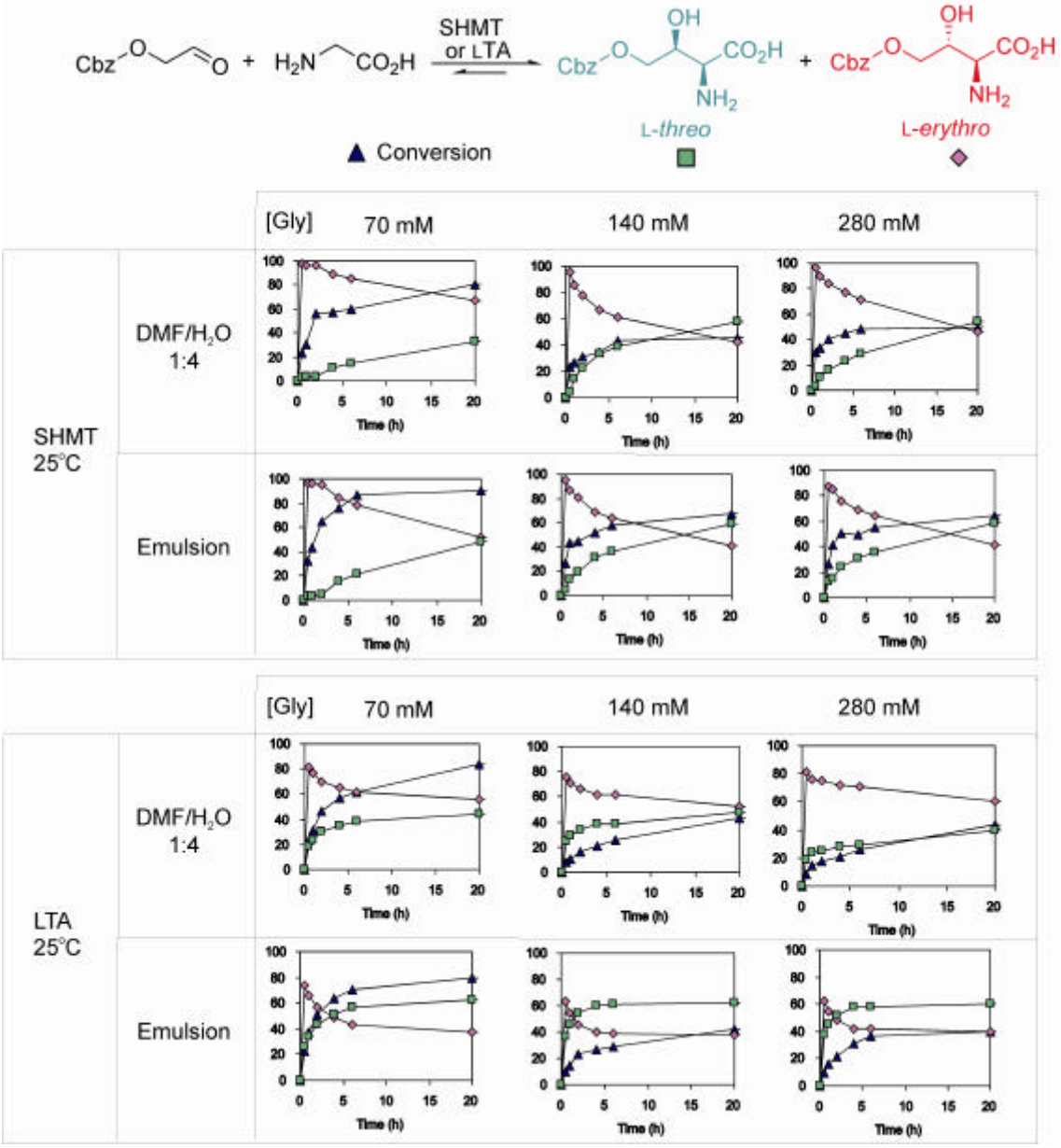


Figure 7. Reaction-time profile for the aldol addition of glycine to benzyloxyacetaldehyde under different reaction conditions at 4°C.

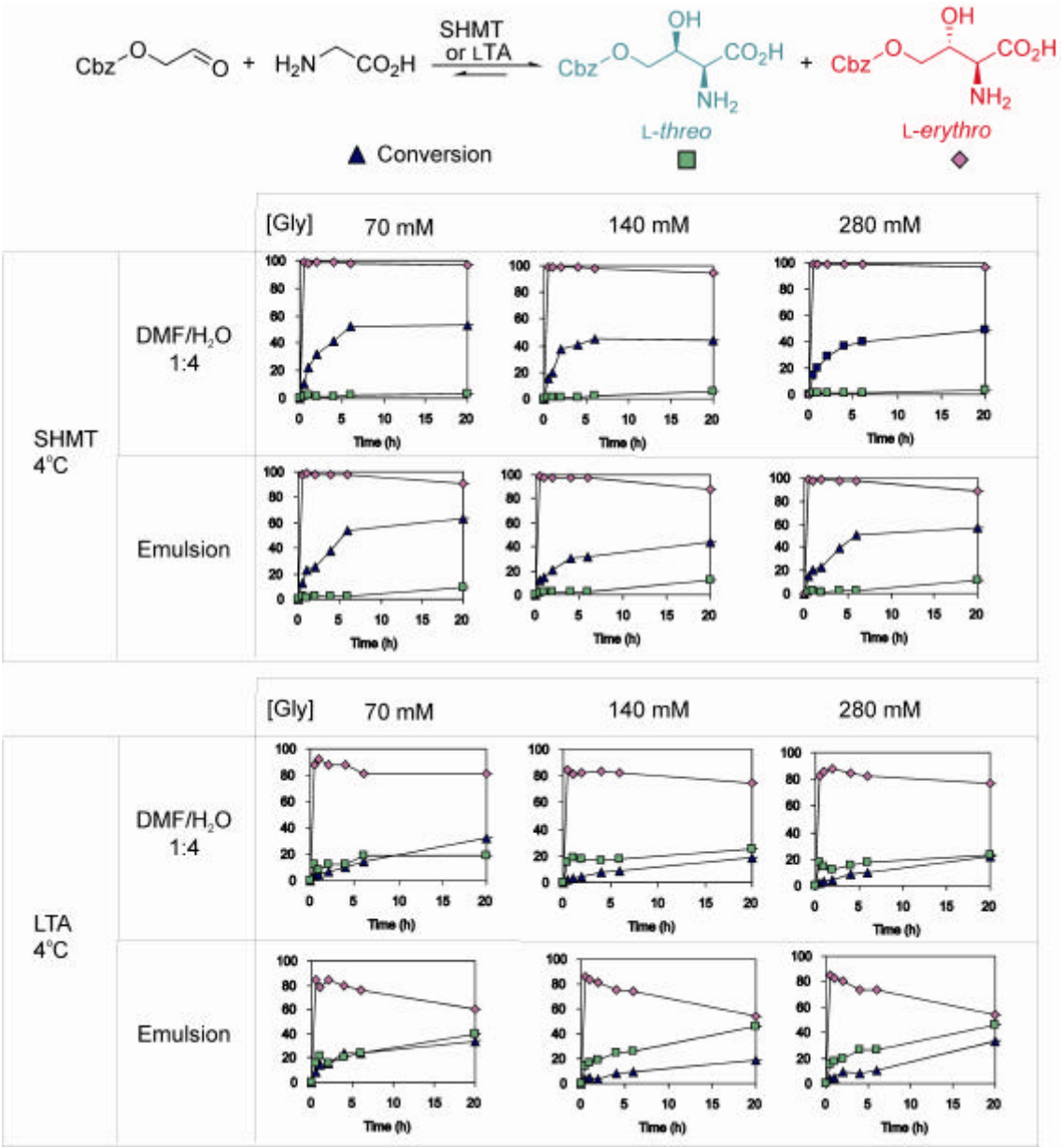


Figure 8. Complete and expanded regions of the ^{1}H NMR spectrum of produc **6a**.

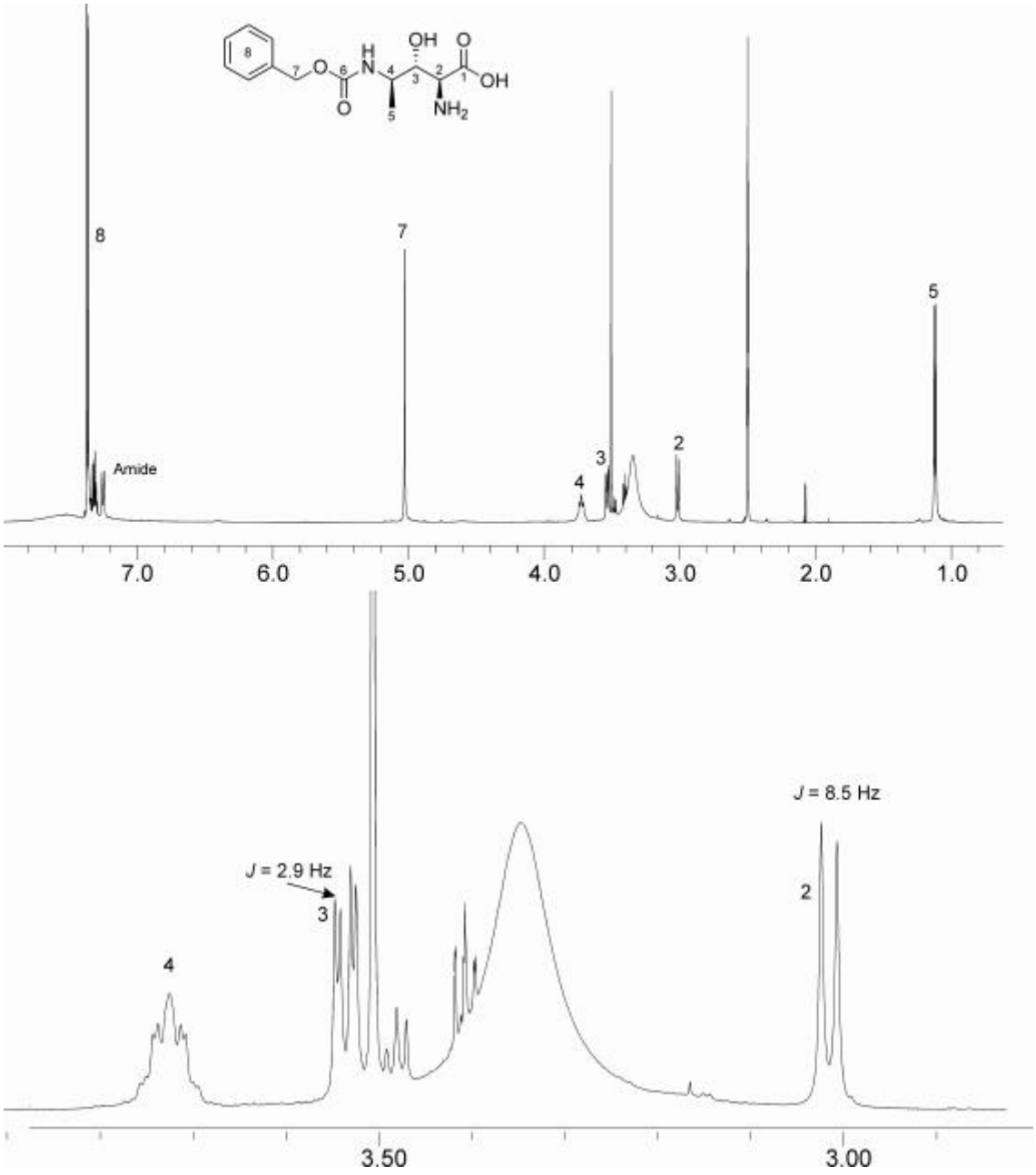


Figure 9. ^{13}C NMR and 2D ^{1}H-^{1}H COSY spectra of product **6a**.

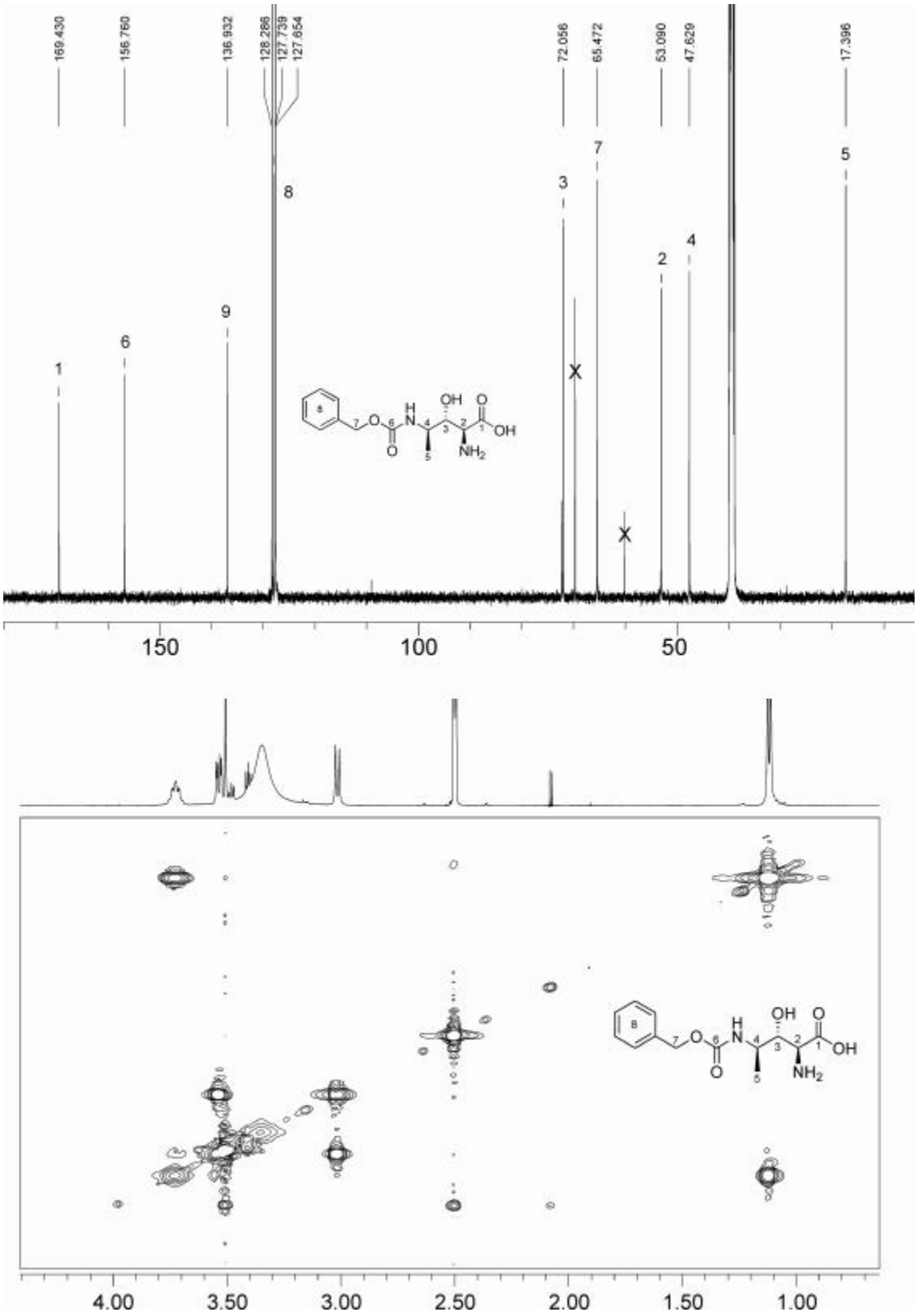


Figure 10. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **6a** and **6b**.

