

# Investigation and Comparison of Catalytic Methods to Produce Green CO<sub>2</sub>-Containing Monomers for Polycarbonates

## -Supporting Information-

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**Table S1. Experimental parameters to determine the influence of the catalyst for reaction with various temperatures.**

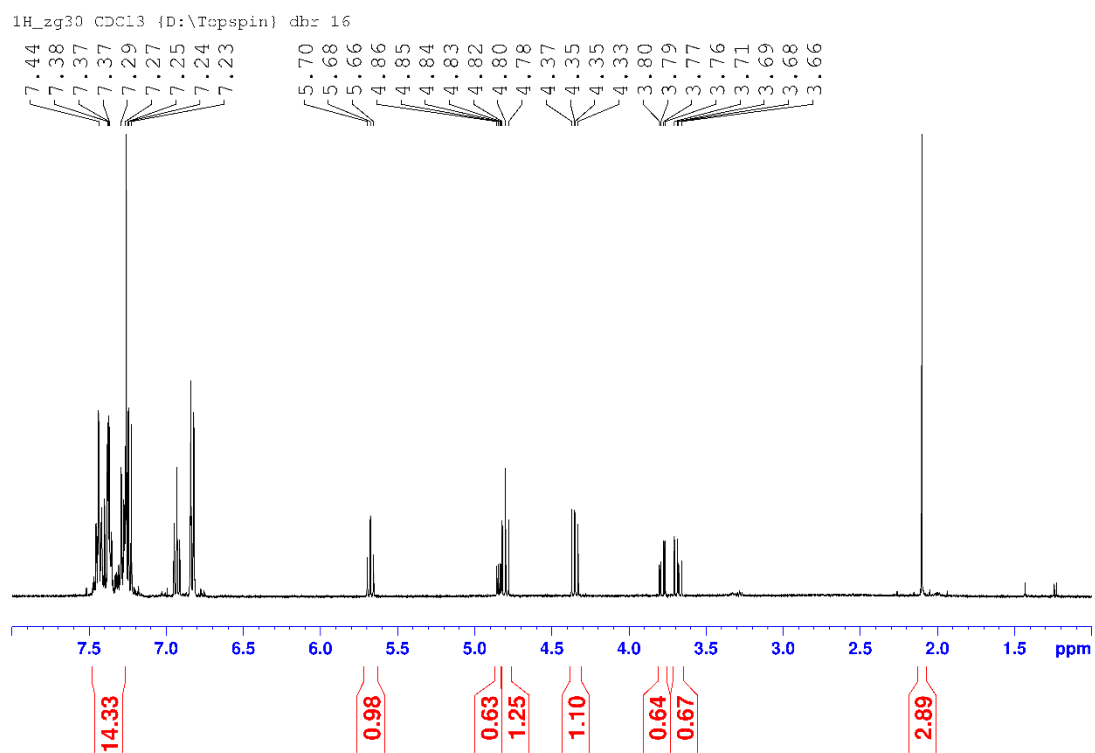
Number	Experiment	T [°C]	t [h]	Cat. [mol %]	m (PED) [g]	m (DMC) [mL]	Figure
22	V2504	30	3.5	2.00	5.0614	2.8037	1
23	V2604	31	4.5	2.00	50.6137	28.074	2
24	V0305	35	3.5	2.00	5.0614	2.8037	3
25	V0805	40	3.5	2.00	5.0614	2.8037	4
26	V0905	45	3.5	2.00	5.0614	2.8037	5
27	V1105	40	3.5	2.00	8.0614	2.8037	6
28	V1605	40	12.0	2.00	4.99419	13.2	7
29	V1705	45	12.0	2.00	5.00753	13.2	8
30	V2205	35	12.0	2.00	5.0019	14	9
31	V2305	50	12.0	2.00	5.00195	15	10
32	V2906	10	12.0	2.00	5.0079	13	11
33	V0307	20	12.0	2.00	5.00889	13	12
34	V0407	55	12.0	2.00	5.0219	13	13
35	V1007	60	5.0	2.00	5.0751	13	14

36	V1707	65	4.0	2.00	5.0016	13.1	15
37	V1807	0	12.0	2.00	5.0045	13.1	16
38	V1907	-5	12.0	2.00	5.0066	13.1	17
39	V2507	0	12.0	1.00	5.0614	2.804	18
40	V2607	0	v	1.00	5.0032	13.1	19
41	V3107	0	3.5	0.8	5.0652	2.804	20
42	V3107-2	10	12.0	0.8	5.0623	2.804	21
43	V0108	20	3.5	0.8	5.0631	2.804	22
44	V0108-2	30	v	0.8	5.0622	2.804	23
45	V0208	40	3.5	0.8	5.0632	2.804	24
46	V0208-2	50	12.0	0.8	5.0612	2.804	25
47	V0308	60	3.5	0.8	5.0620	2.804	26
48	V0308-2	30	12.0	0.6	5.0609	2.804	27
49	V0408	20	3.5	0.6	5.0613	2.804	28
50	V0708	0	3.5	0.6	5.0610	2.804	29
51	V0808	10	3.5	0.6	5.0613	2.804	30
52	V0808-2	40	v	0.6	5.0613	2.804	31
53	V0908	50	3.5	0.6	5.0614	2.804	32

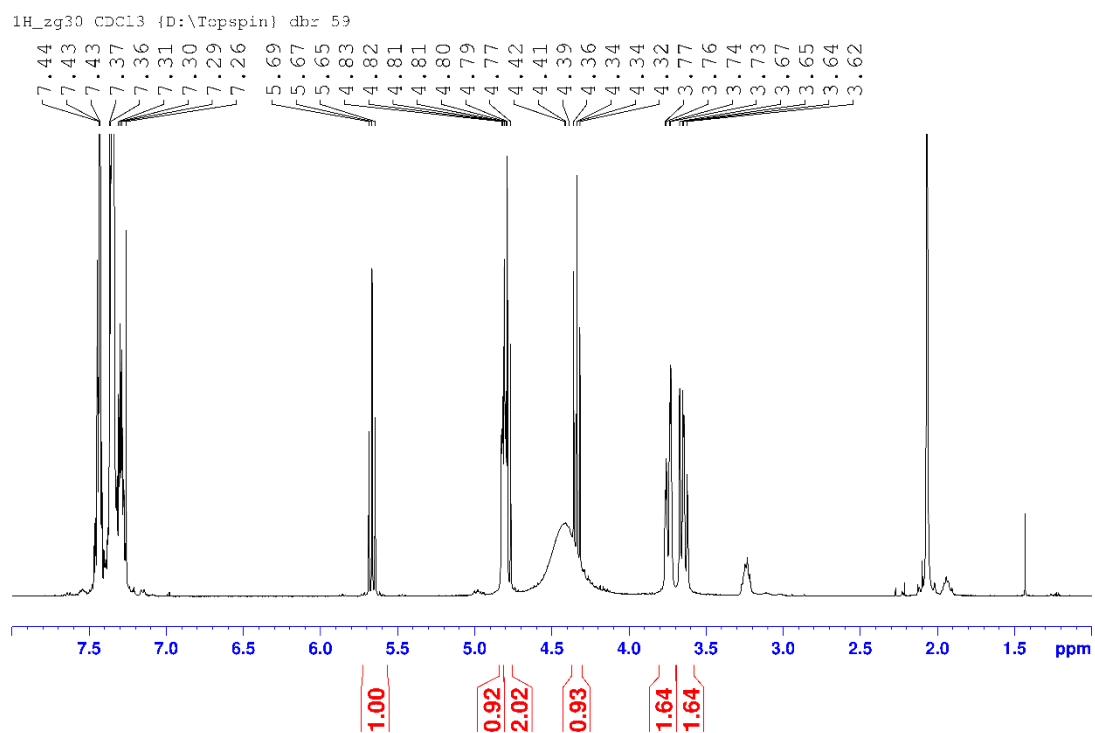
### NMR-Analytic of the Experiments

In the following section, the  $^1\text{H}$ -NMR spectra of Styrene carbonate in reaction with the catalyst 1,5,7-triazabicyclo[4.4.0]dec-5-ene at different temperatures and catalyst loadings are shown.

