

Supporting information

***In Situ* Evaluation of Lipase Performances Through Dynamic Asymmetric Cyanohydrin Resolution**

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



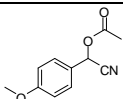
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Preference factors (F_p)

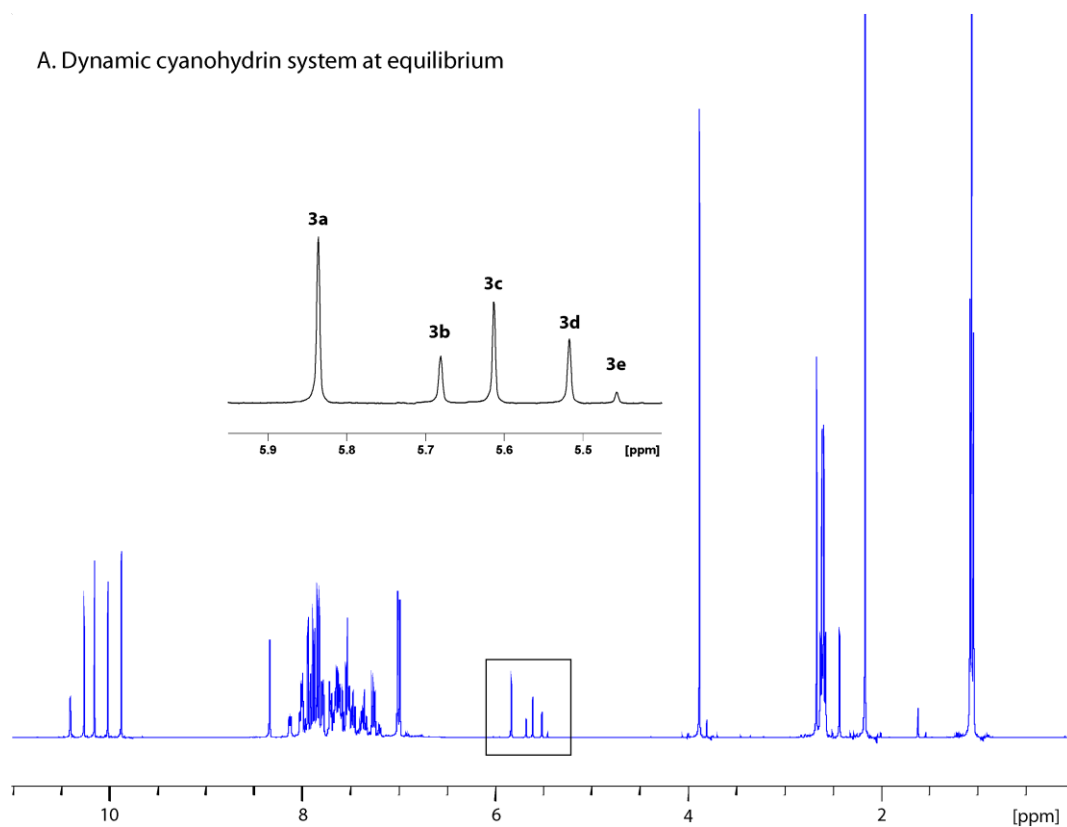
Table S1 Preference factors of ester products **4a-e** at different reaction conditions.

Reaction condition	Preference factor of ester product				
	 4a	 4b	 4c	 4d	 4e
10 mg of lipase at RT	-0.42	0.26	0.20	0.40	0.30
6 mg of lipase at RT	-0.63	0.55	0.15	0.79	0.59
3 mg of lipase at RT	-0.66	0.79	-0.03	0.89	0.63
3 mg of lipase at 0°C	-0.72	0.75	-0.03	1.15	0.28
3 mg of lipase at -18°C ^[a]	-0.78	0.83	-0.36	1.68	0.45

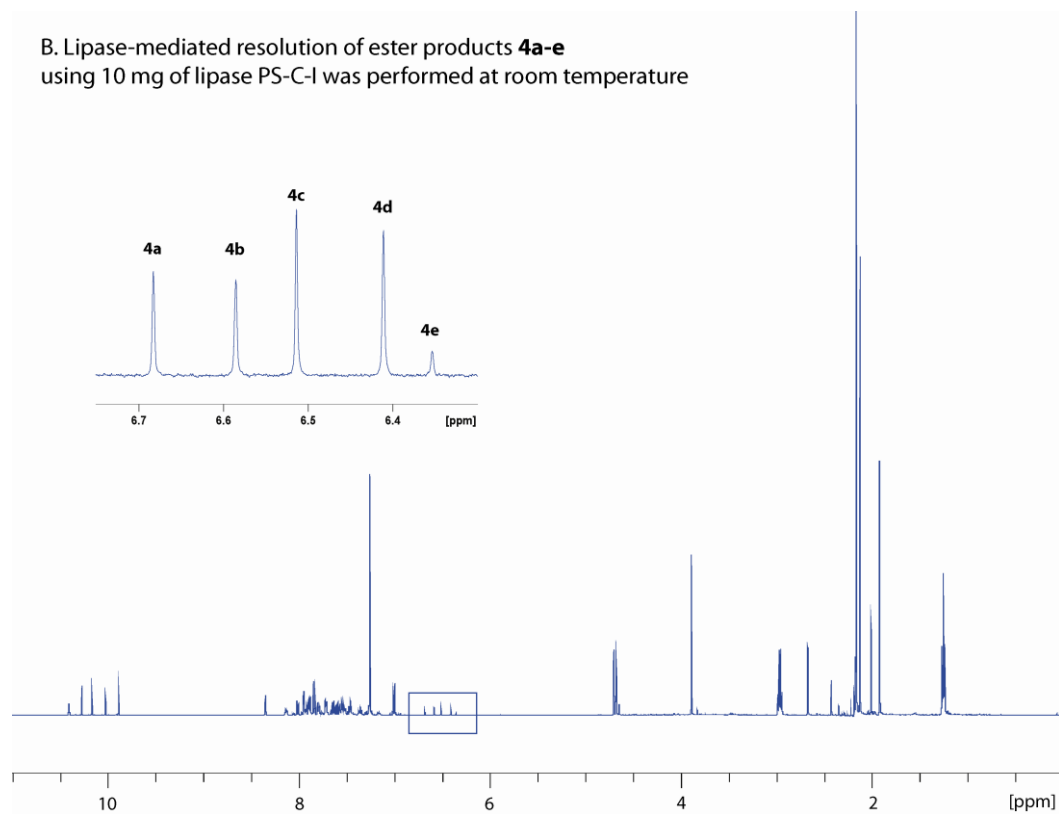
^[a] The lipase-mediated resolution of the dynamic cyanohydrin system at -18°C was slow and was stopped at <50% conversion.