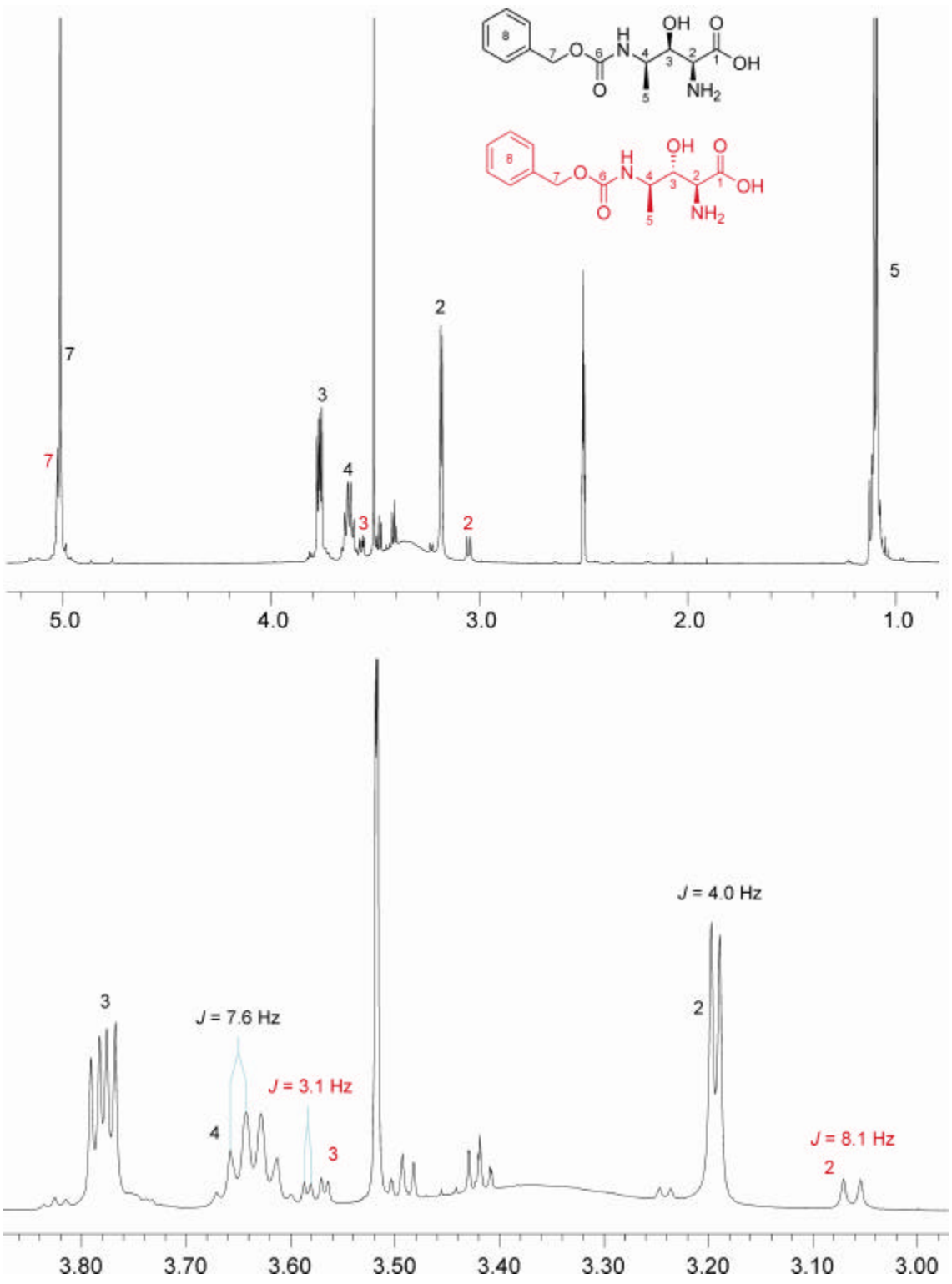


Figure 11. ^{13}C NMR and 2D ^{1}H-^{1}H COSY spectra of the mixture of products **6a** and **6b**.

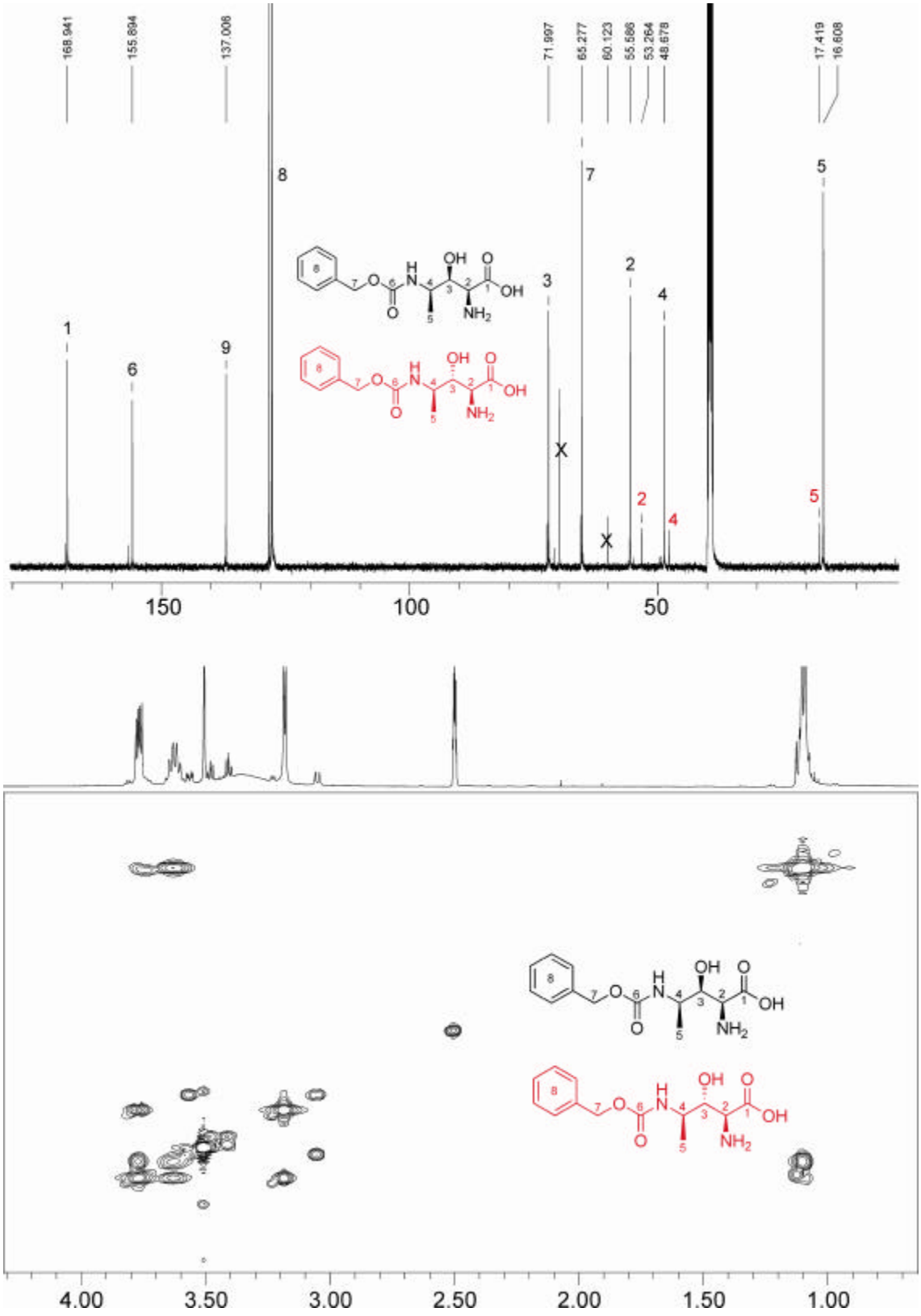


Figure 12. Expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone derivatives from products **6a** and **6b**, respectively.

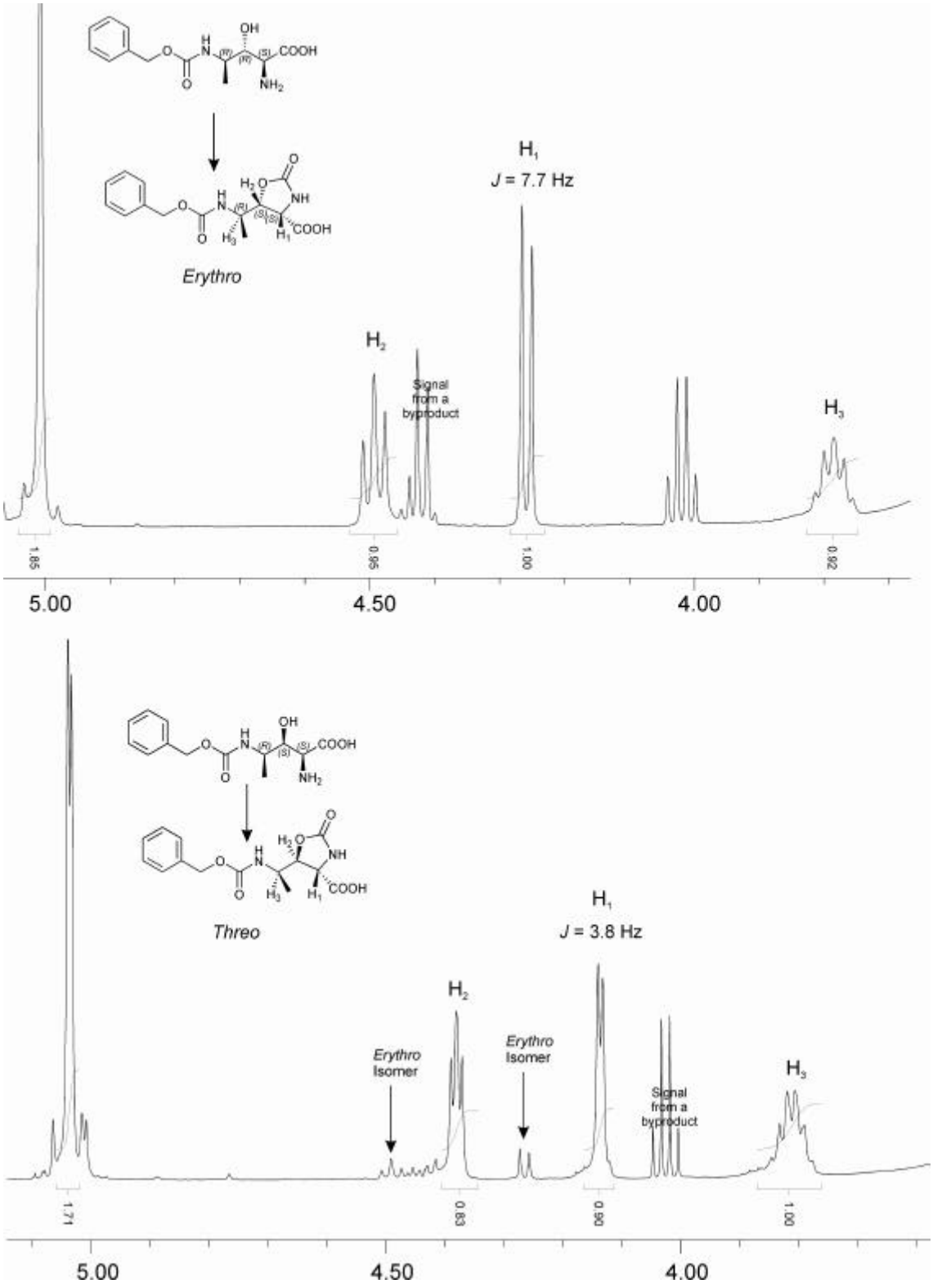


Figure 13. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **7a**.

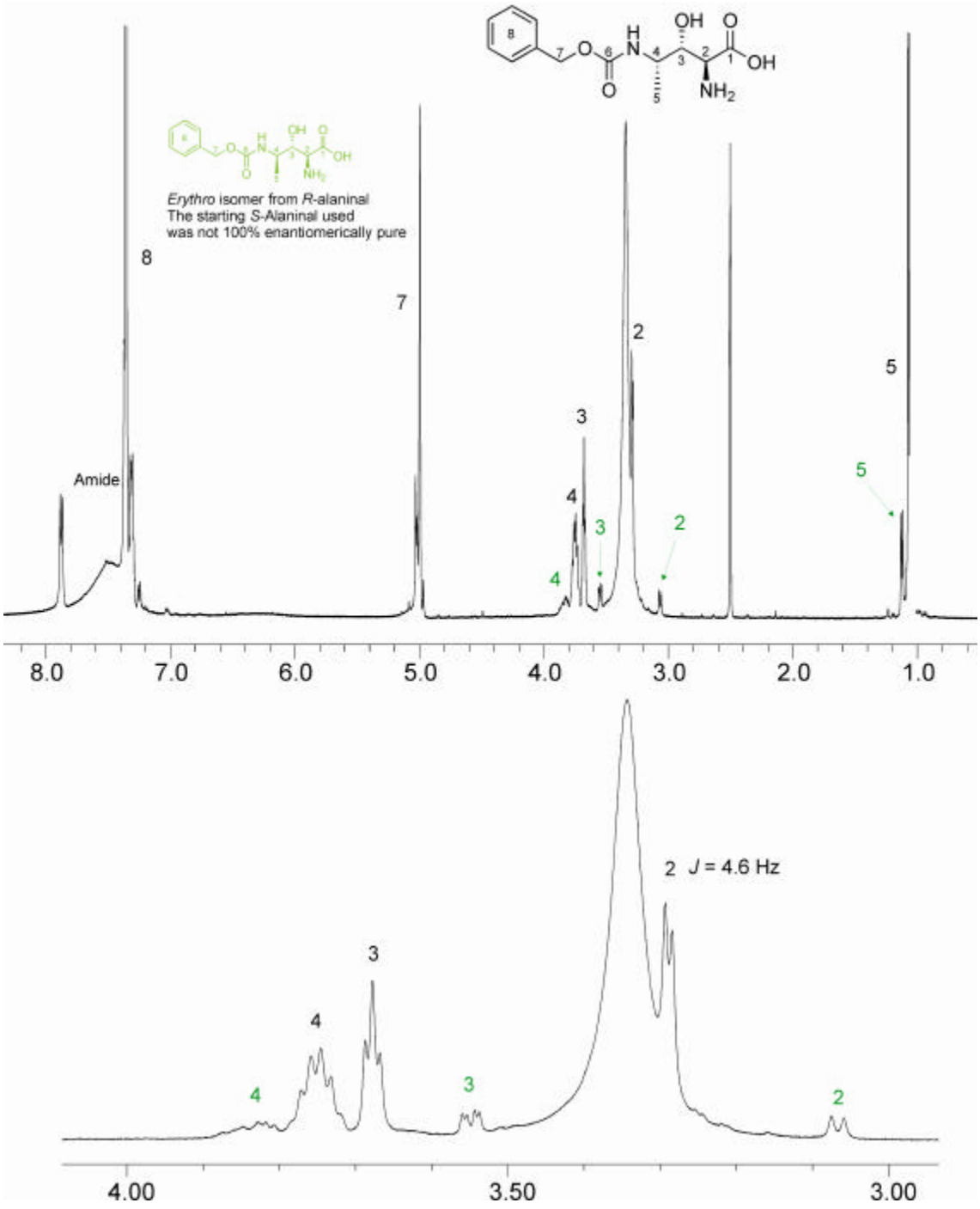


Figure 14. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **7a** and **7b**.