#### Dimethyl carbonate, 2.00 mol % catalyst loading

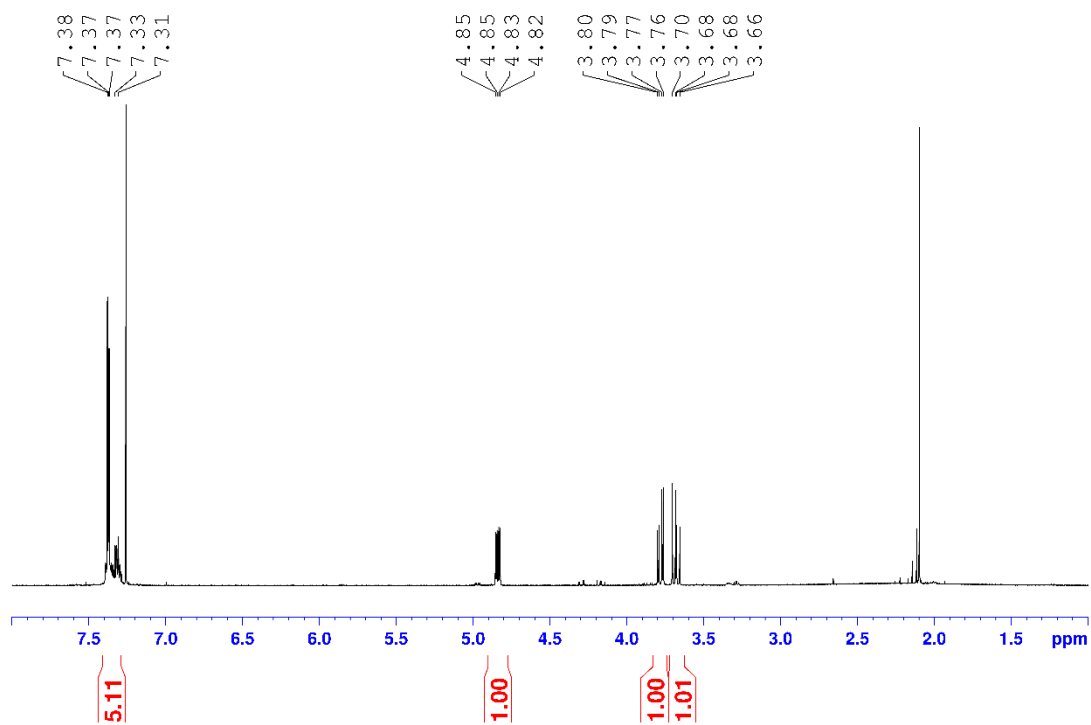


**Figure S1.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 30 °C. For reaction conditions see Table 1.

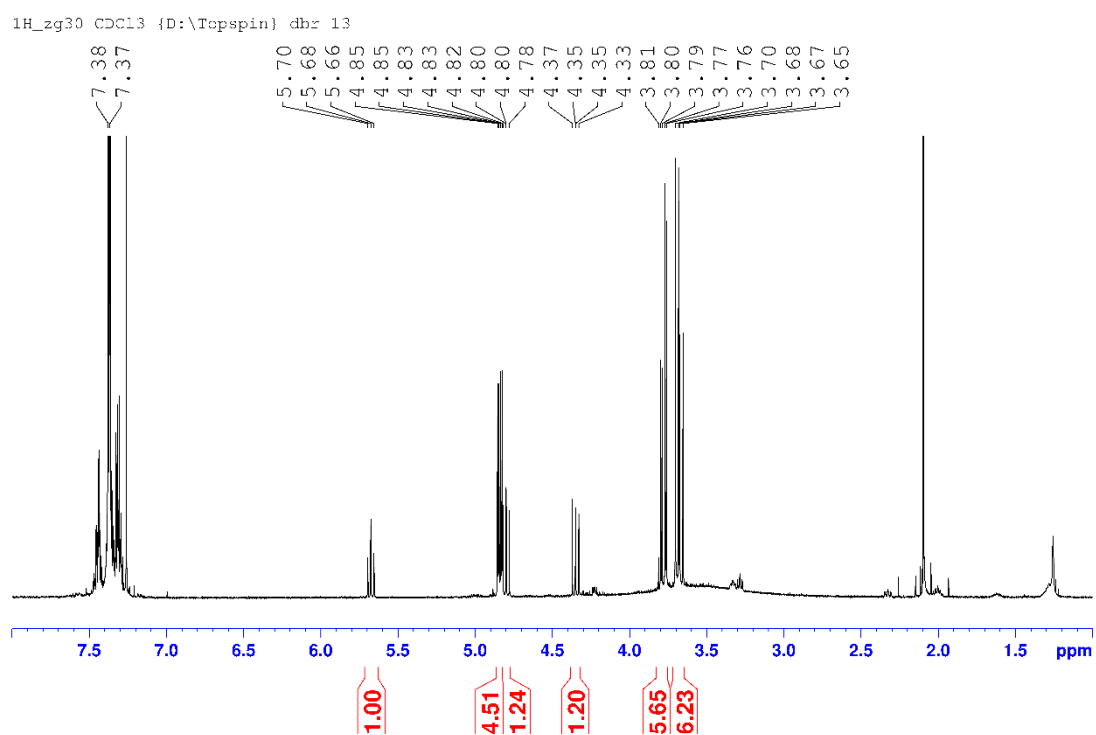


**Figure S2.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 31 °C. For reaction conditions Table 1.

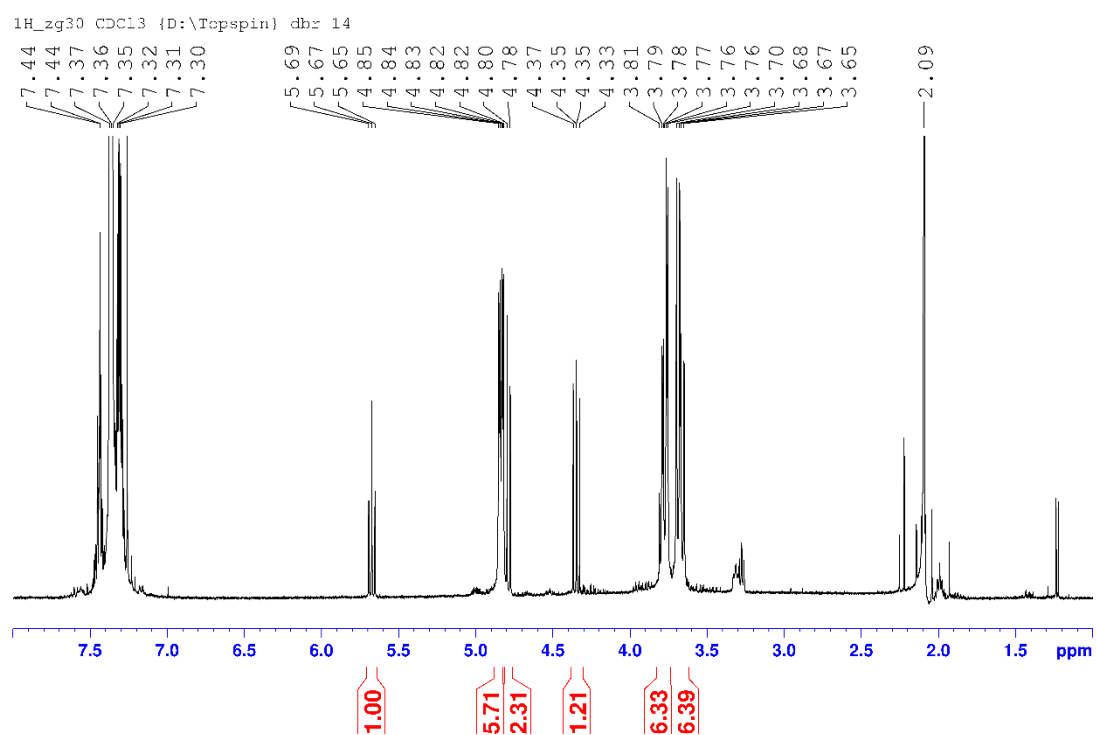
1H\_zg30 CDCl3 {D:\Topspin} yhle 37



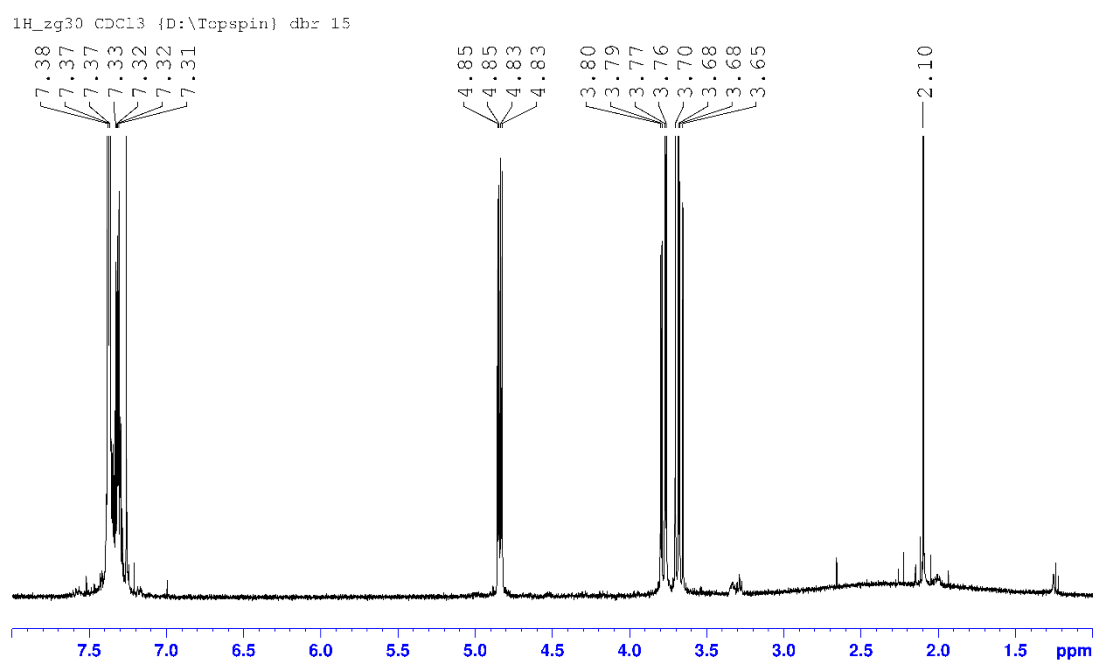
**Figure S3.** <sup>1</sup>H-NMR spectrum in deuterated chloroform at a reaction temperature of 35 °C. For reaction conditions Table 1.