¹H-NMR-analyses

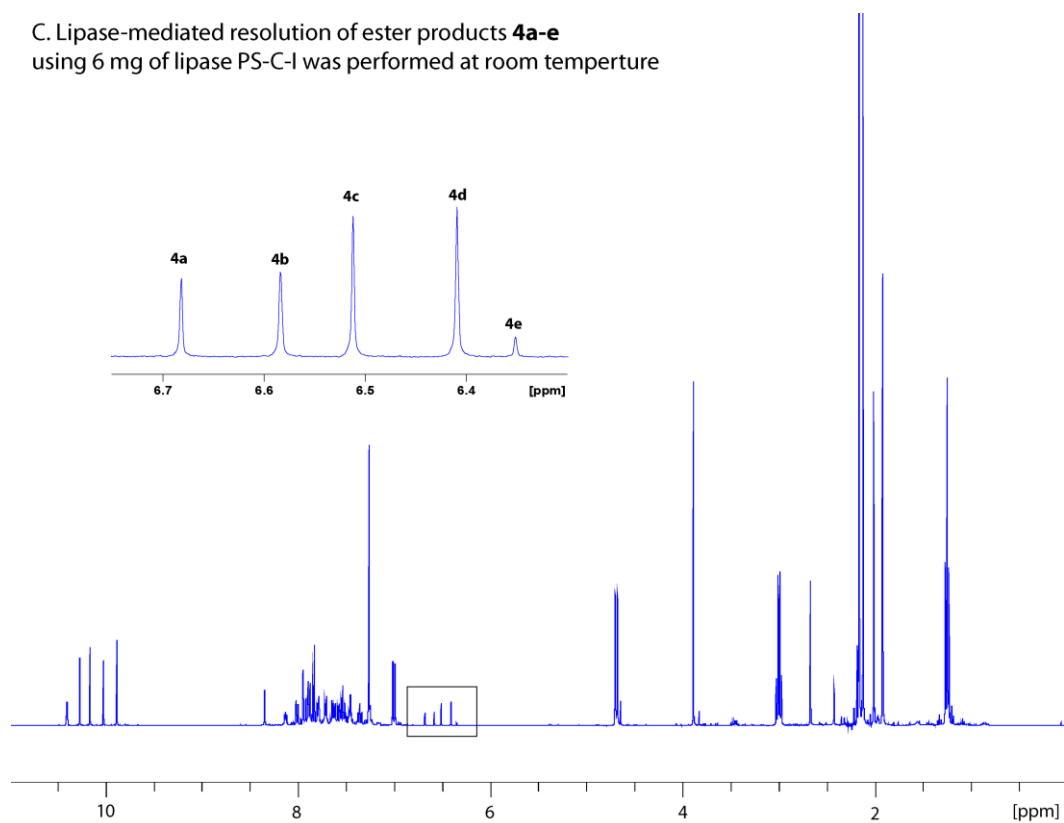
A. Dynamic cyanohydrin system at equilibrium



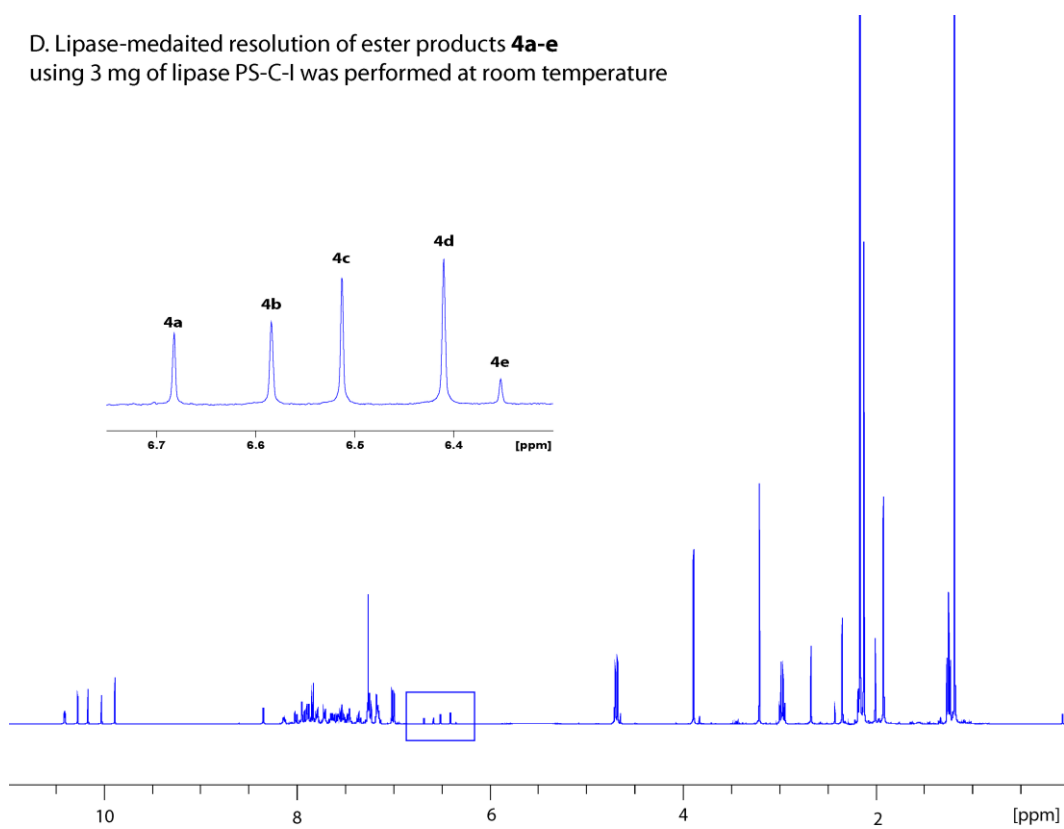
B. Lipase-mediated resolution of ester products 4a-e using 10 mg of lipase PS-C-I was performed at room temperature