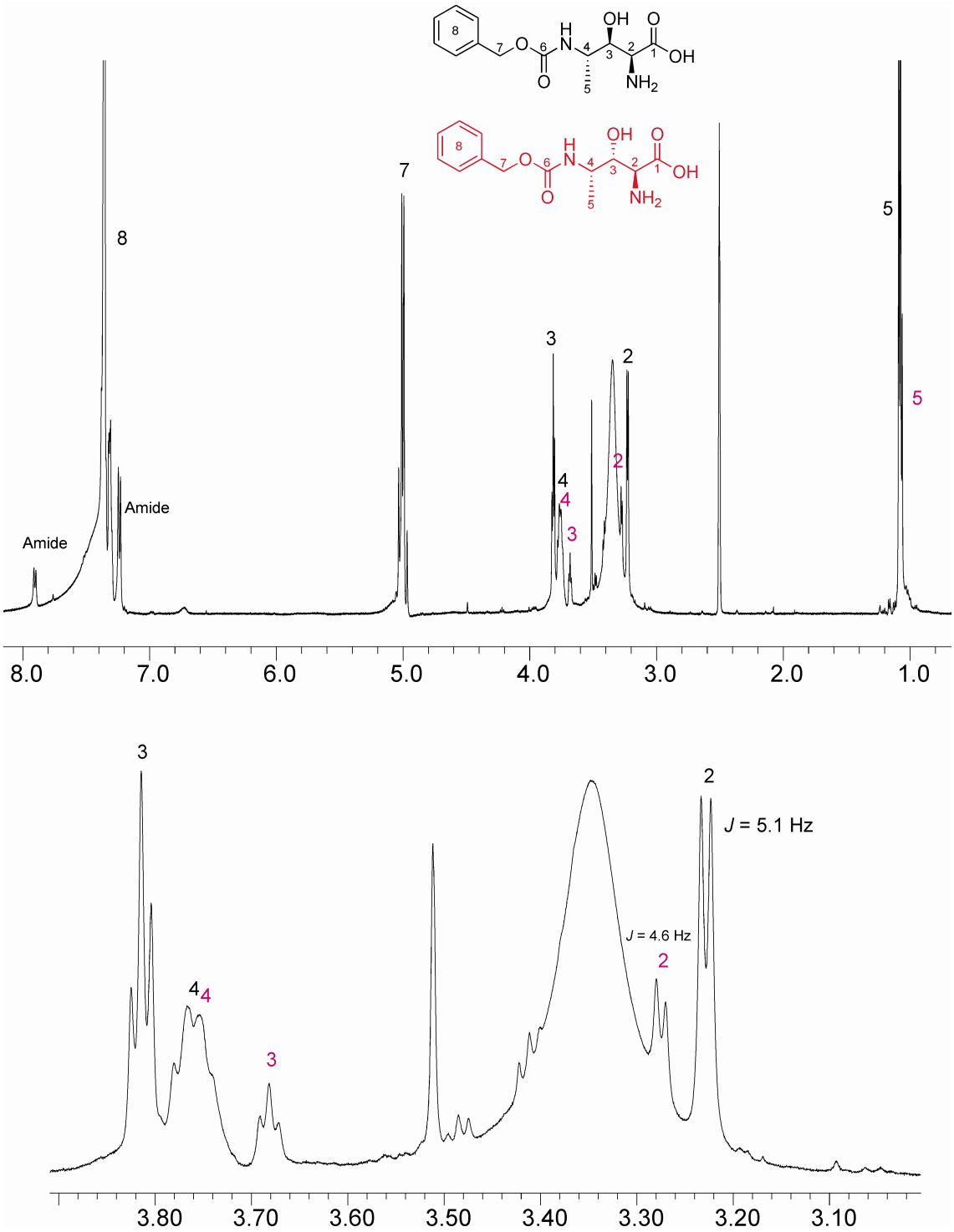


Figure 15. ^{13}C NMR spectra of the mixture of products **7a** and **7b**

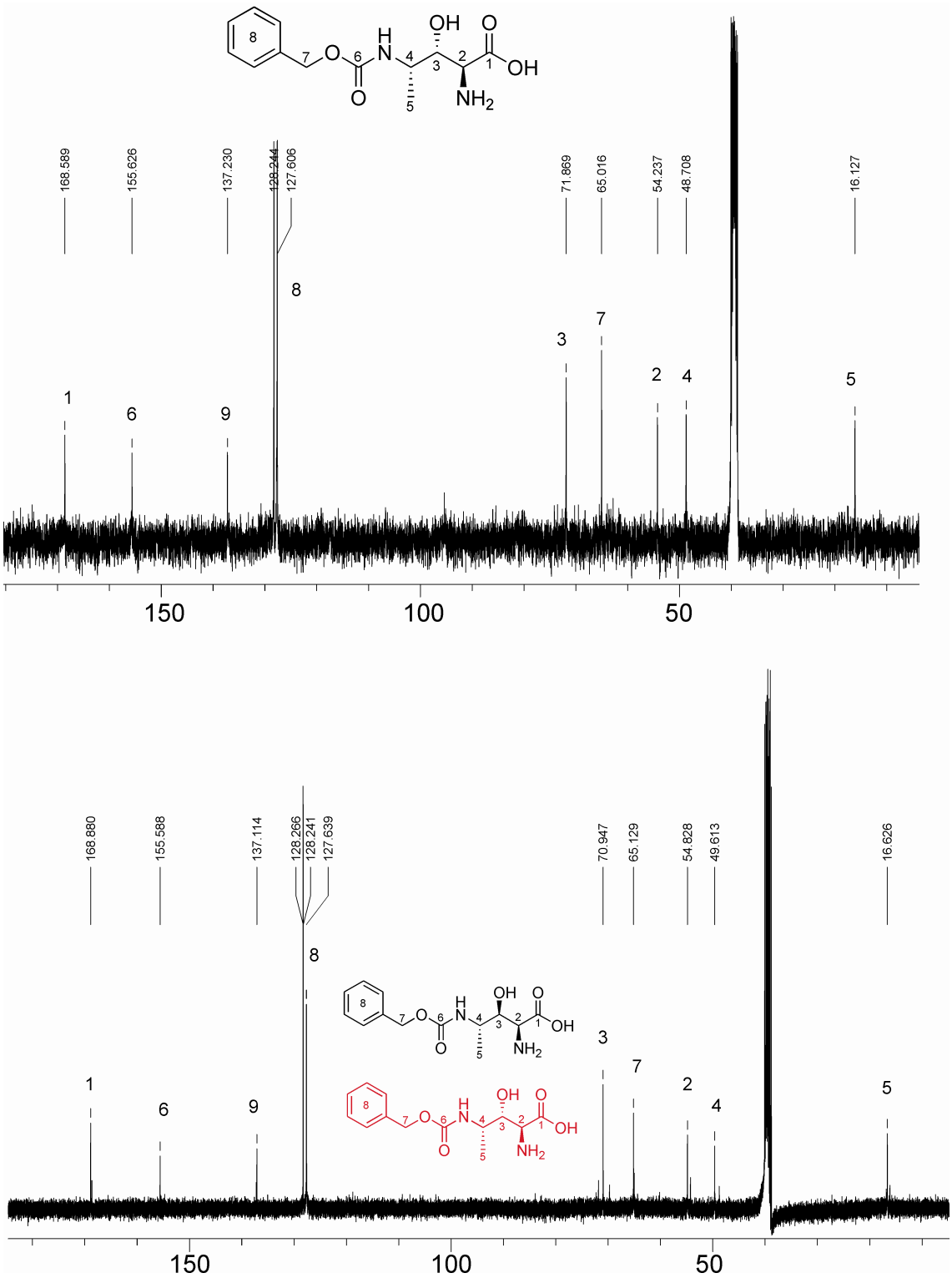


Figure 16. Expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone derivatives from products **7a** and **7b**, respectively.

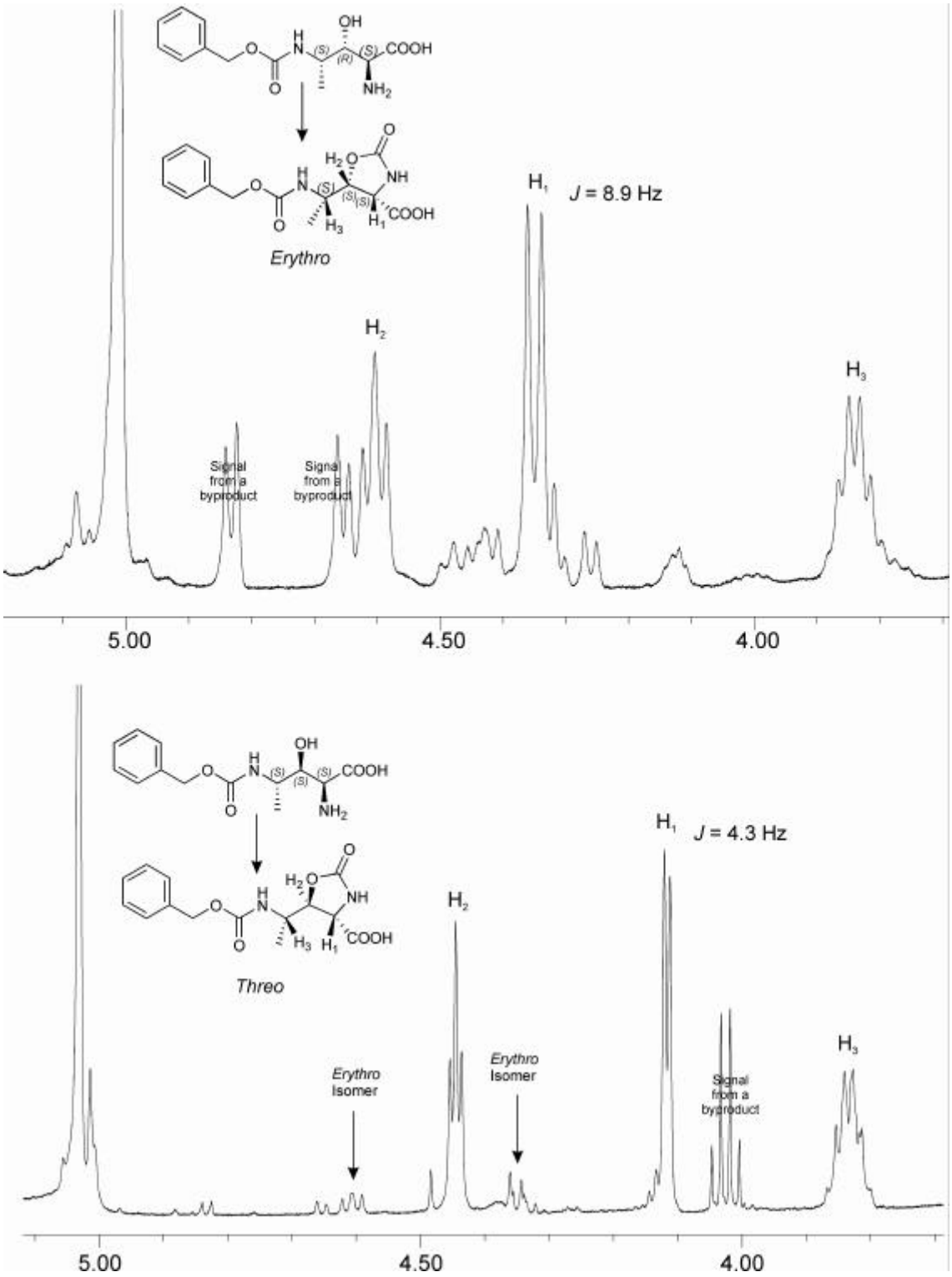


Figure 17. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **8a** and **8b**.

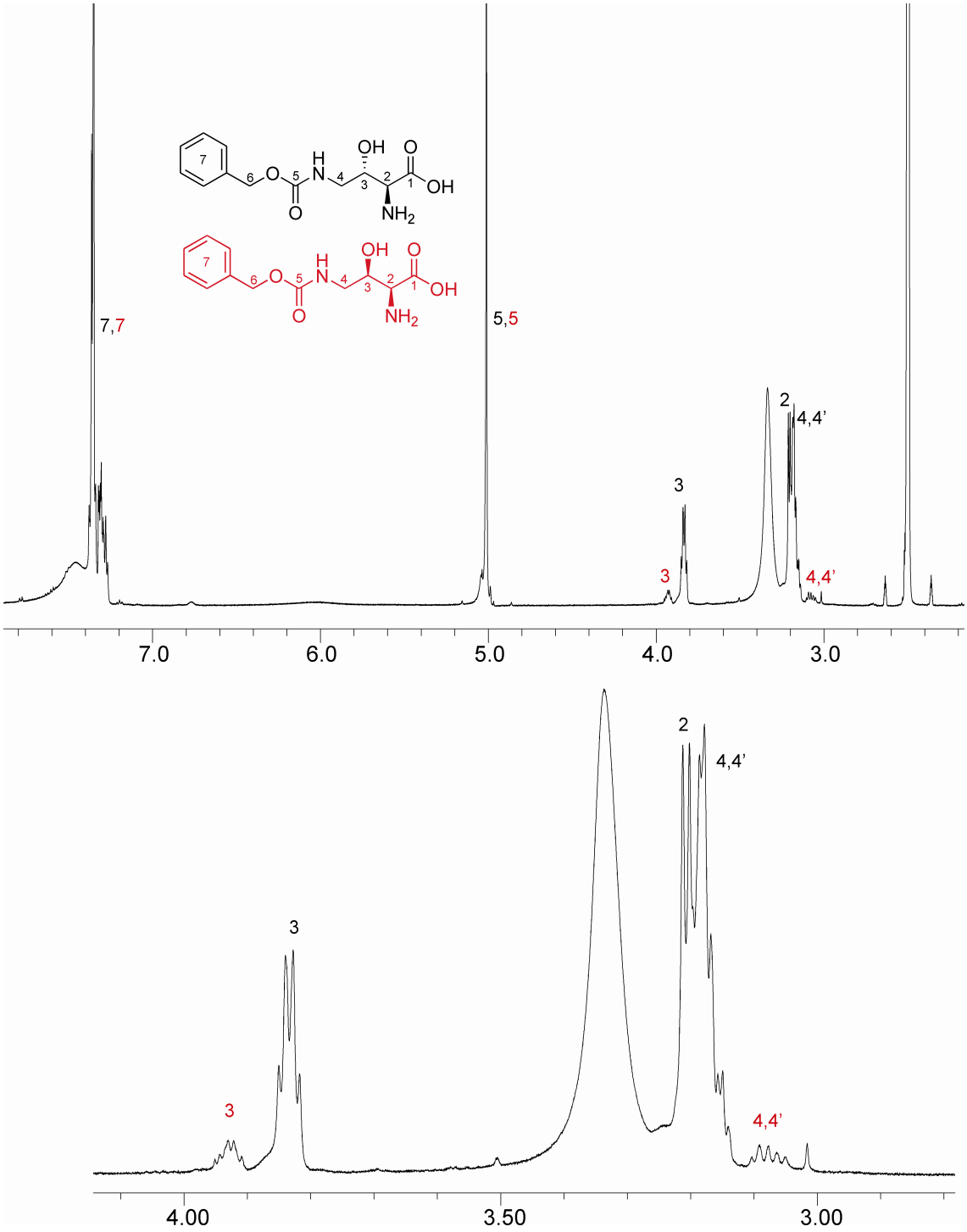


Figure 18. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **8a** and **8b**.