**Figure S4.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 40 °C. For reaction conditions Table 1.

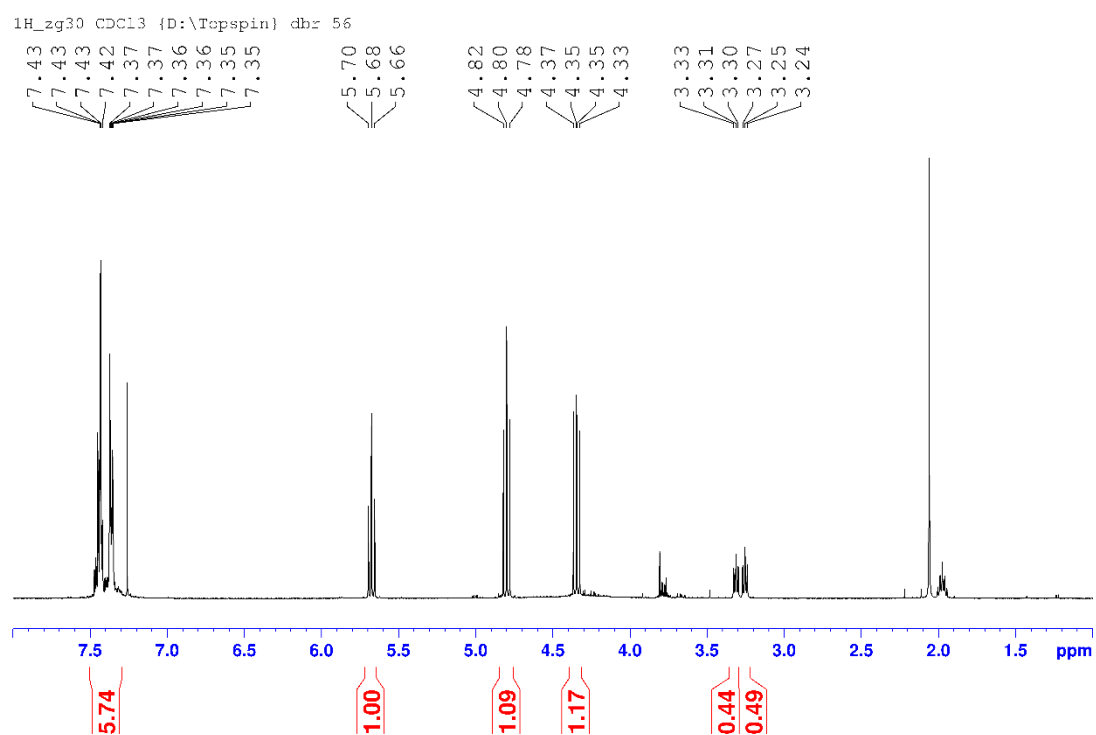


**Figure S5.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 45 °C. For reaction conditions Table 1.

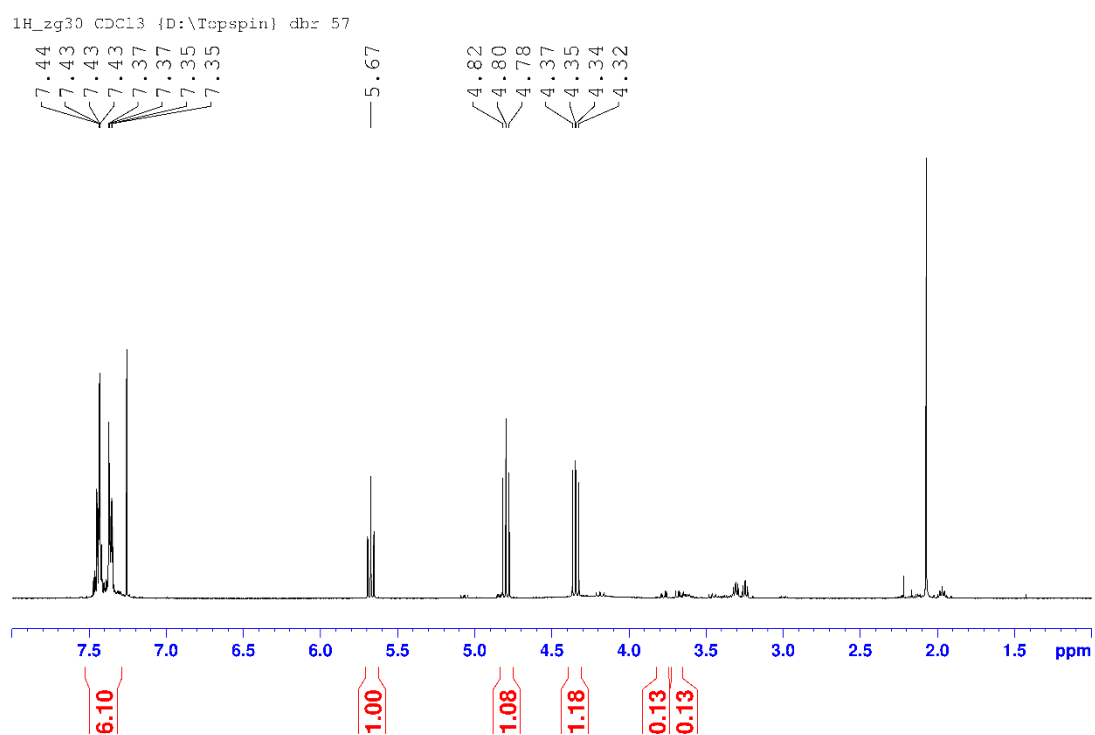


**Figure S6.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 40 °C. For reaction conditions Table 1.

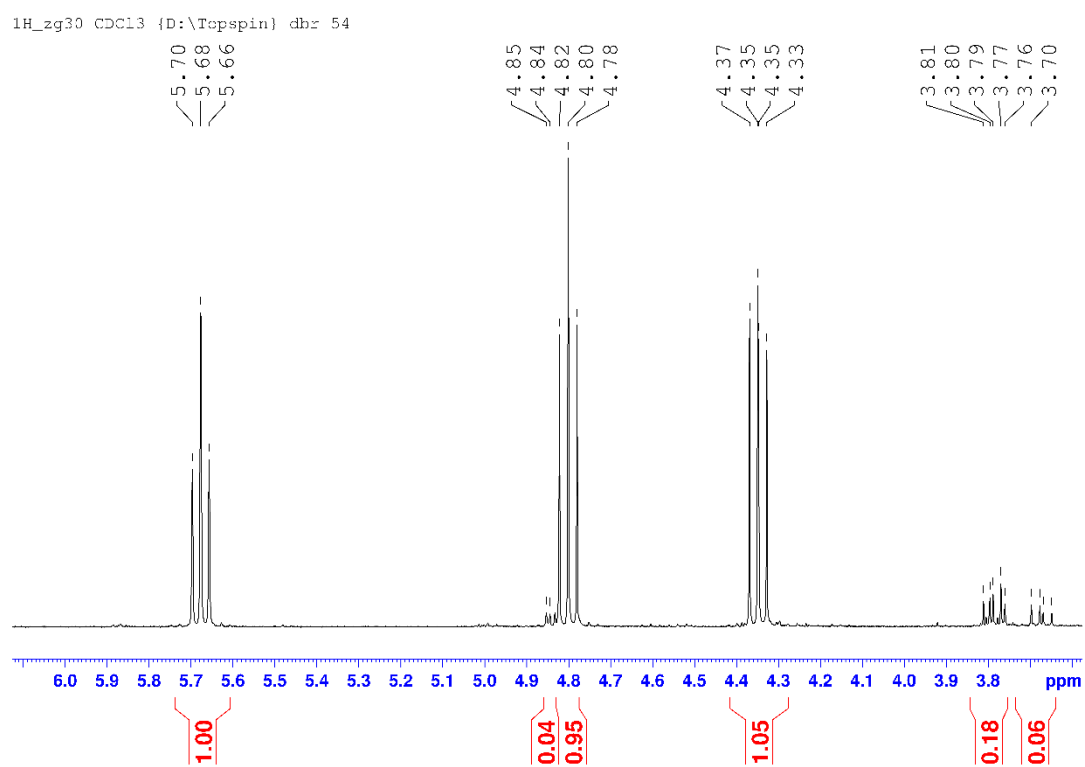




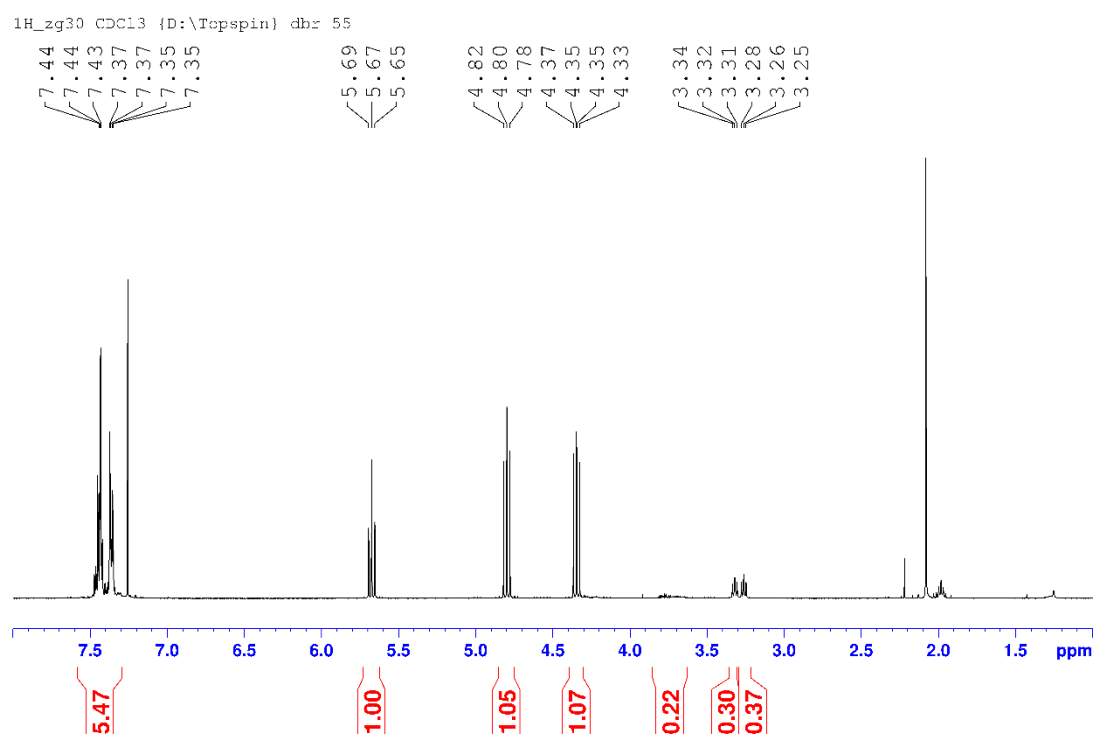
**Figure S7.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 40 °C. For reaction conditions Table 1.