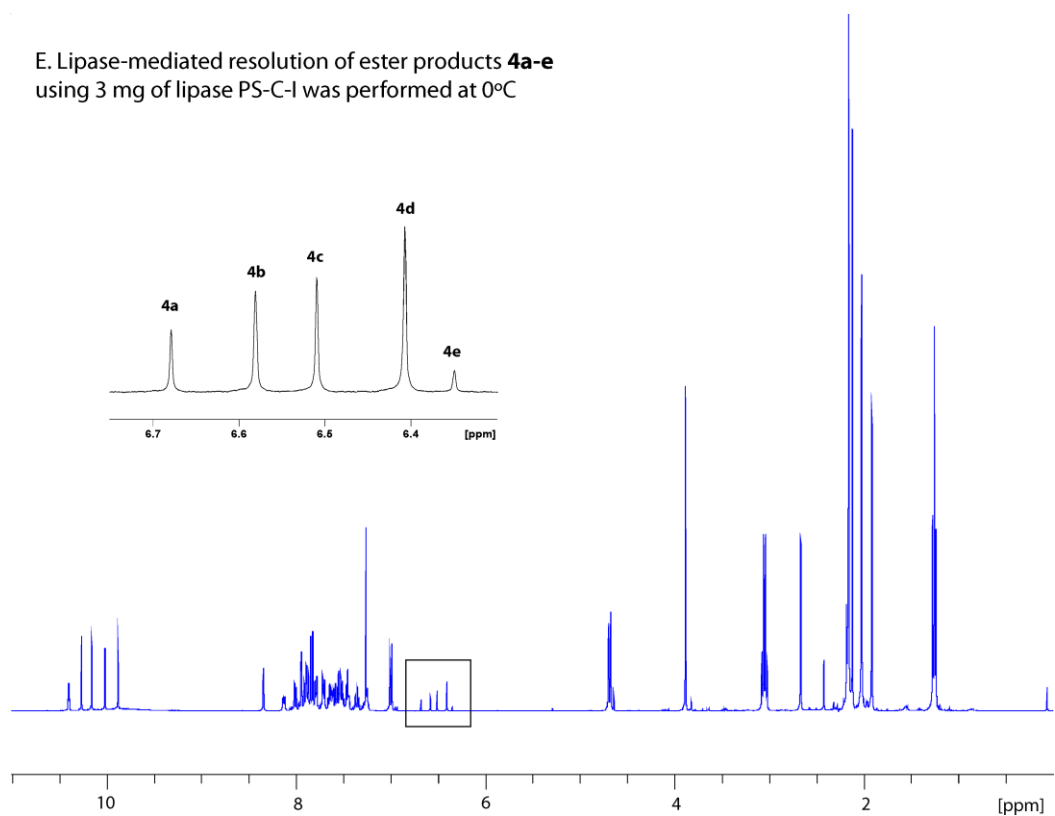
C. Lipase-mediated resolution of ester products **4a-e**
using 6 mg of lipase PS-C-I was performed at room temperature



D. Lipase-mediated resolution of ester products **4a-e**
using 3 mg of lipase PS-C-I was performed at room temperature



E. Lipase-mediated resolution of ester products **4a-e**
using 3 mg of lipase PS-C-I was performed at 0°C



F. Lipase-mediated resolution of ester products **4a-e**
using 3 mg of lipase PS-C-I at -18°C

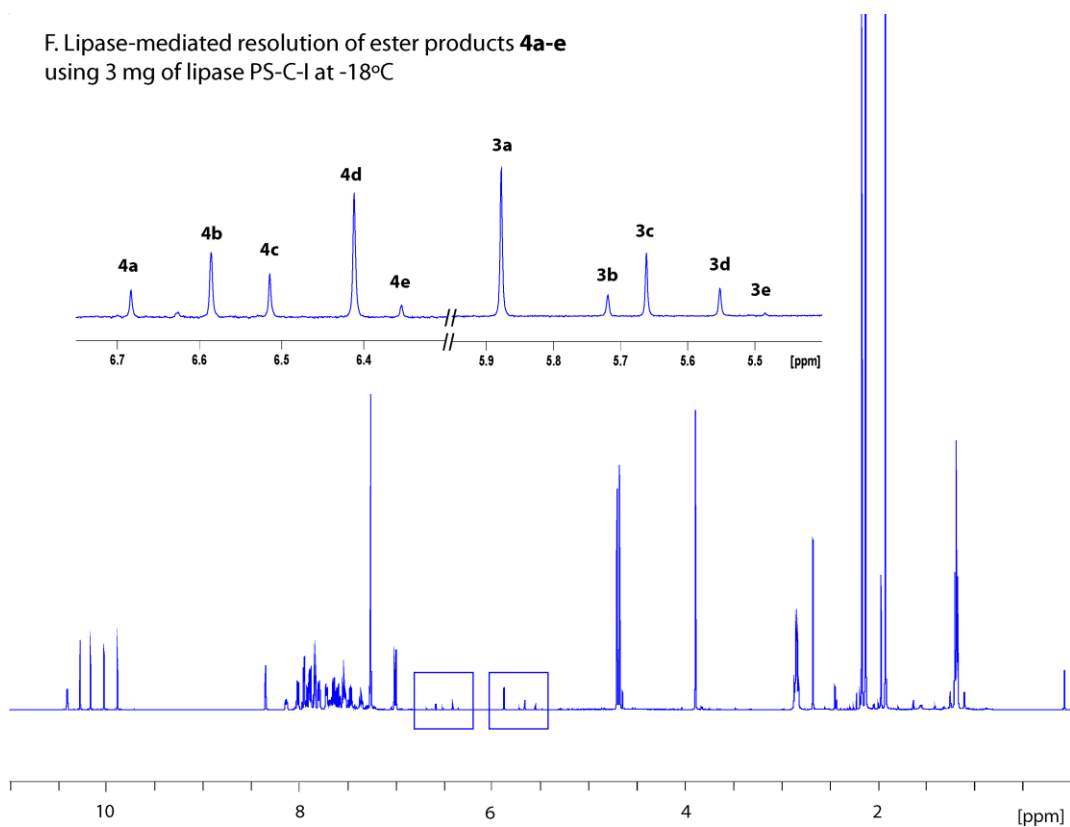


Figure S1. ¹H-NMR spectra of A. dynamic cyanohydrin intermediate at equilibrium; and lipase-mediated resolution using B. 10 mg of lipase at room temperature; C. 6 mg of lipase at room temperature; D. 3 mg of lipase at room temperature; E. 3 mg of lipase at 0°C; F. 3 mg of lipase at -18°C.