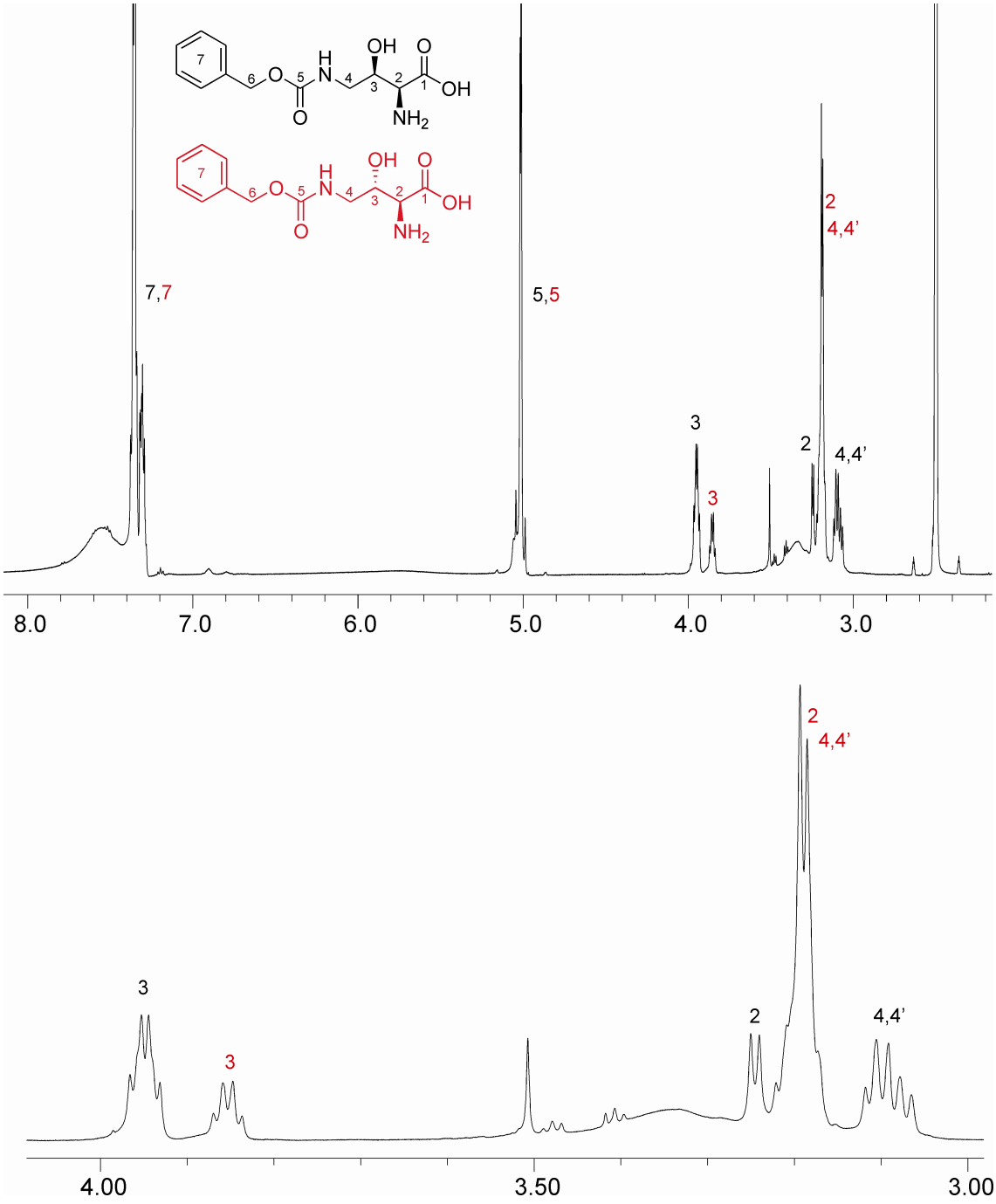


Figure 19. ^{13}C NMR spectra of the mixture of products **8a** and **8b**

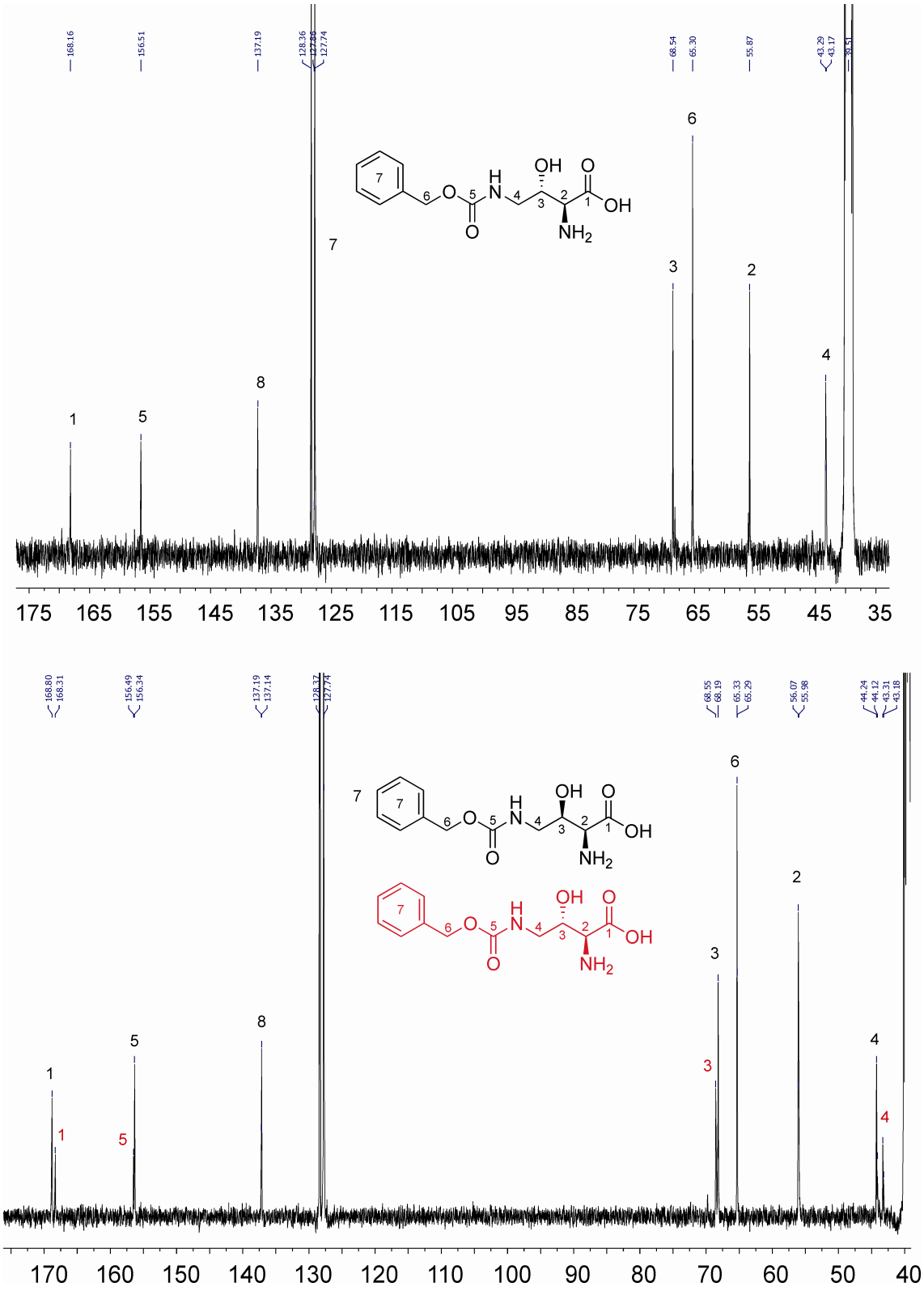


Figure 20. Expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone derivatives from products **8a** and **8b**, respectively.

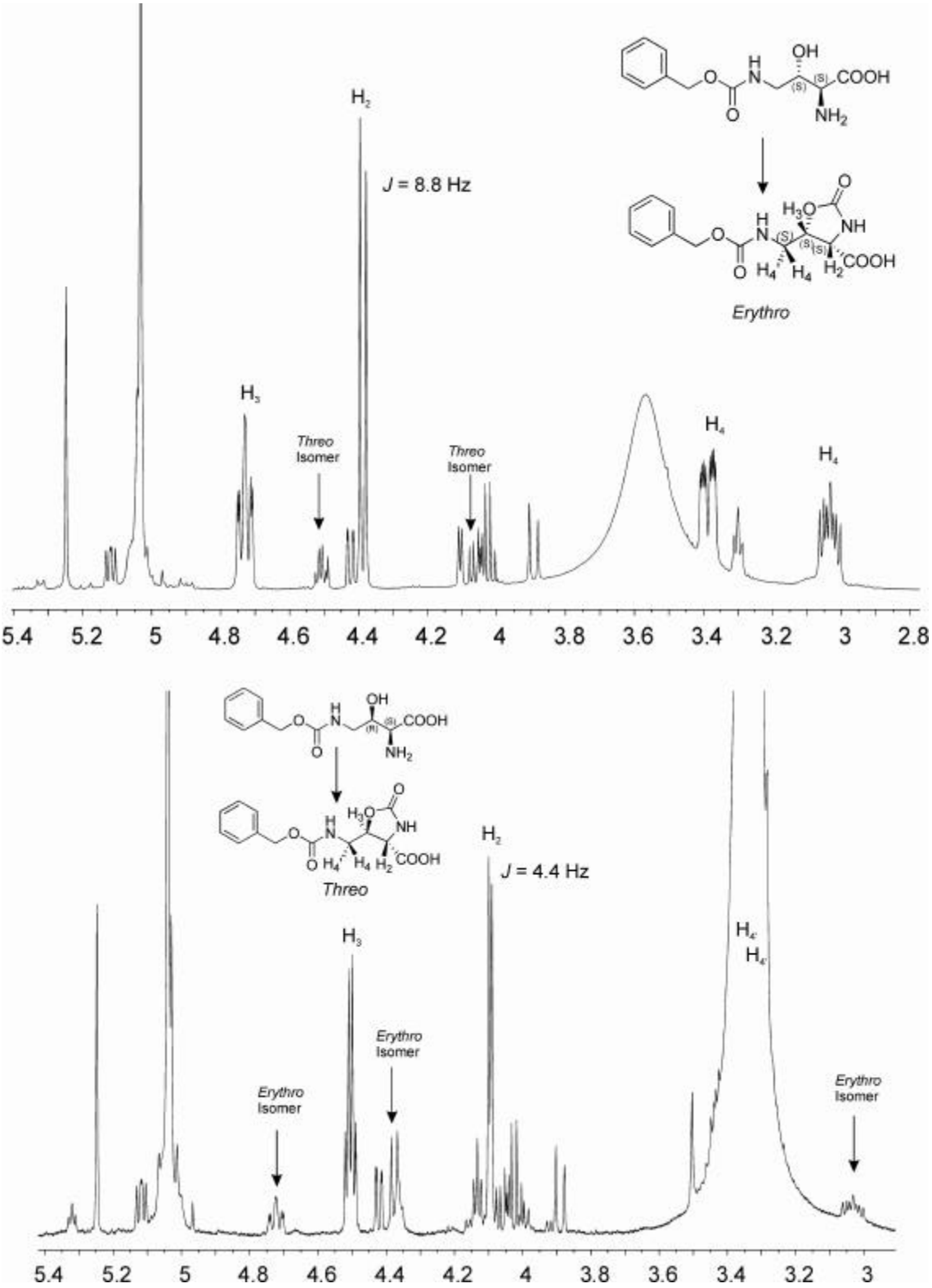


Figure 21. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **9a** and **9b**.

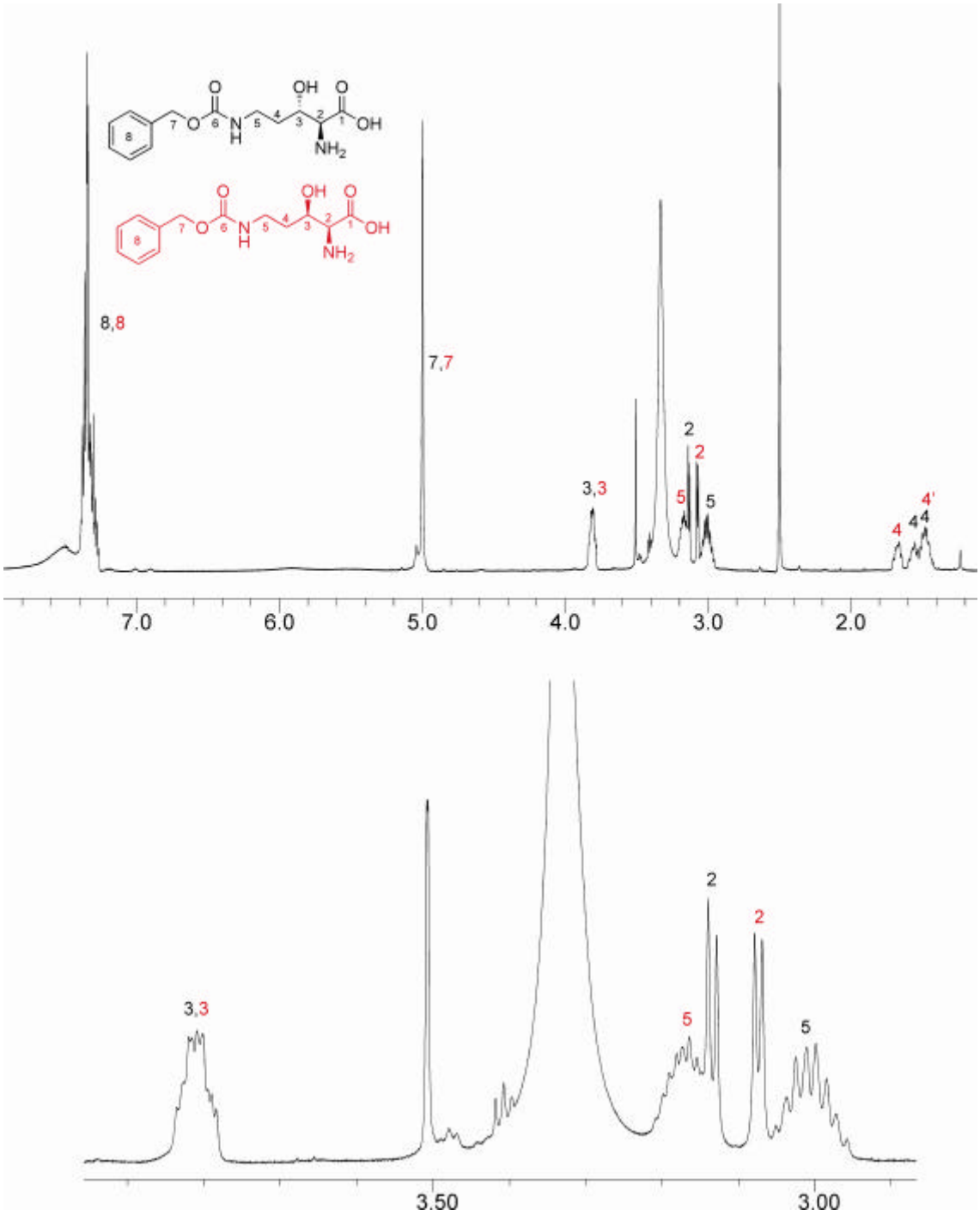


Figure 22. ^{13}C NMR spectra of the mixture of products **9a** and **9b** obtained using SHMT and LTA catalysts, respectively.