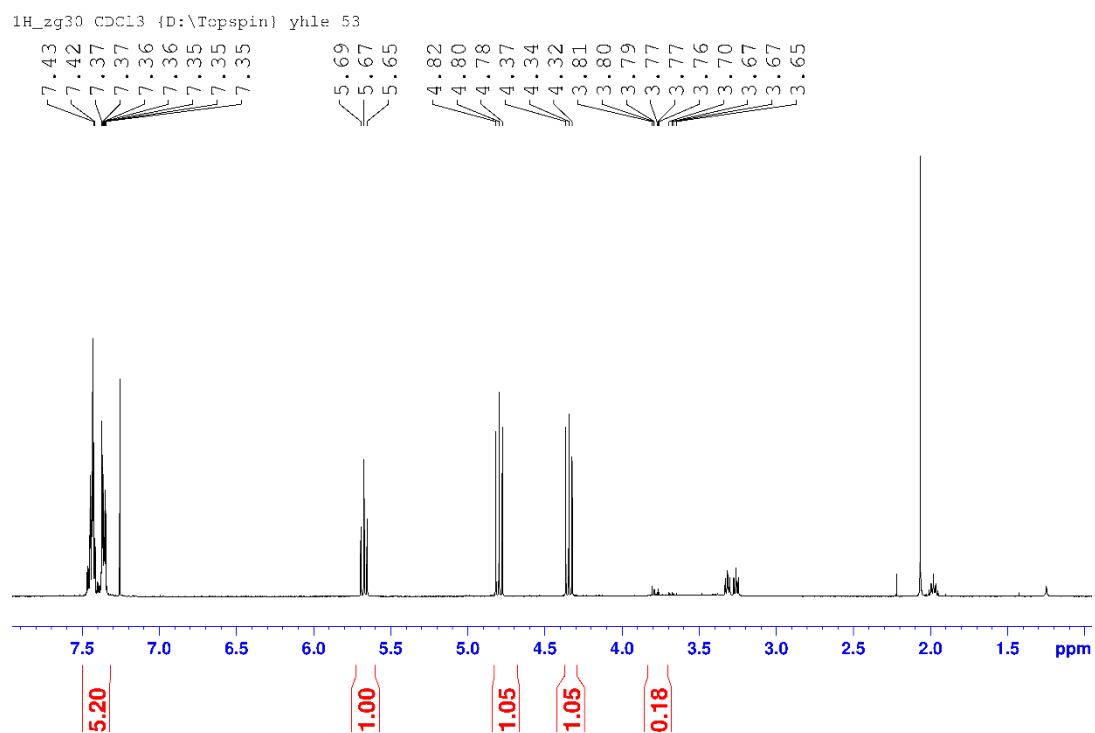
**Figure S8.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 45 °C. For reaction conditions Table 1.



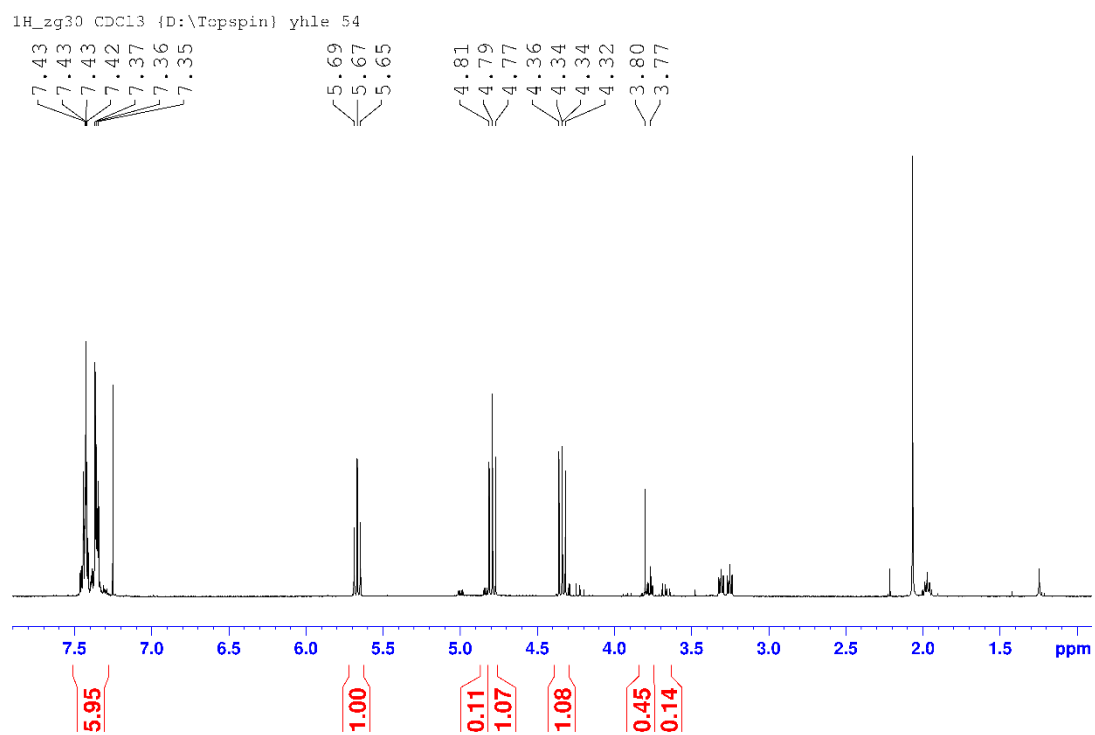
**Figure S9.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 35 °C. For reaction conditions Table 1.



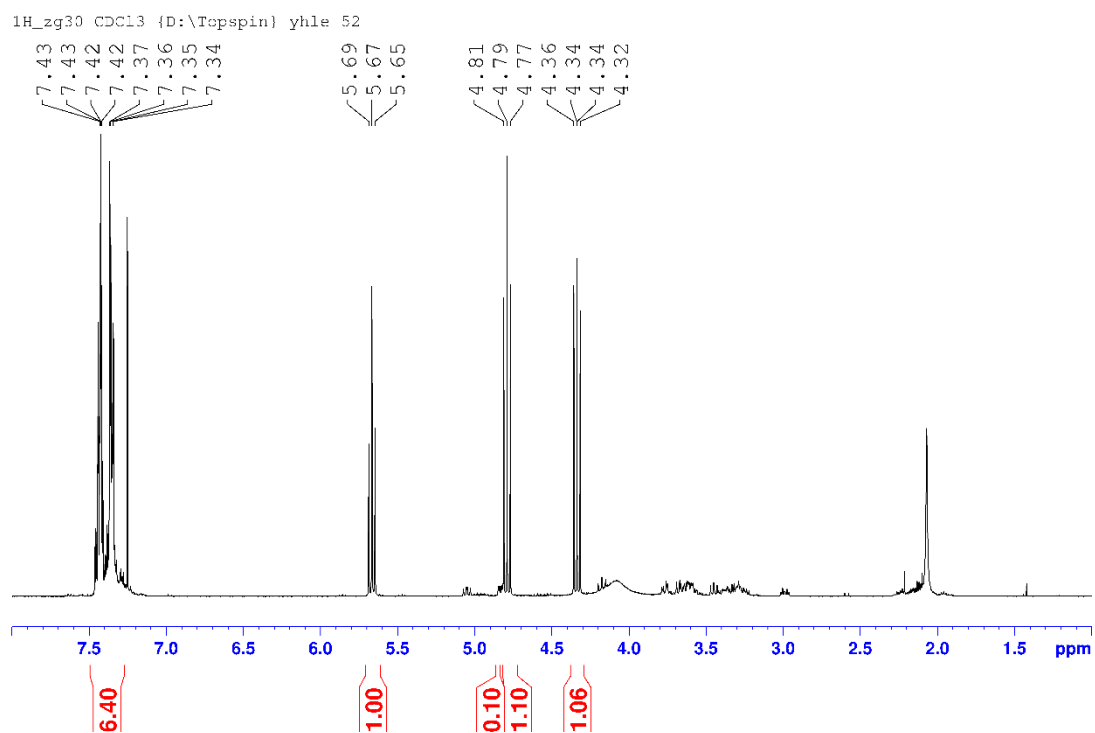
**Figure S10.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 50  $^{\circ}\text{C}$ . For reaction conditions Table 1.