Chiral HPLC-analyses

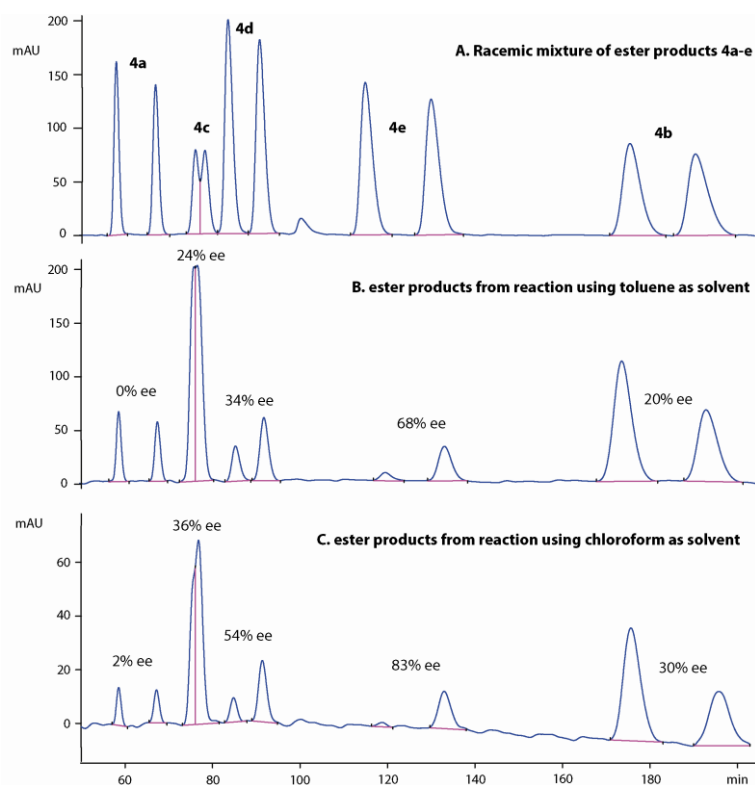
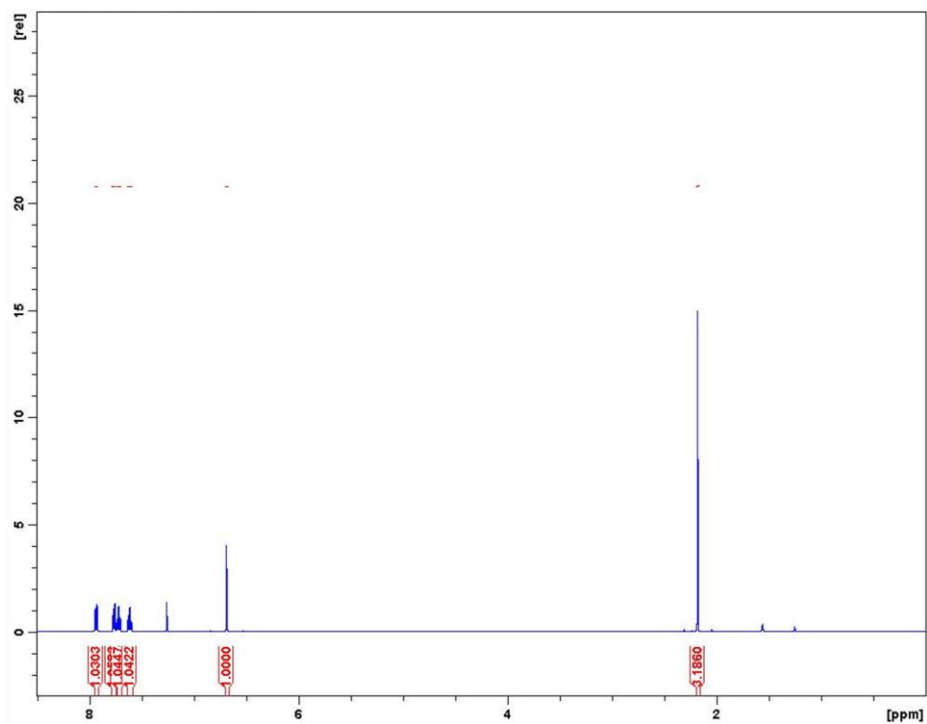
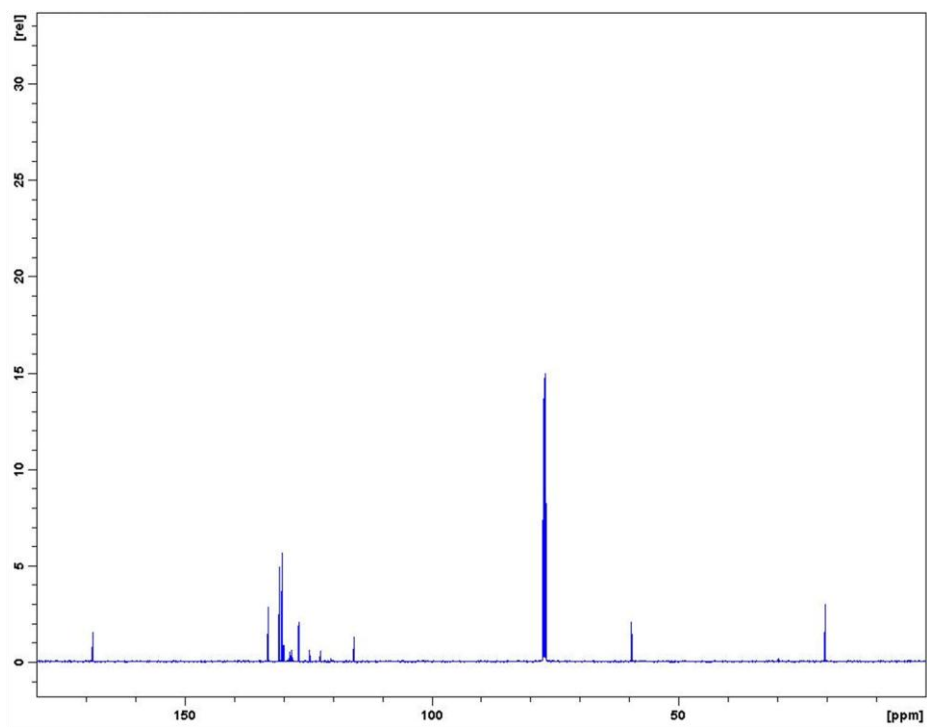