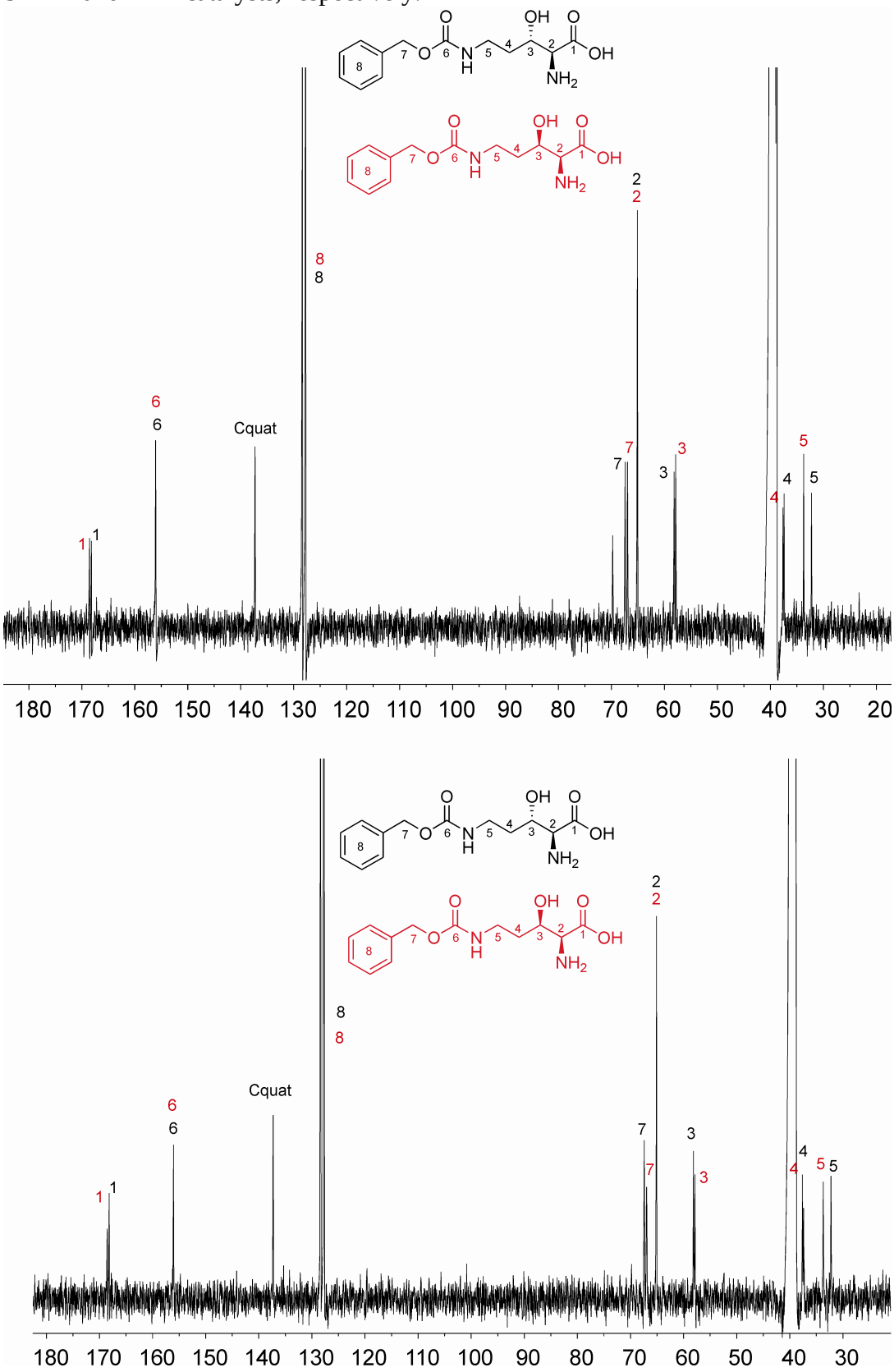


Figure 23. Expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone derivatives from products **9a** and **9b**, respectively.

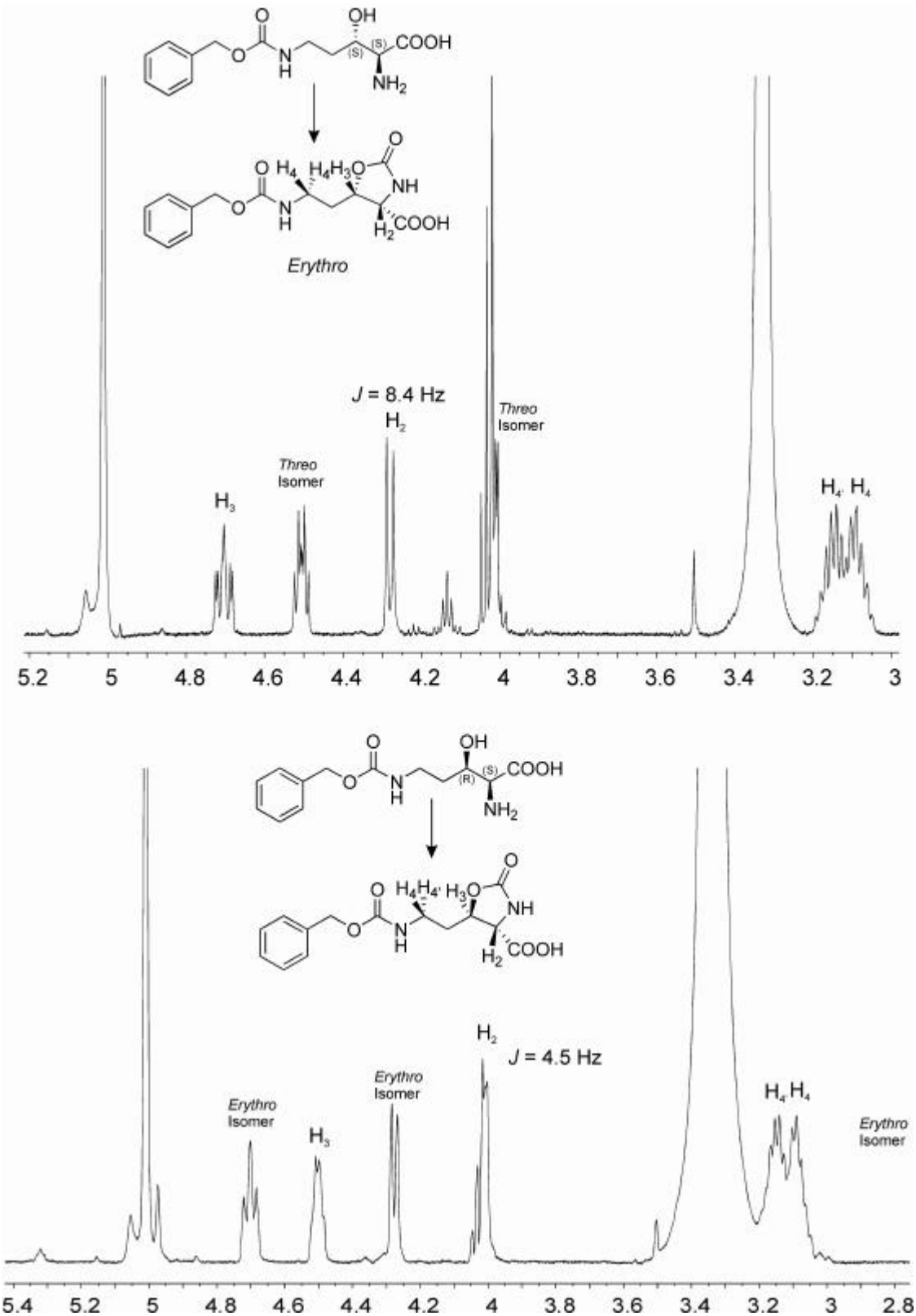


Figure 24. ^{1}H and ^{13}C NMR spectra of **9a** obtained using SHMT.

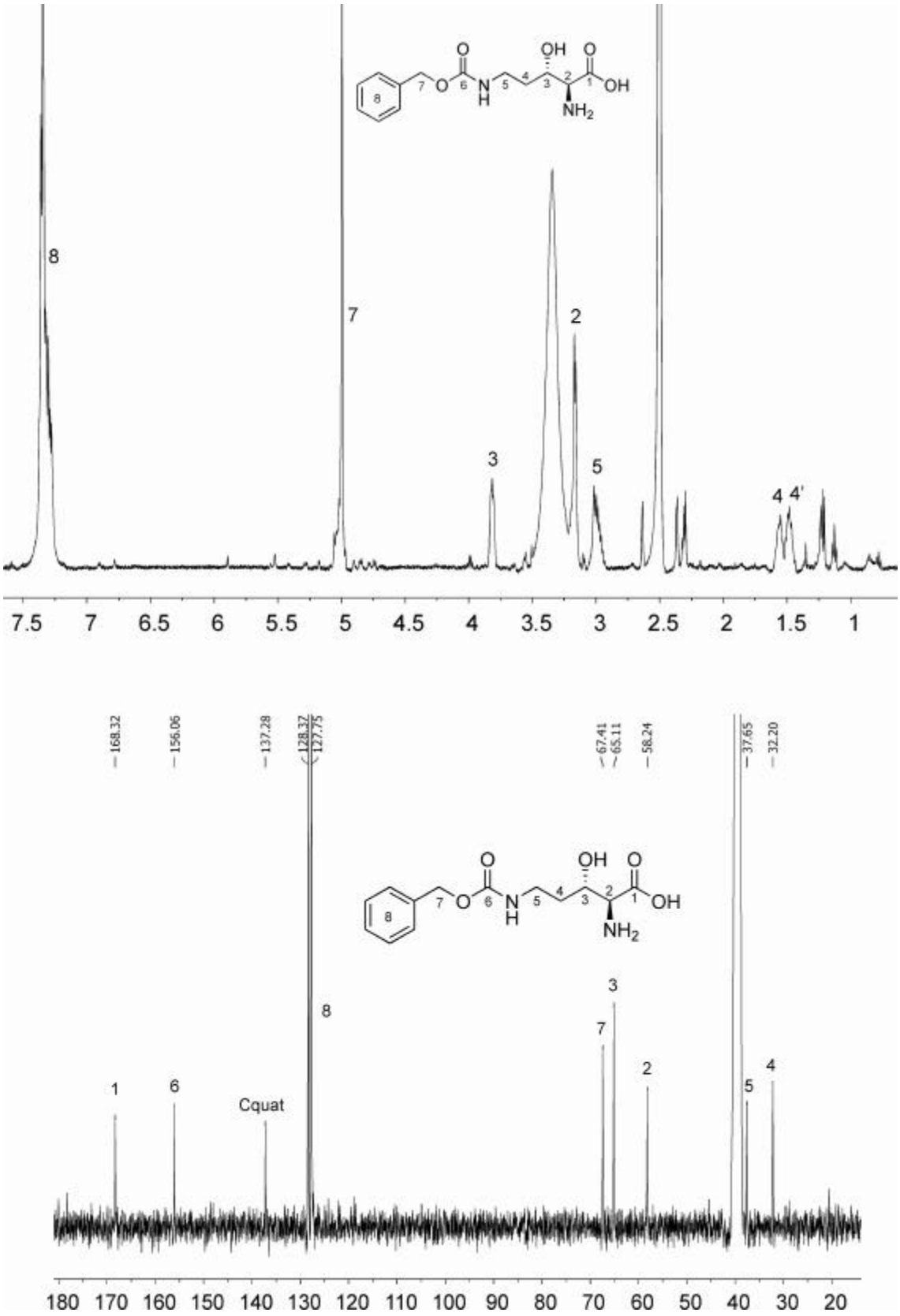


Figure 25. Complete and expanded regions of the ^{1}H NMR spectrum of **10a**.

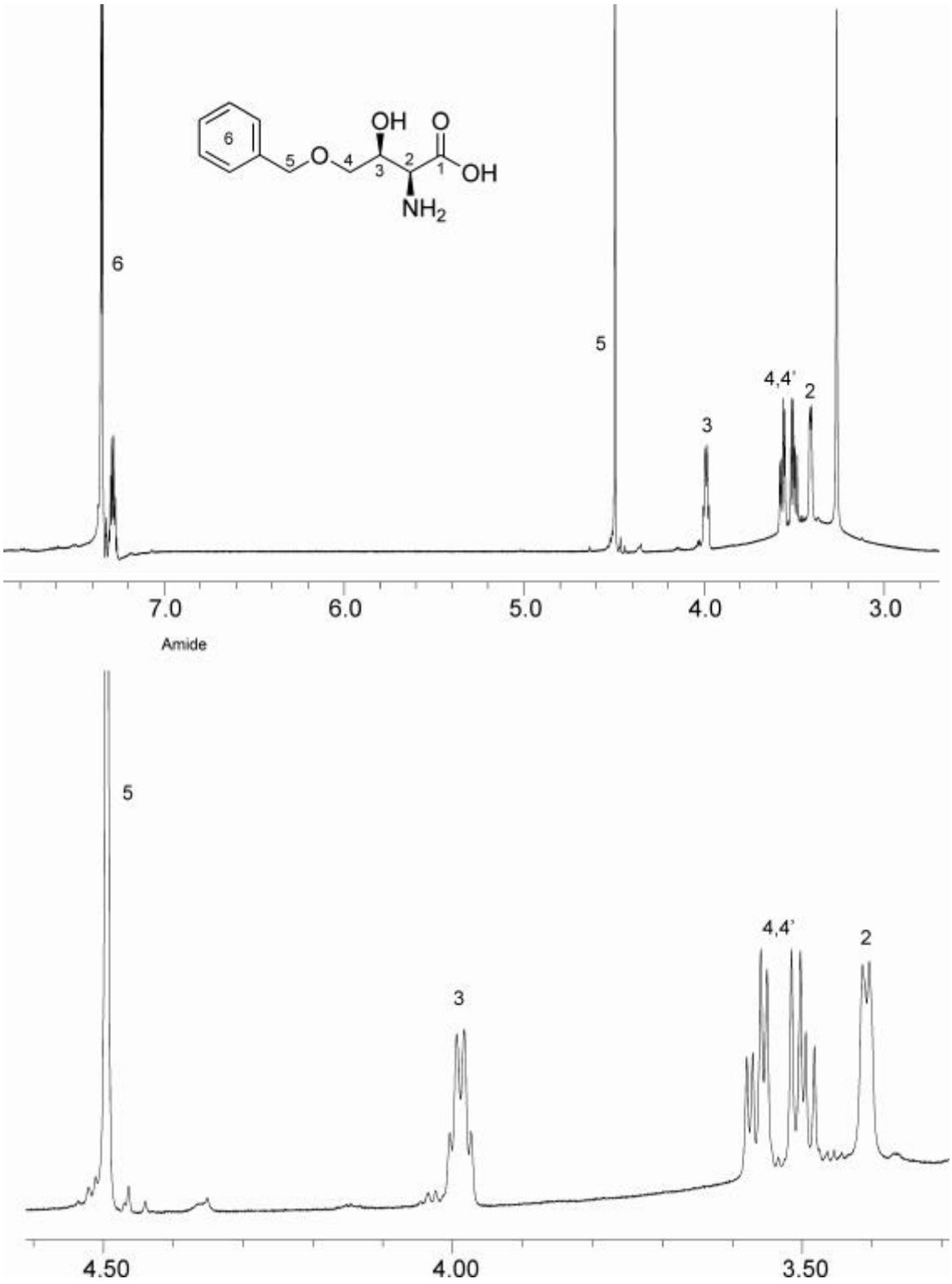


Figure 26. Complete and expanded regions of the ^{1}H NMR spectrum of a mixture of products **10a** and **10b**.