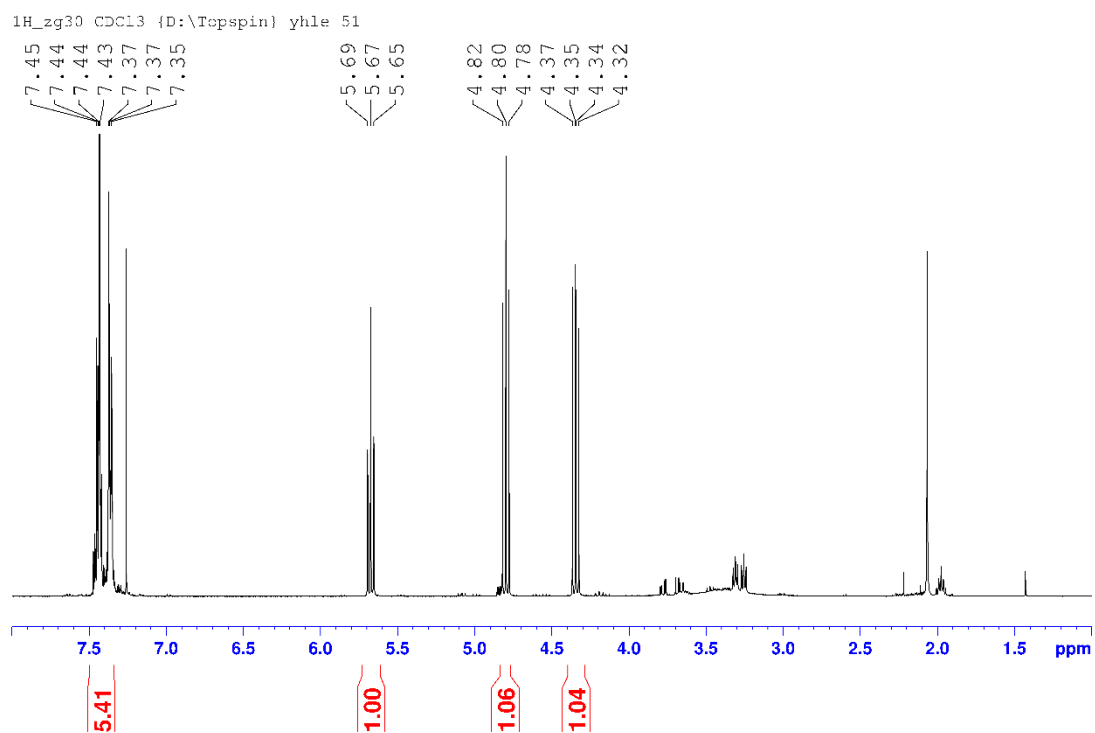
**Figure S11.** H-NMR spectrum in deuterated chloroform at a reaction temperature of 10 °C. For reaction conditions see Table 1.



**Figure S12.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 20  $^\circ\text{C}$ . For reaction conditions Table 1.