Figure S2. HPLC spectra. A. mixture of racemic ester compounds **4a-e**; B. mixture of ester products **4a-e** from the dynamic resolution using dry toluene as solvent; C. mixture of ester products **4a-e** from the dynamic resolution using chloroform-*d* as solvent.

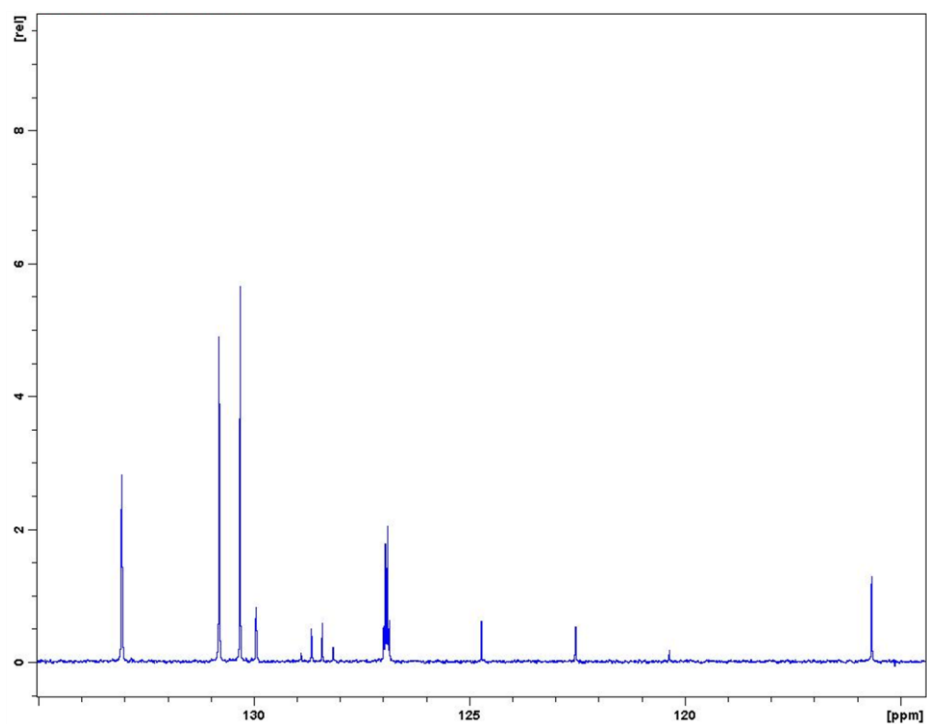
NMR spectra of ester product **4a**:



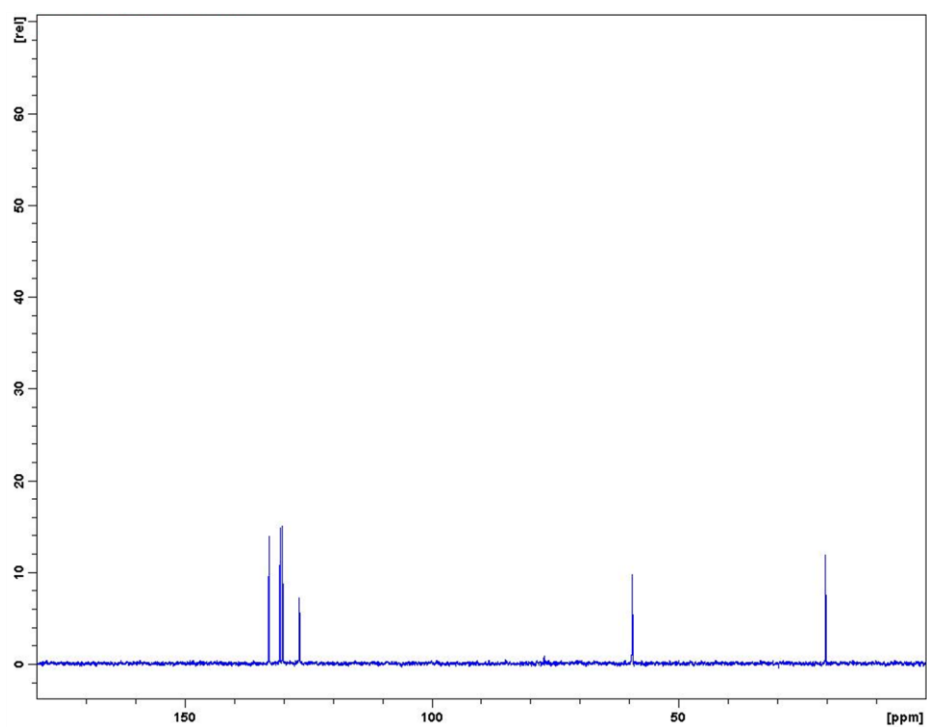
^1H NMR spectrum of ester product **4a**.



^{13}C NMR spectrum of ester product **4a**.