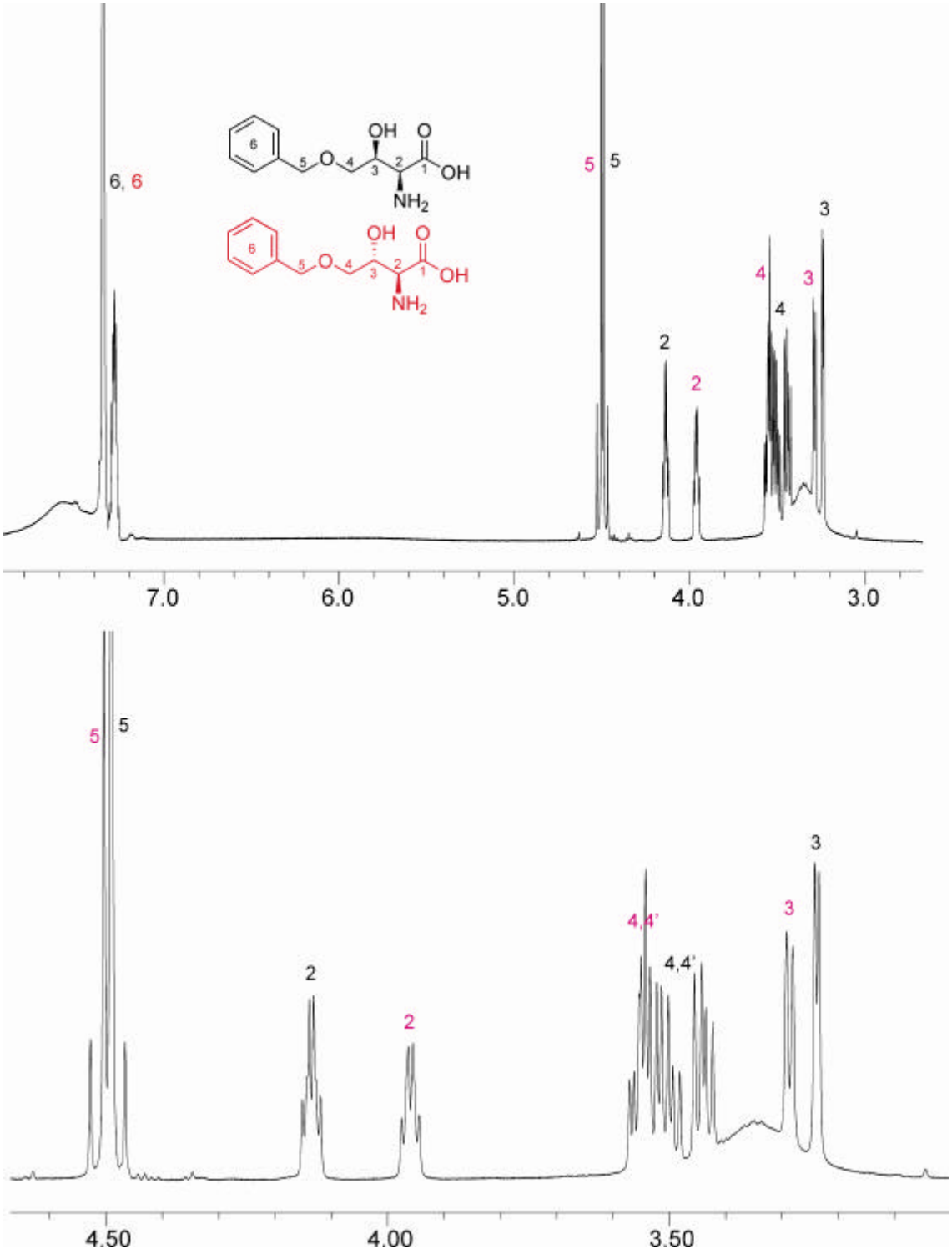


Figure 27. ^{13}C NMR spectra of the mixture of products **10a** and **10b** obtained using SHMT and LTA catalysts, respectively.

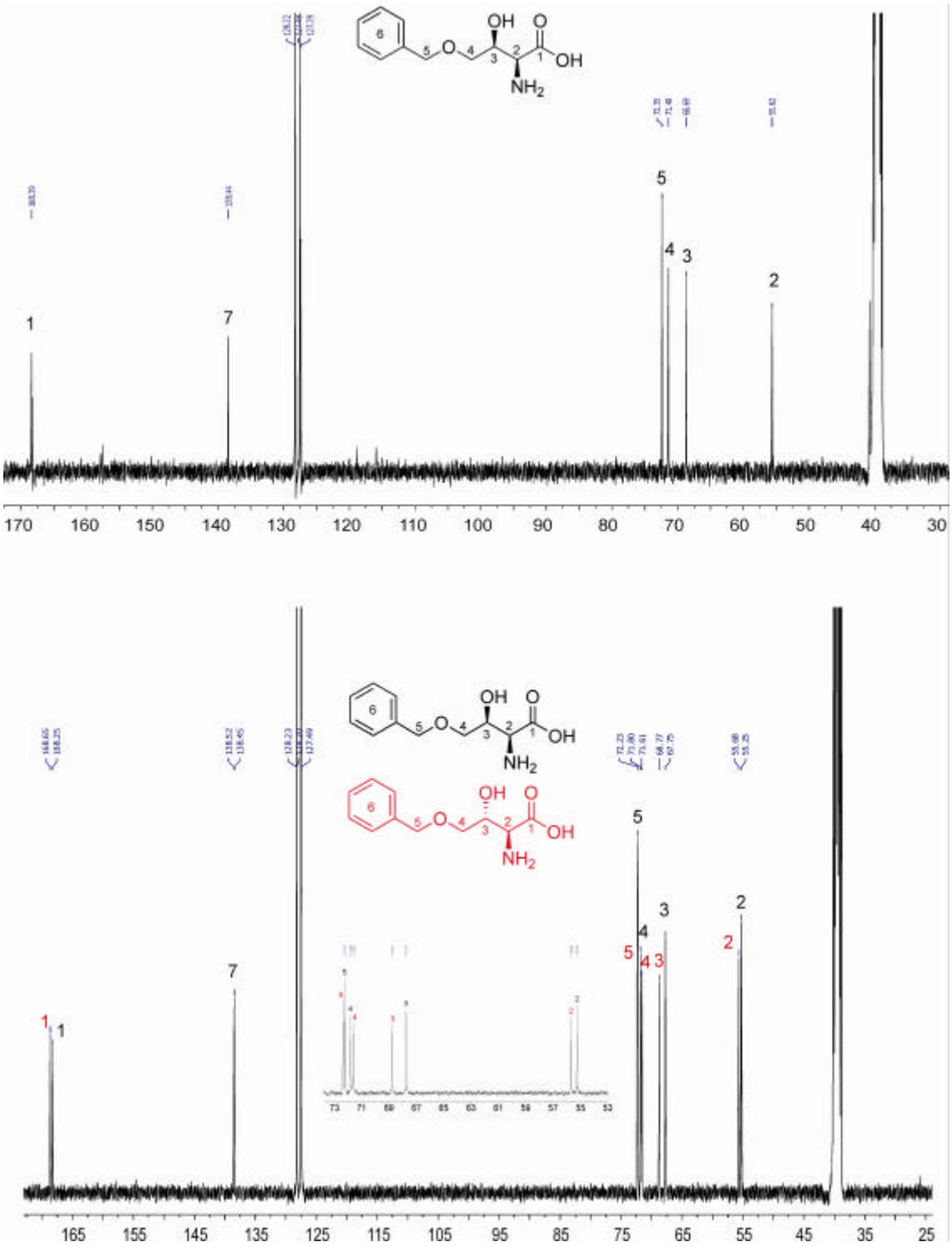


Figure 28. Expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone derivatives from products **9a** and **9b**, respectively.

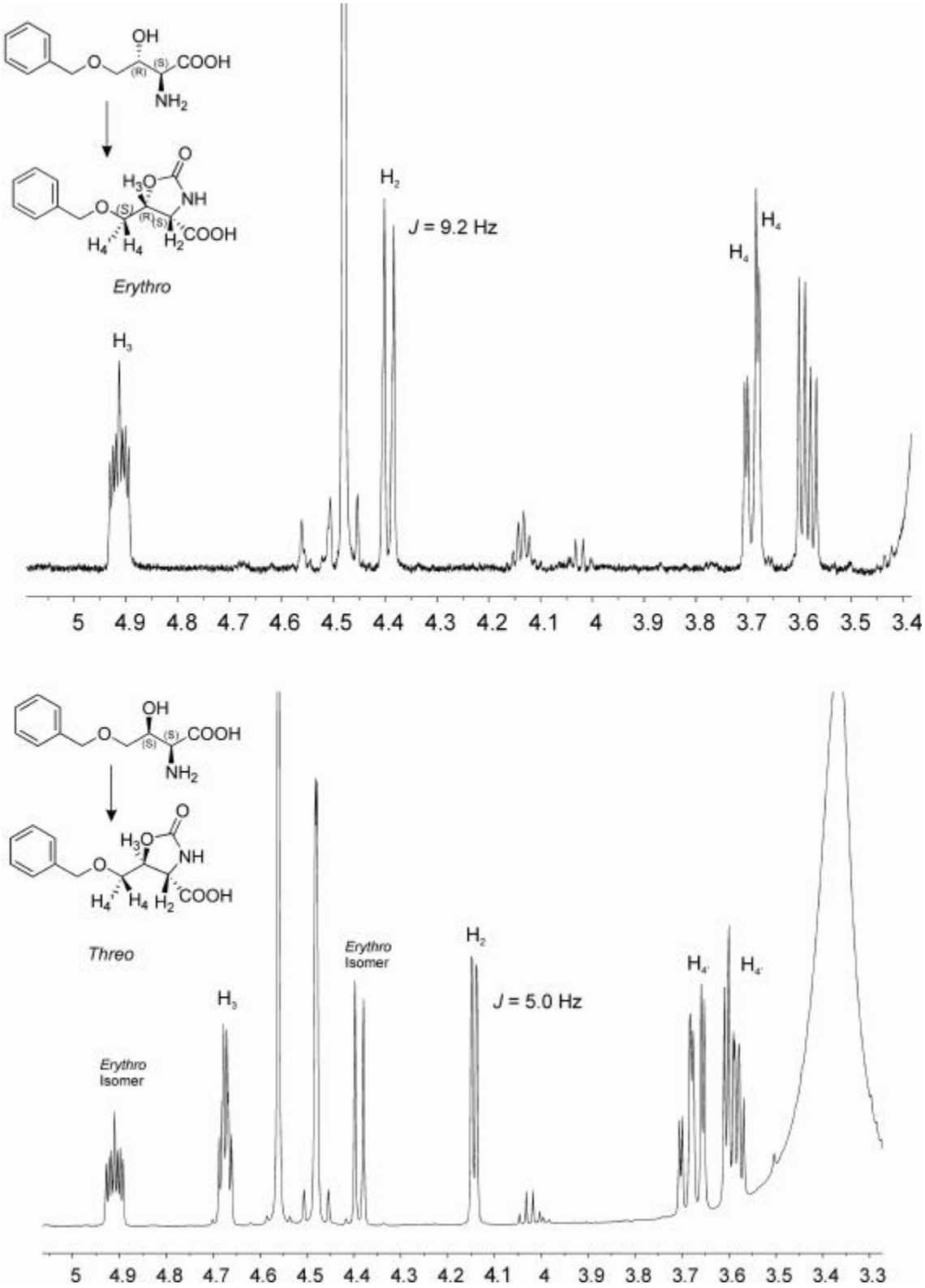


Table 2. The most relevant ^{1}H and ^{13}C chemical shifts and HH coupling constants (in DMSO) of *N*-Cbz-γ-amino-β-hydroxy-α-amino acid derivatives and 2-amino-4-(benzyloxy)-3-hydroxybutanoic acid.

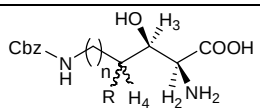
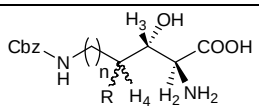
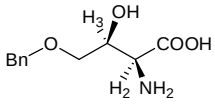
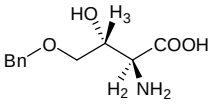
n, R	 *Threo*					 *Erythro*				
	$\delta (H_2)$	$\delta (H_3)$	$\delta (H_4)$	$^{3}J_{H2H3}$	$^{3}J_{H3H4}$	$\delta (H_2)$	$\delta (H_3)$	$\delta (H_4)$	$^{3}J_{H2H3}$	$^{3}J_{H3H4}$
0, (*R*)CH_3	3.19	3.77	3.65	4.0	7.5	3.02	3.54	3.73	8.4	3.0
0, (*S*)CH_3	3.23	3.81	3.76	5.1	5.3	3.27	3.68	3.67	4.6	4.9
0, H	3.25	3.95	3.69	5.6	nd	3.21	3.81	3.18	5.2	nd
1, H	3.10	3.81	3.17	4.9	nd	3.16	3.82	3.00	5.5	nd
	 *Threo*					 *Erythro*				
	$\delta (H_2)$	$\delta (H_3)$	$\delta (H_4)$	$^{3}J_{H2H3}$	$^{3}J_{H3H4}$	$\delta (H_2)$	$\delta (H_3)$	$\delta (H_4)$	$^{3}J_{H1H2}$	$^{3}J_{H3H4}$
	3.23	4.13	3.52	3.6	nd	3.28	3.96	3.52-3.43	5.5	nd

Figure 29. Complete and expanded regions of the ^{1}H NMR spectrum of 2-oxazolidinone **11a** from aldol adduct **6a**.

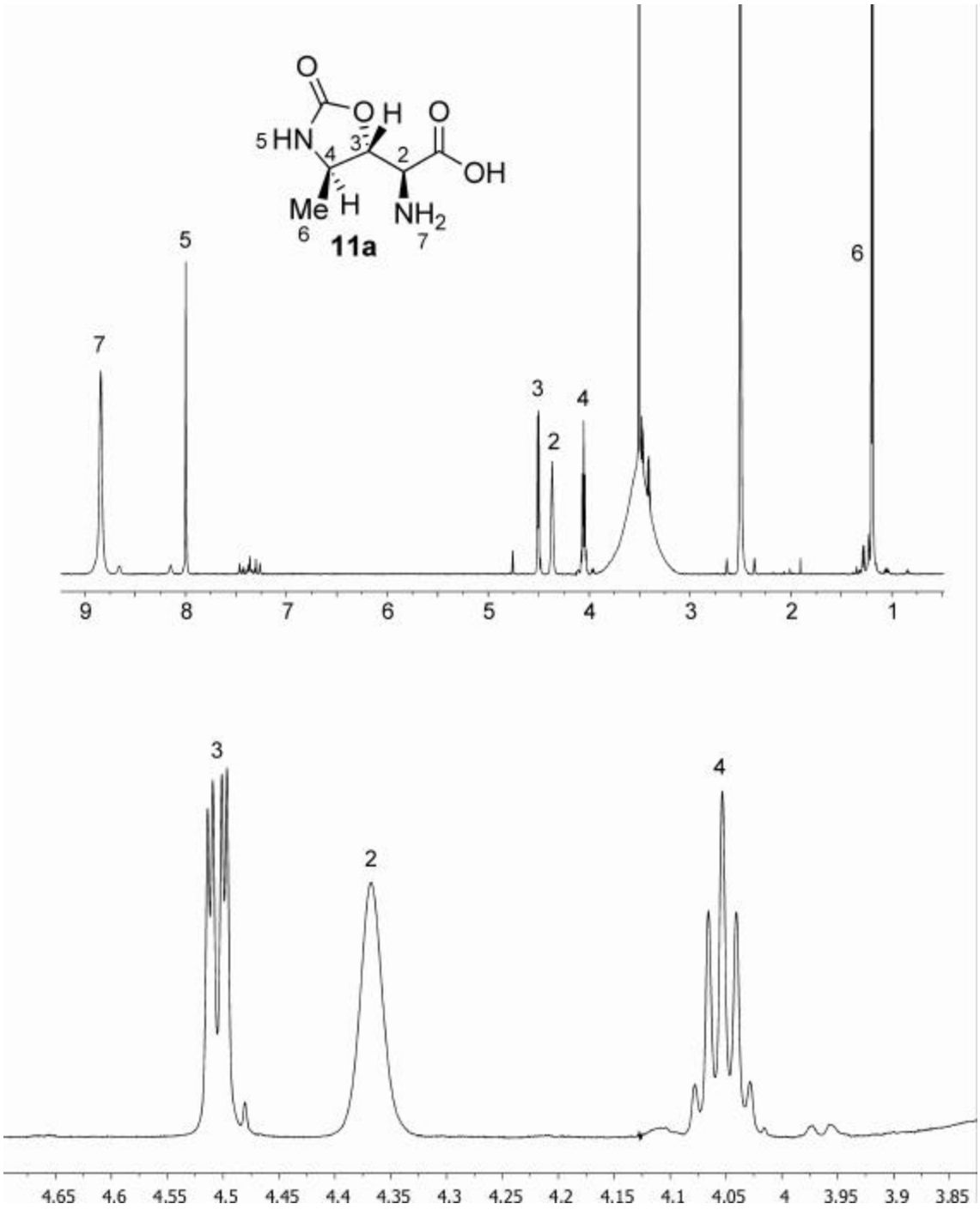


Figure 30. 2D ^{1}H-^{1}H COSY and 2D ^{1}H-^{13}C HSQC spectra of 2-oxazolidinone **11a**.