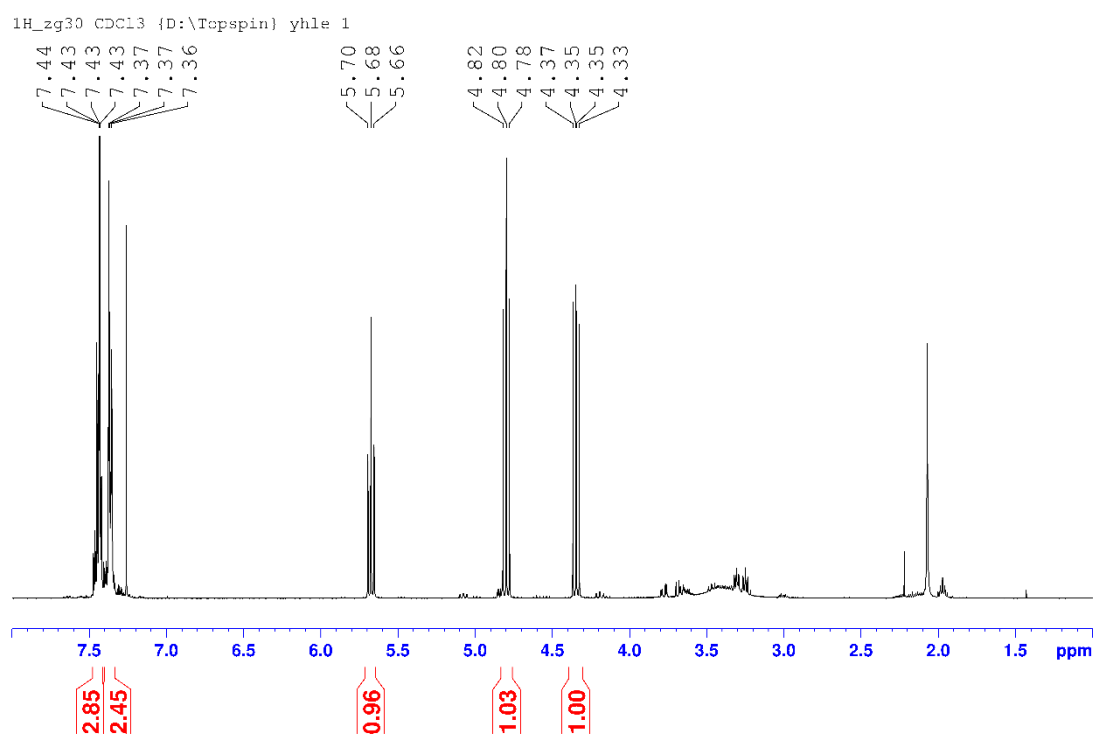


**Figure S13.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 55 °C. For reaction conditions see Table 1.

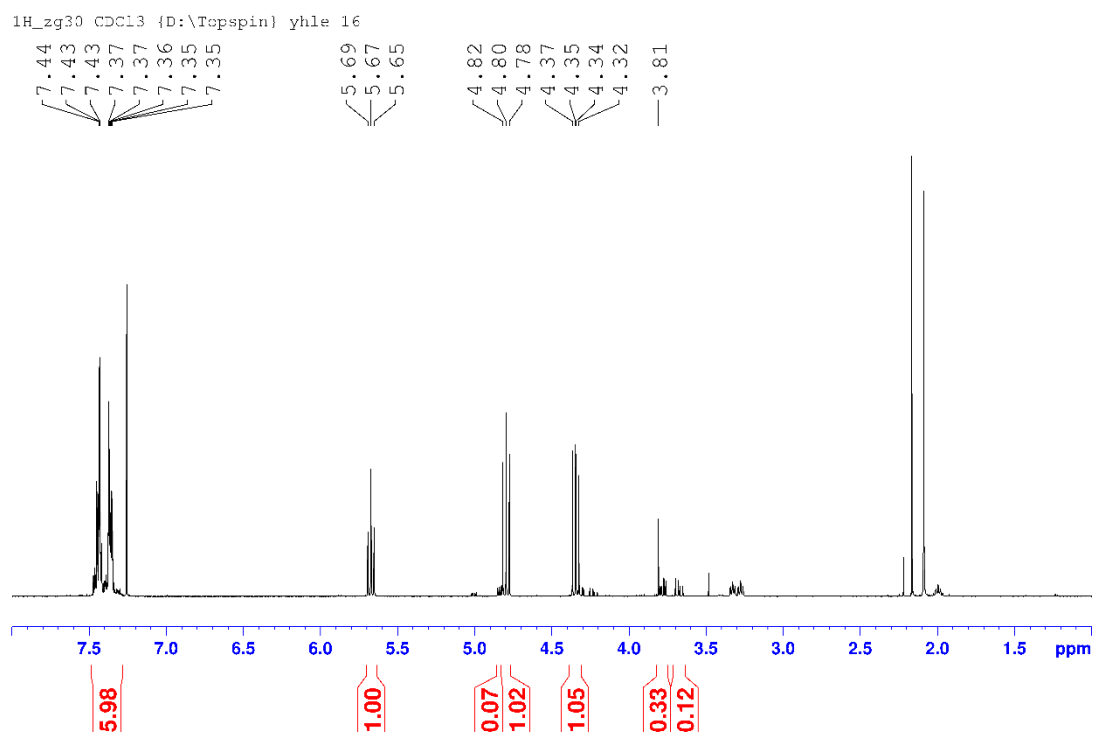


**Figure S14.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 60  $^\circ\text{C}$ . For reaction conditions Table 1.