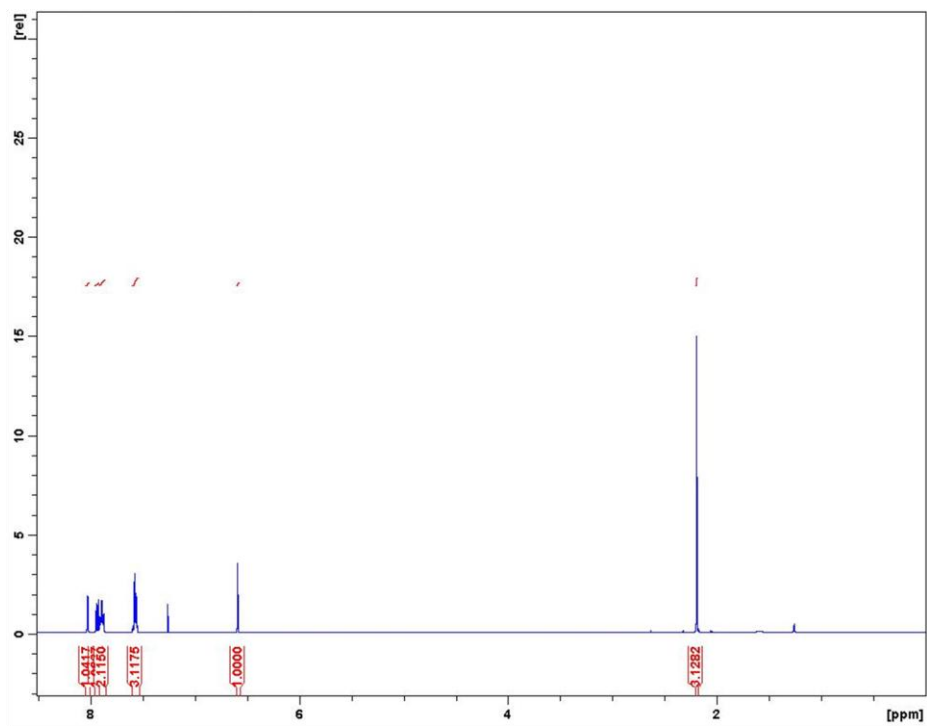


^{13}C NMR spectrum (enlarged at aromatic area) of ester product **4a**.

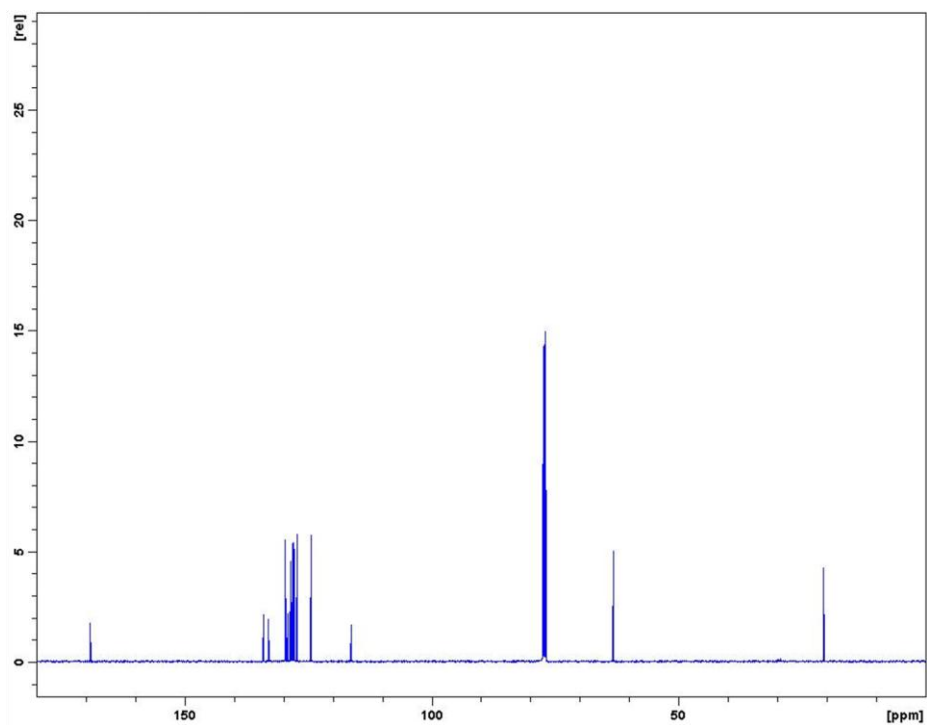


DEPT 45 NMR spectrum of **4a**.

NMR spectra of ester product **4b**:

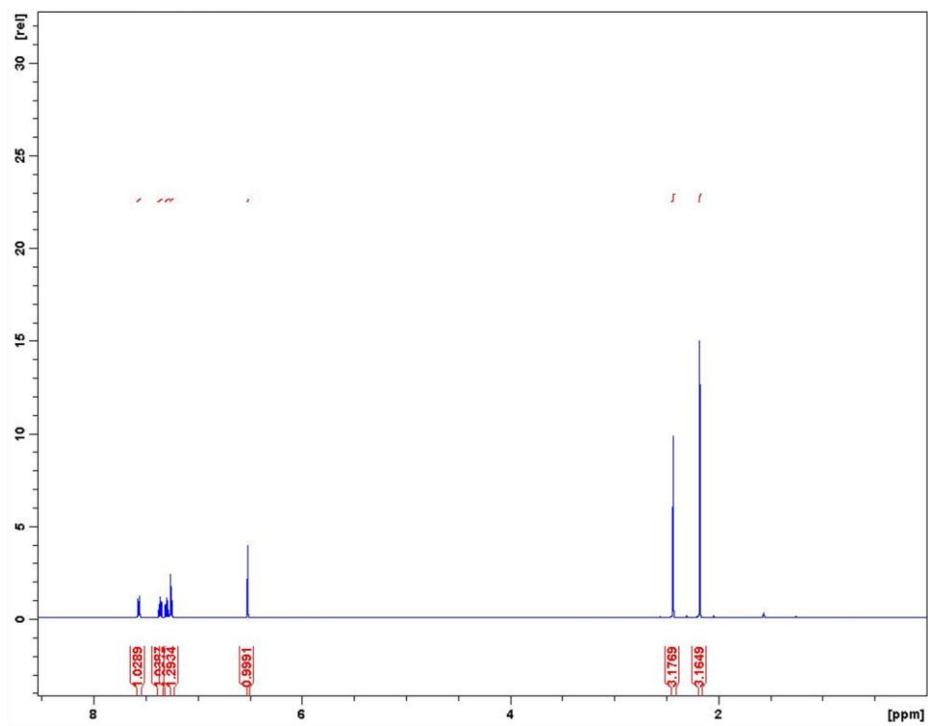


^1H NMR spectrum of ester product **4b**.