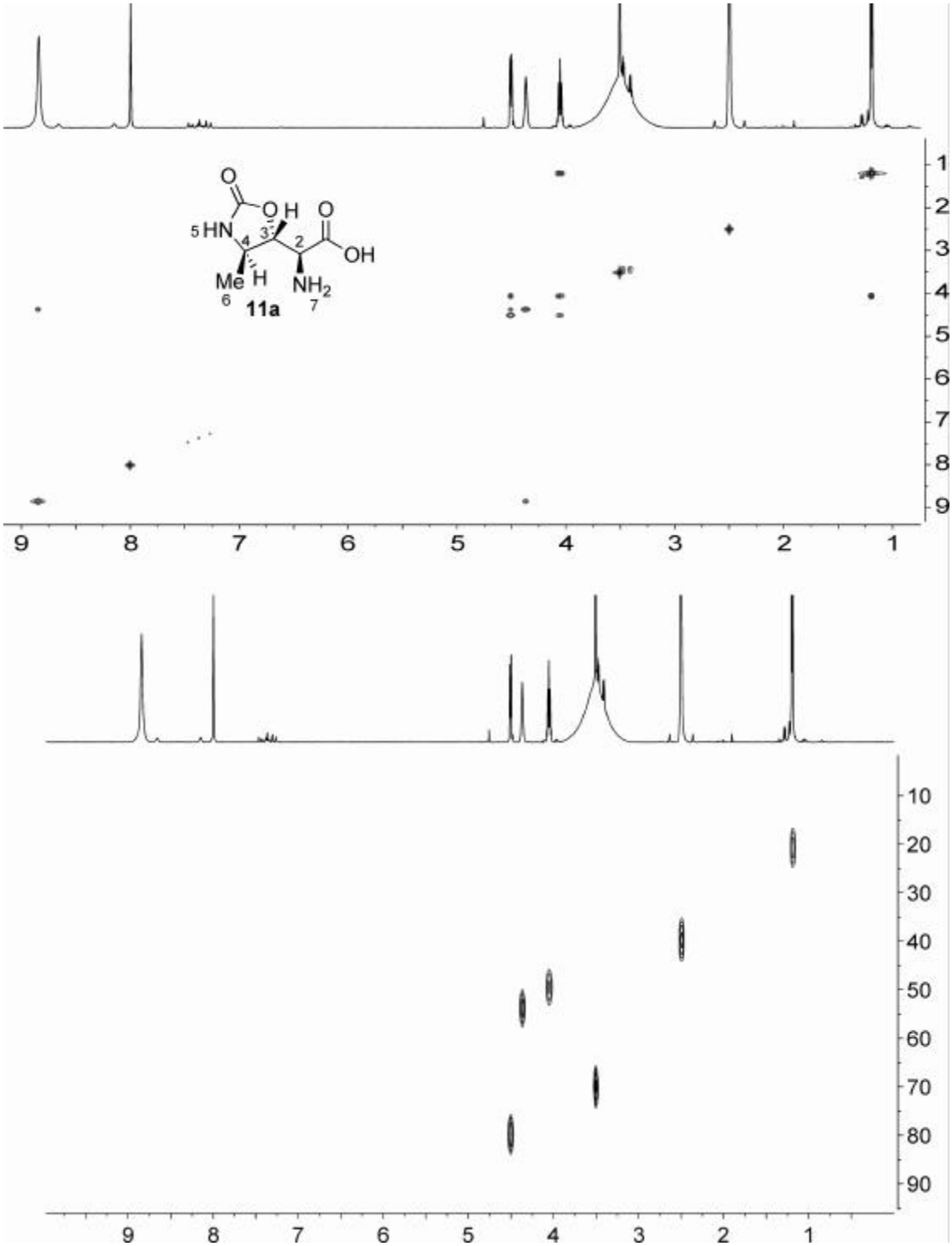


Figure 31. Some selective 1D NOESY spectra and 2D HMBC spectra of 2-oxazolidinone **11a**.

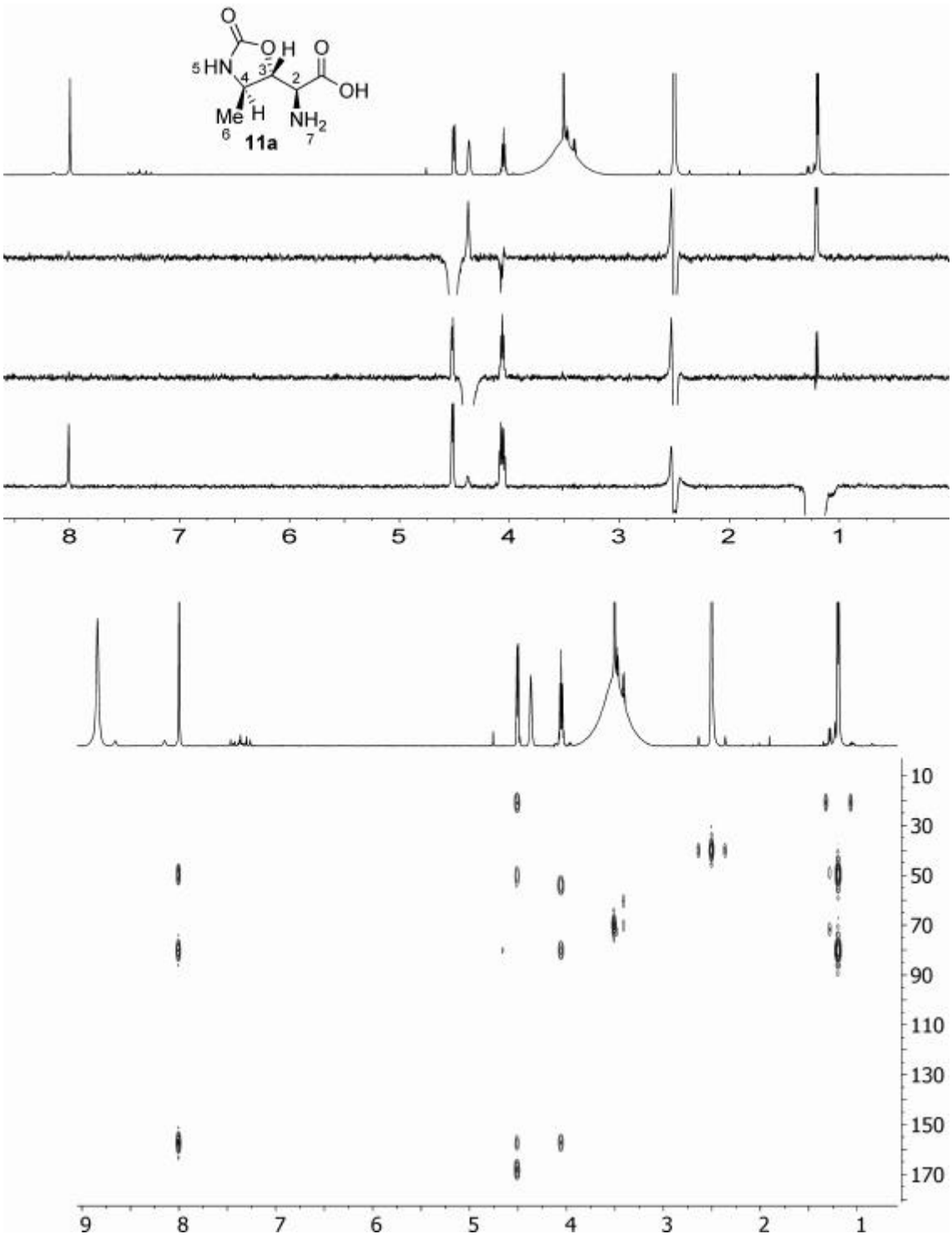


Figure 32. Multiplicity-edited 2D ^{1}H-^{15}N spectrum of 2-oxazolidinone **11a**.

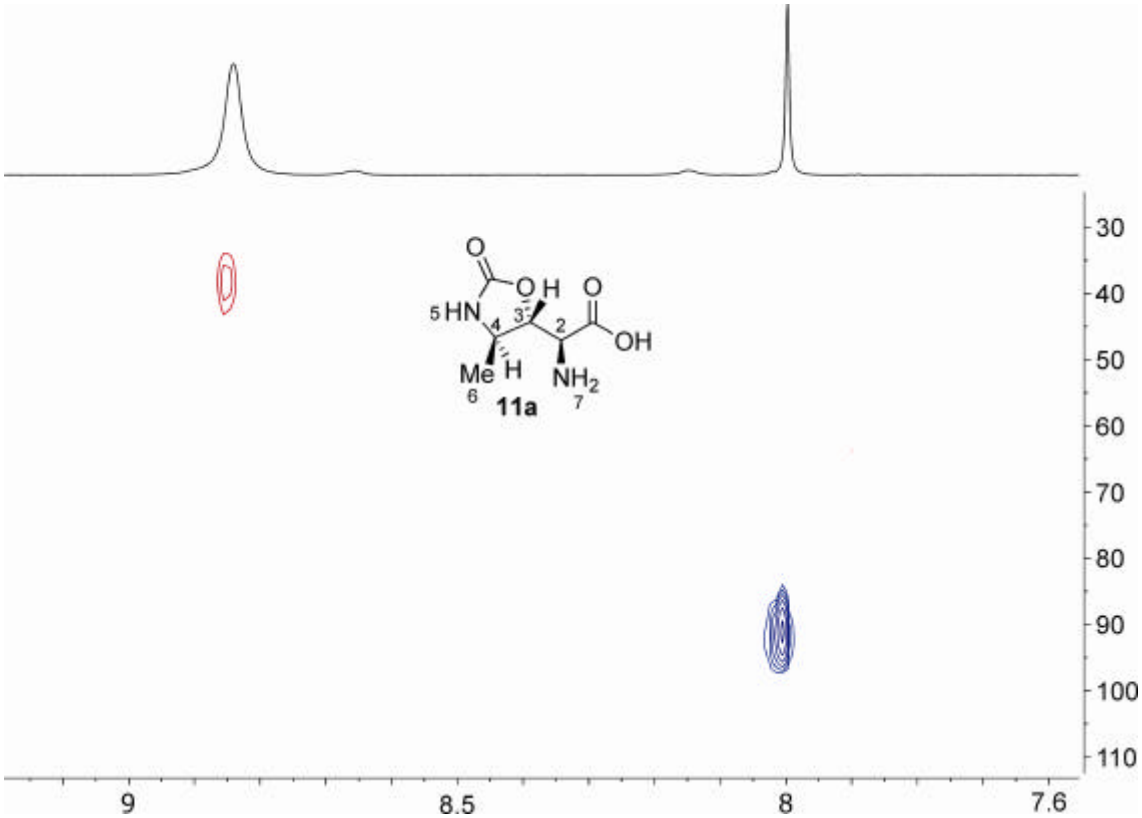


Figure 33. Complete and expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone mixture **11a**-**11b**.

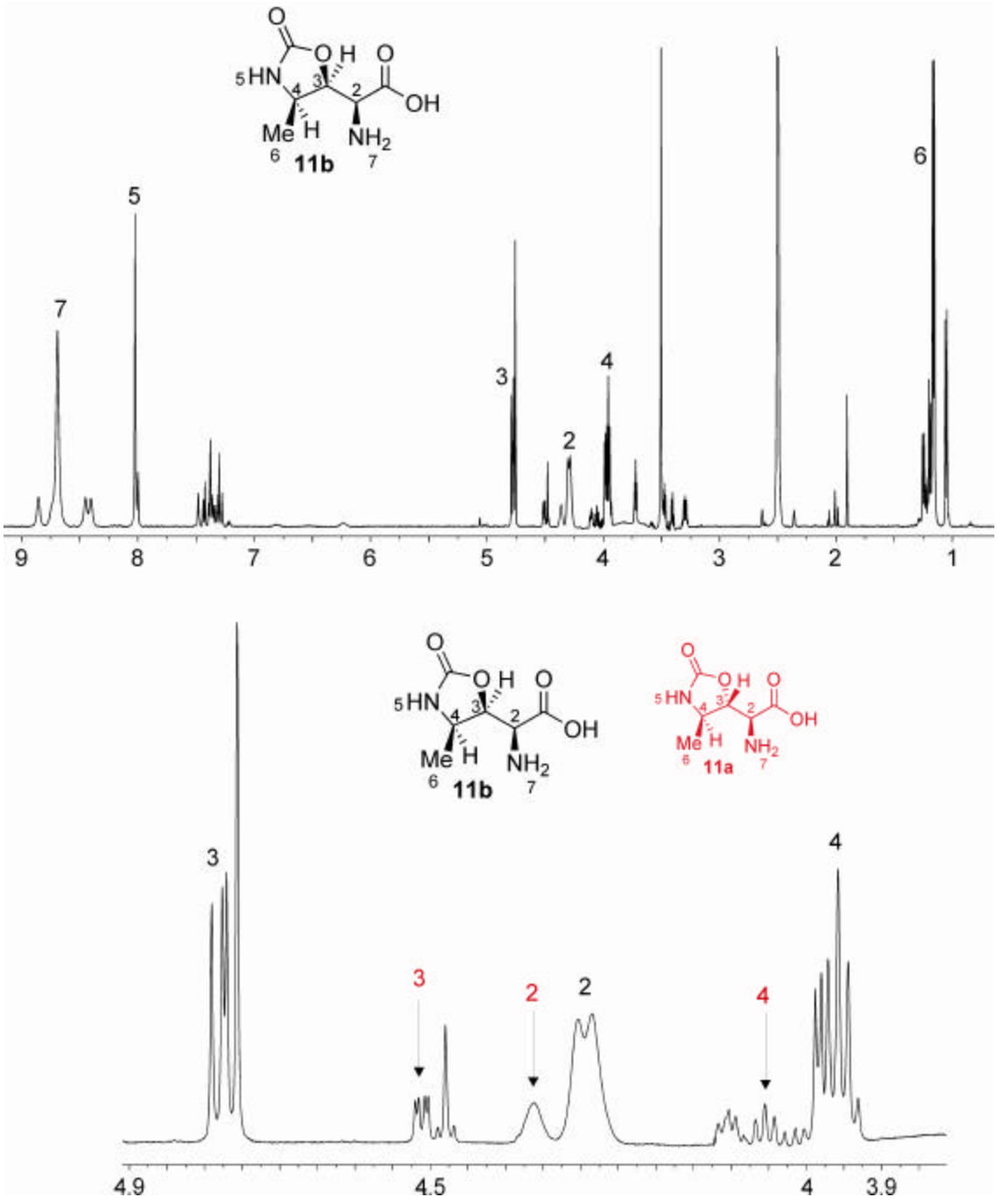


Figure 34. 2D ^{1}H-^{13}C HSQC and some selective 1D NOESY spectra of 2-oxazolidinone **11b**.