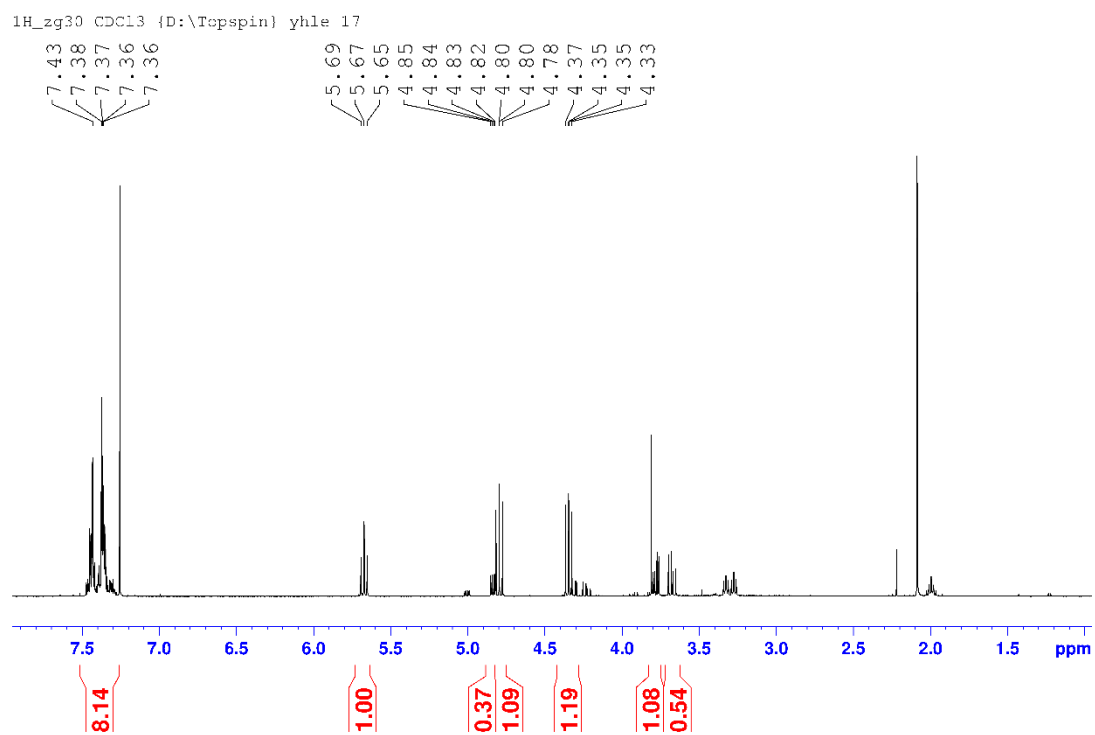




**Figure S15.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 65 °C. For reaction conditions Table 1.

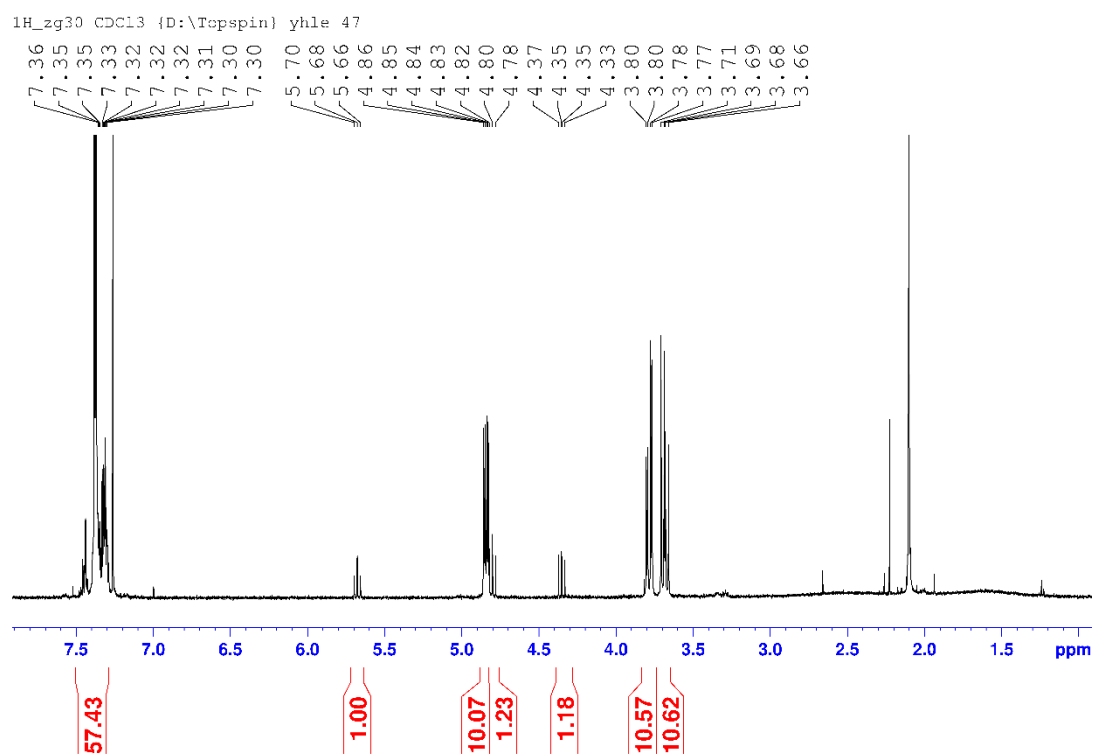


**Figure S16:**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 0 °C. For reaction conditions Table 1.



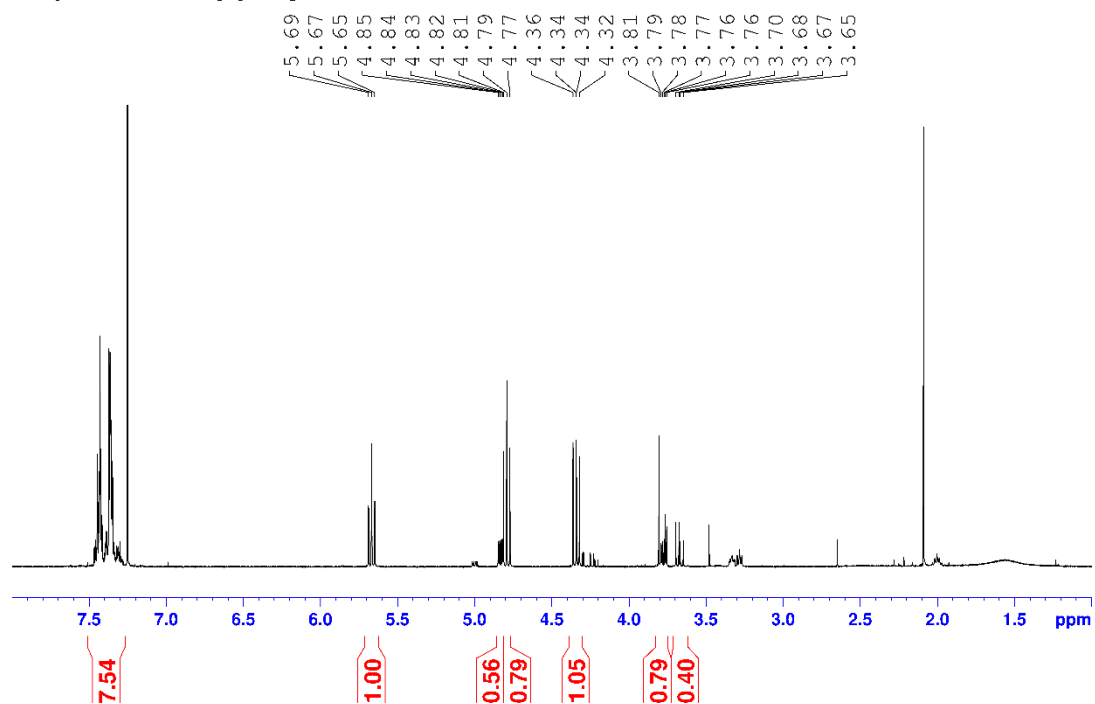
**Figure S17.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of  $-5\text{ }^\circ\text{C}$ . For reaction conditions Table 1.