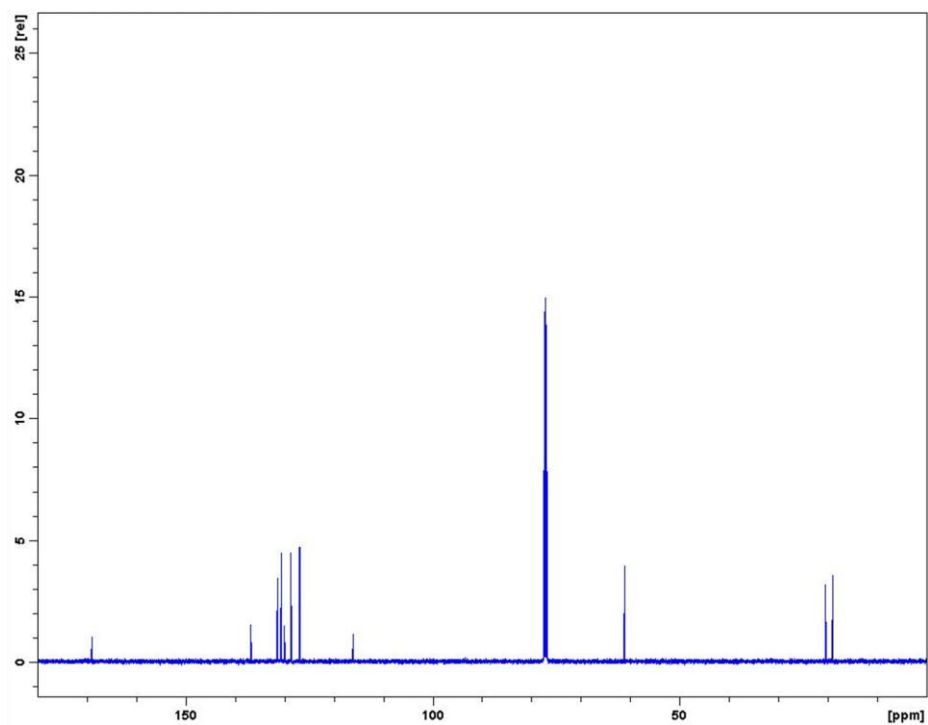


^{13}C NMR spectrum of ester product **4b**.

NMR spectra of ester product **4c**:

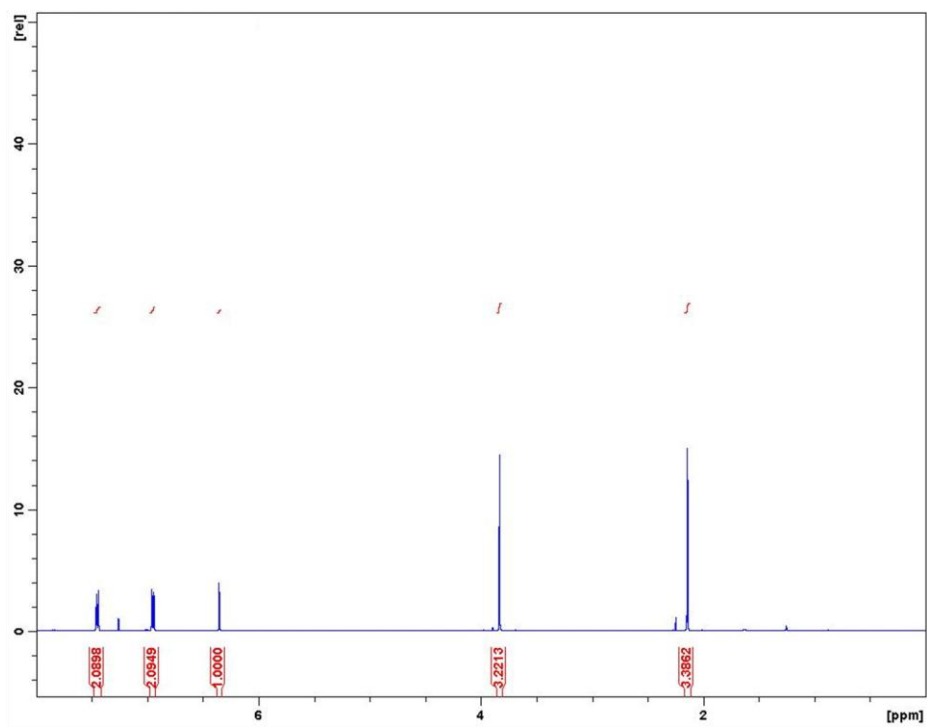


¹H NMR spectrum of ester product **4c**.