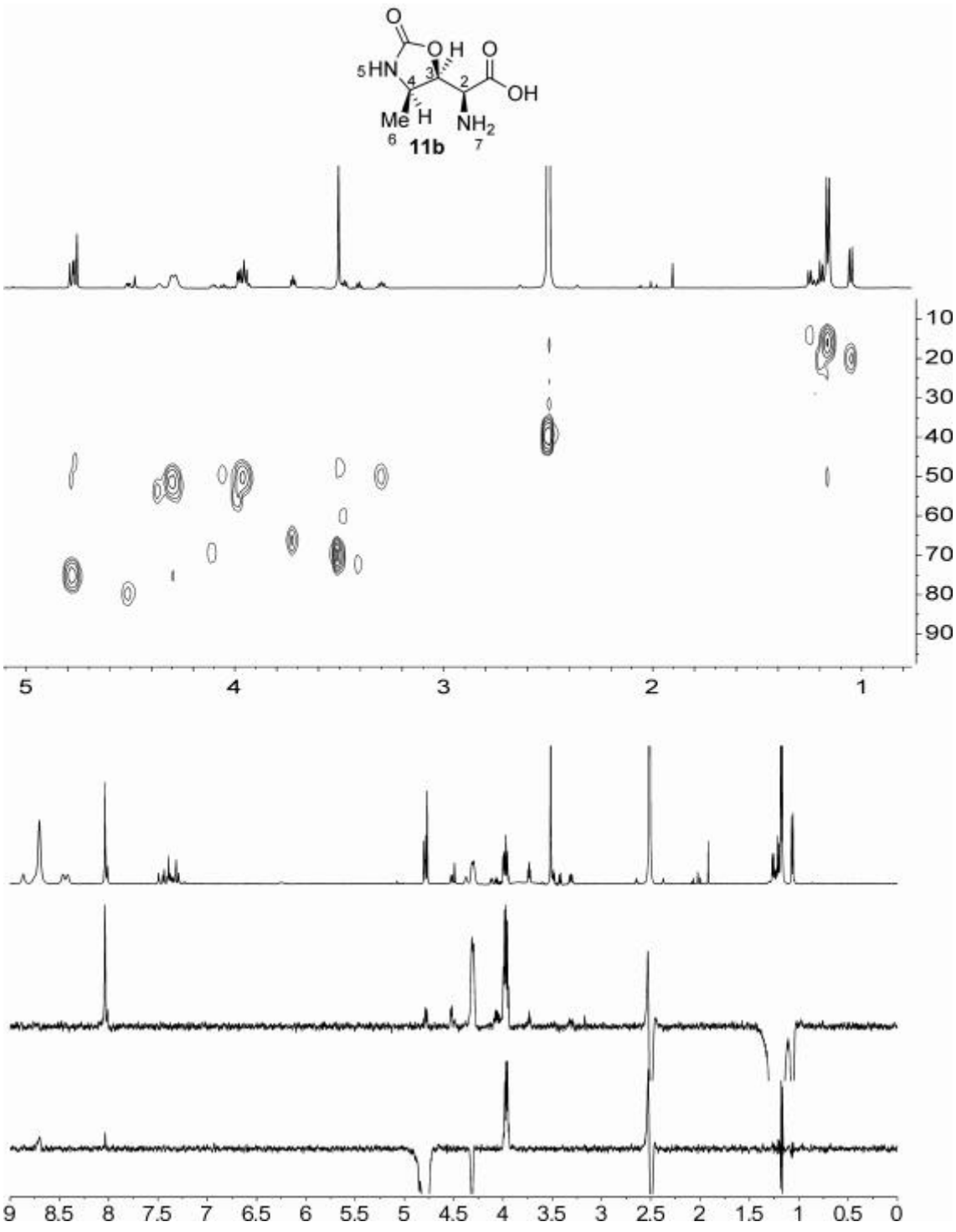


Figure 35. Complete and expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone mixture **11c**-**11a**.

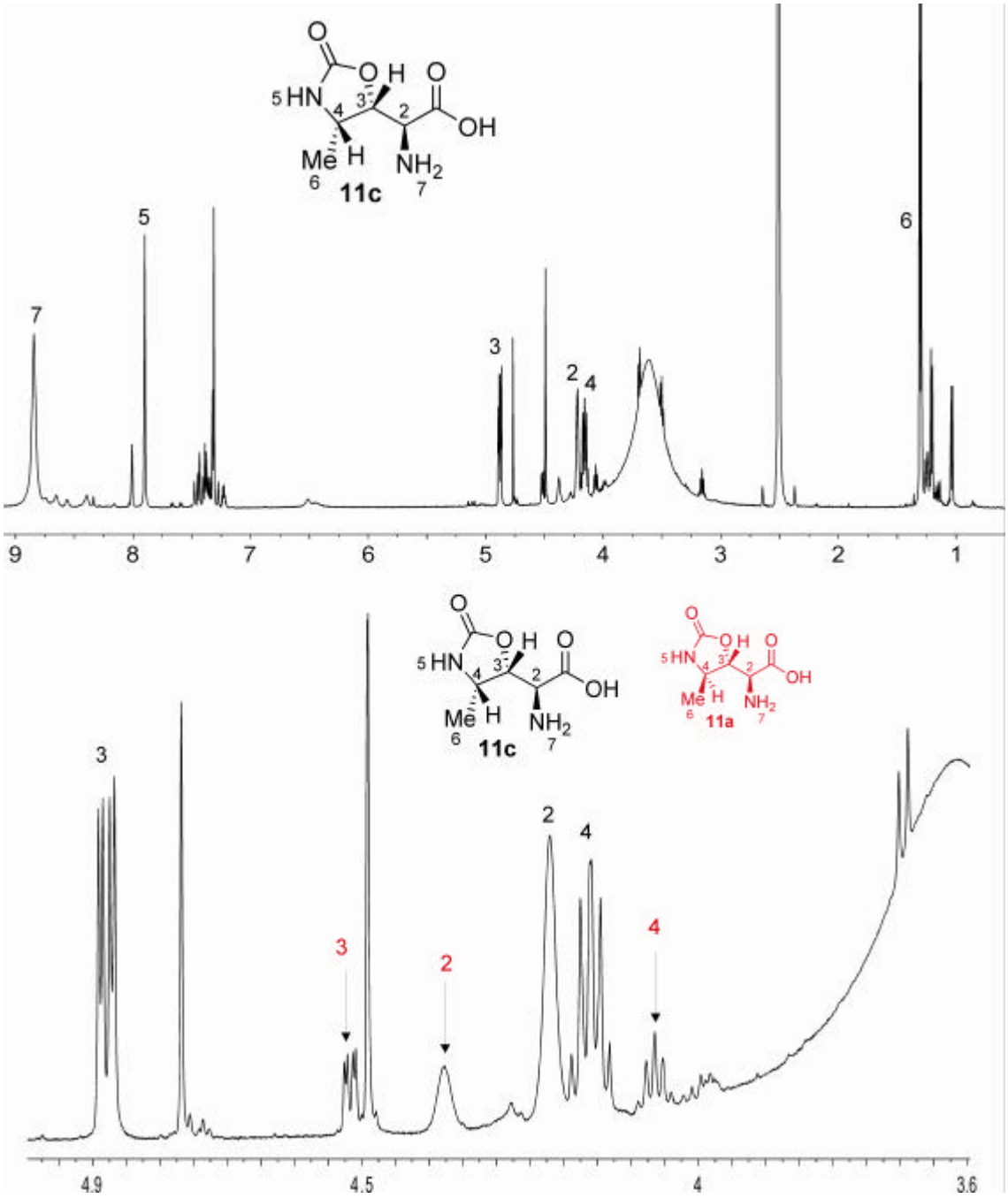


Figure 36. 2D ^{1}H-^{13}C HSQC and some selective 1D NOESY spectra of 2-oxazolidinone **11b**.

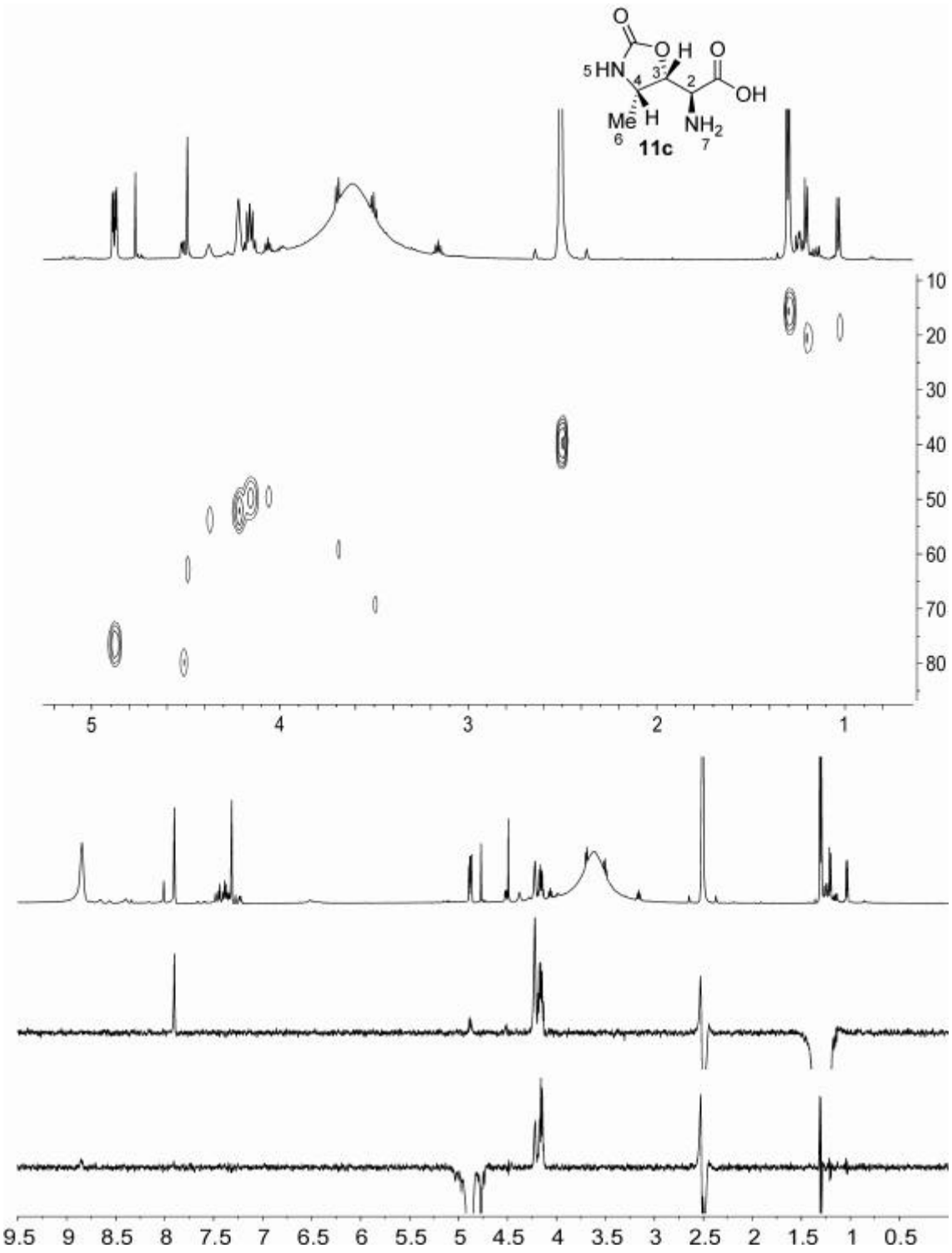


Figure 37. Complete and expanded regions of the ^{1}H NMR spectrum of the 2-oxazolidinone mixture **11d**.

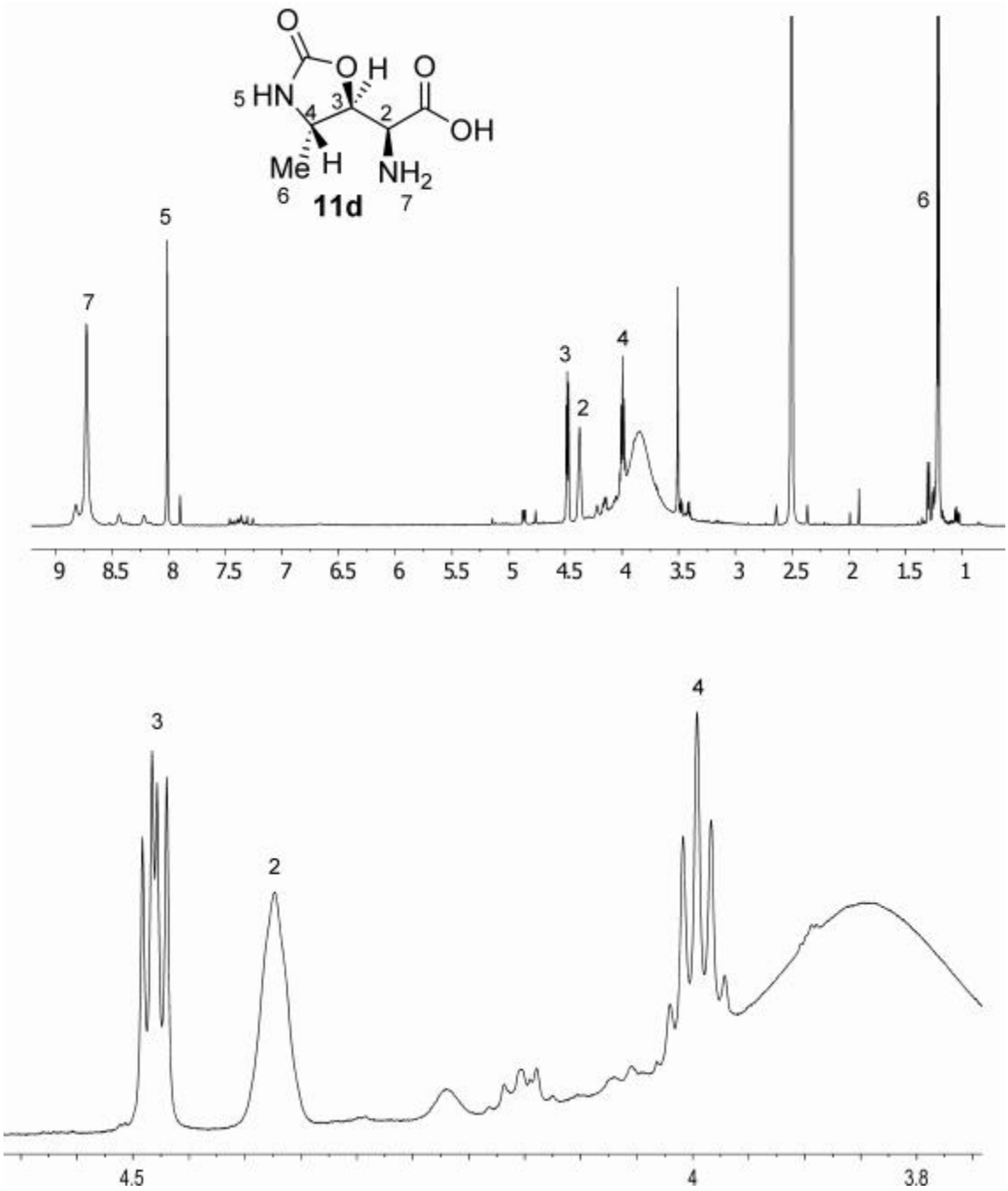


Table 3. The most relevant ^{1}H and ^{13}C chemical shifts and HH coupling constants (in DMSO) of stereoisomeric 2-oxazolidone derivatives (**11a-11d**) from compounds **6a-7b**.

Product	δ (H_2)	δ_H(H_3)	δ_H(H_4)	δ_c(CH_3)	$^{3}J_{H2H3}$	$^{3}J_{H3H4}$
11a	4.37	4.51	4.05	21.1	2.2	6.1
11b	4.29	4.77	3.96	16.1	9.7	7.1
11c	4.21	4.87	4.15	16.7	3.1	8.4
11d	4.37	4.48	3.99	20.6	4.3	6.5