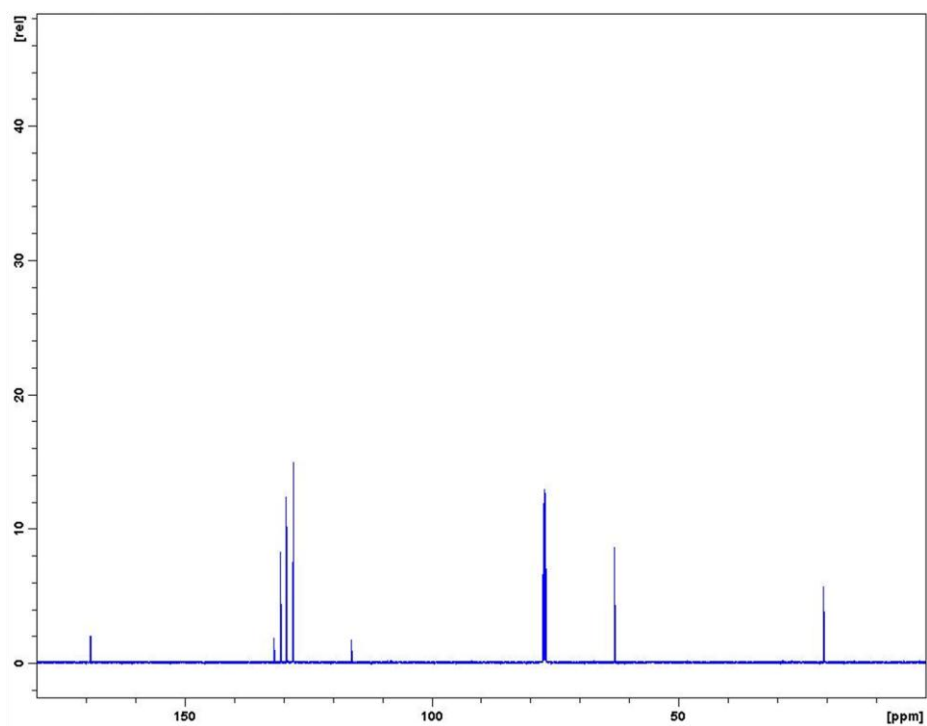


¹³C NMR spectrum of ester product **4c**.

NMR spectra of ester product **4d**:

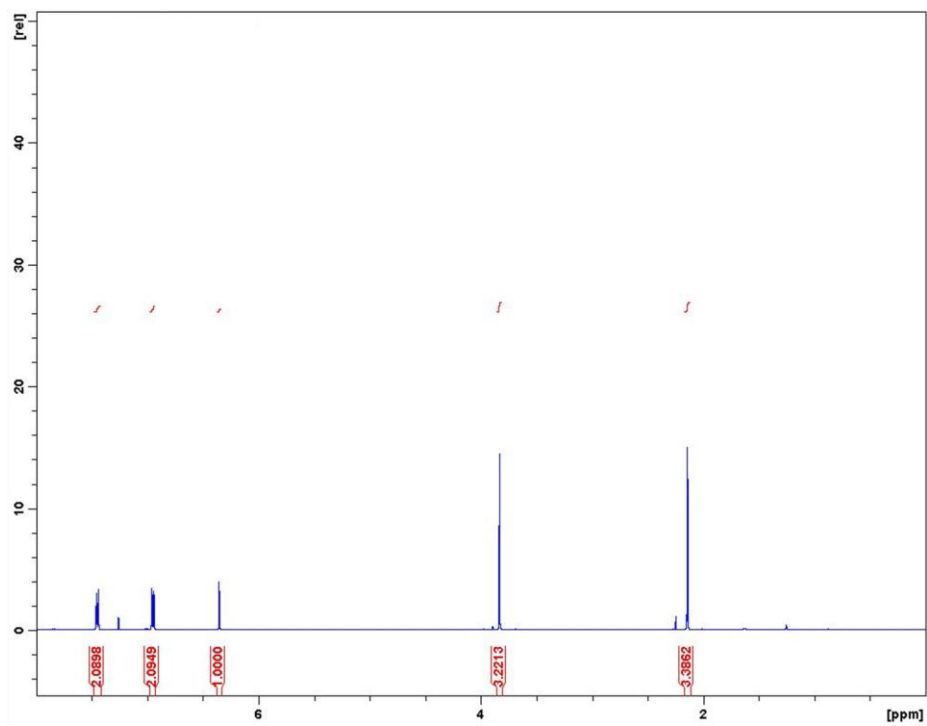


¹H NMR spectrum of ester product **4d**.

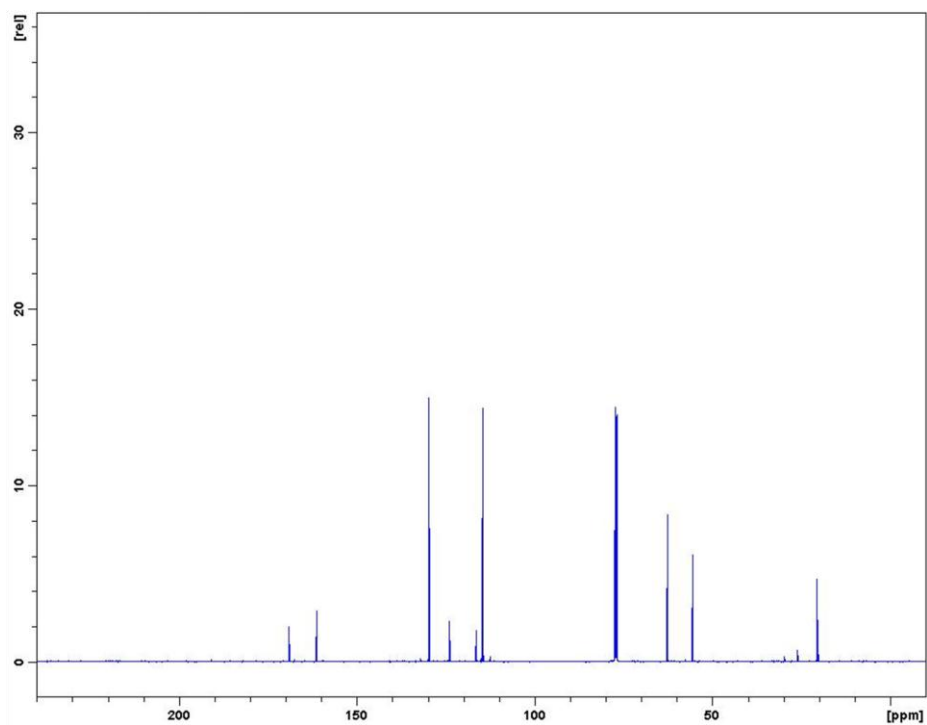


¹³C NMR spectrum of ester product **4d**.

NMR spectra of ester product **4e**:



¹H NMR spectrum of ester product **4e**.



¹³C NMR spectrum of ester product **4e**.