**Dimethyl carbonate, 1.00 mol % catalyst loading**



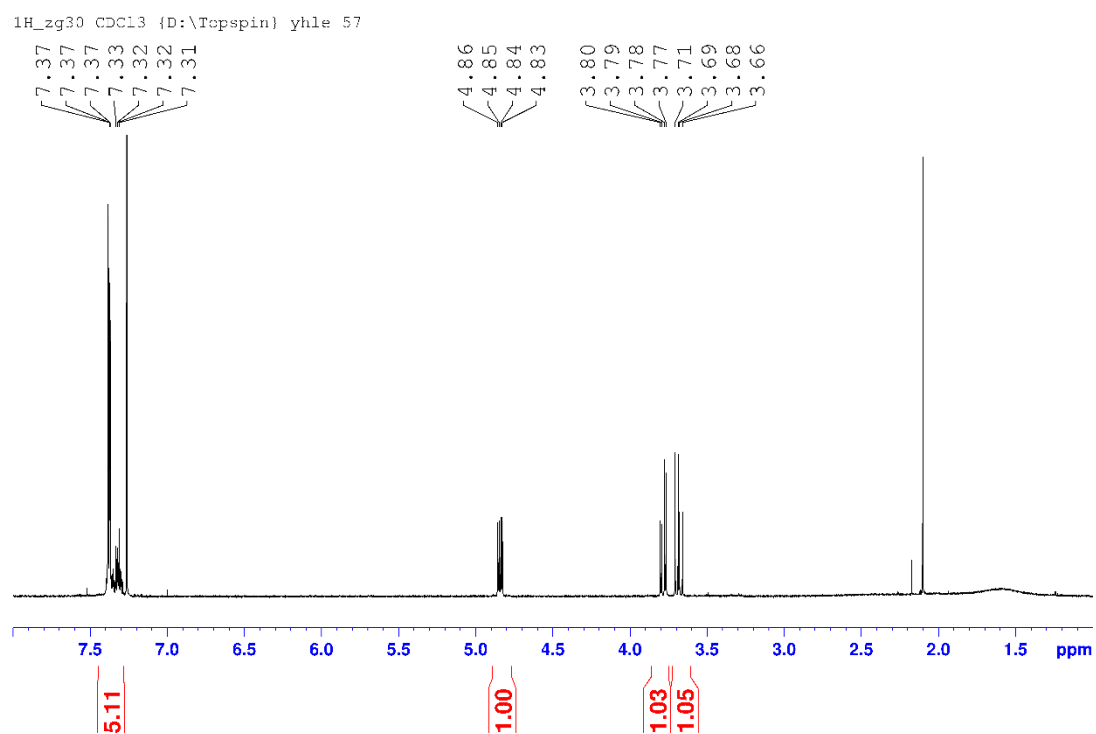
**Figure S18.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 0 °C. For reaction conditions Table 1.

1H\_zg30 CDCl3 {D:\Topspin} yhle 54

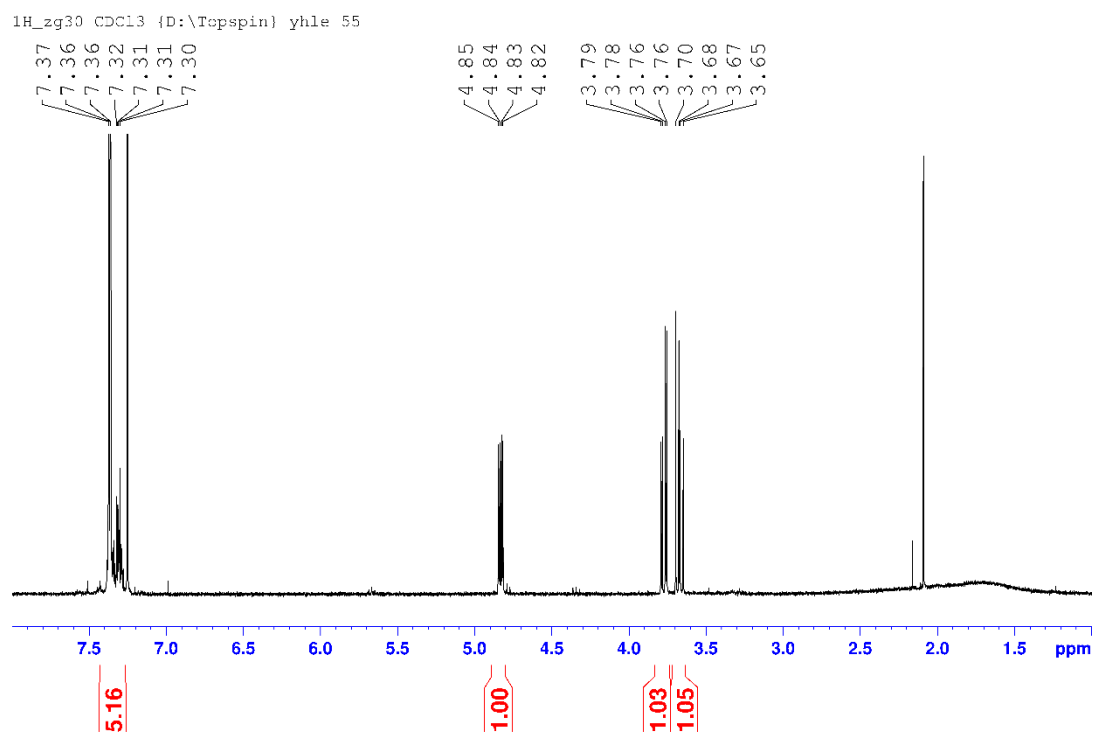


**Figure S19.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 0 °C. For reaction conditions Table 1.

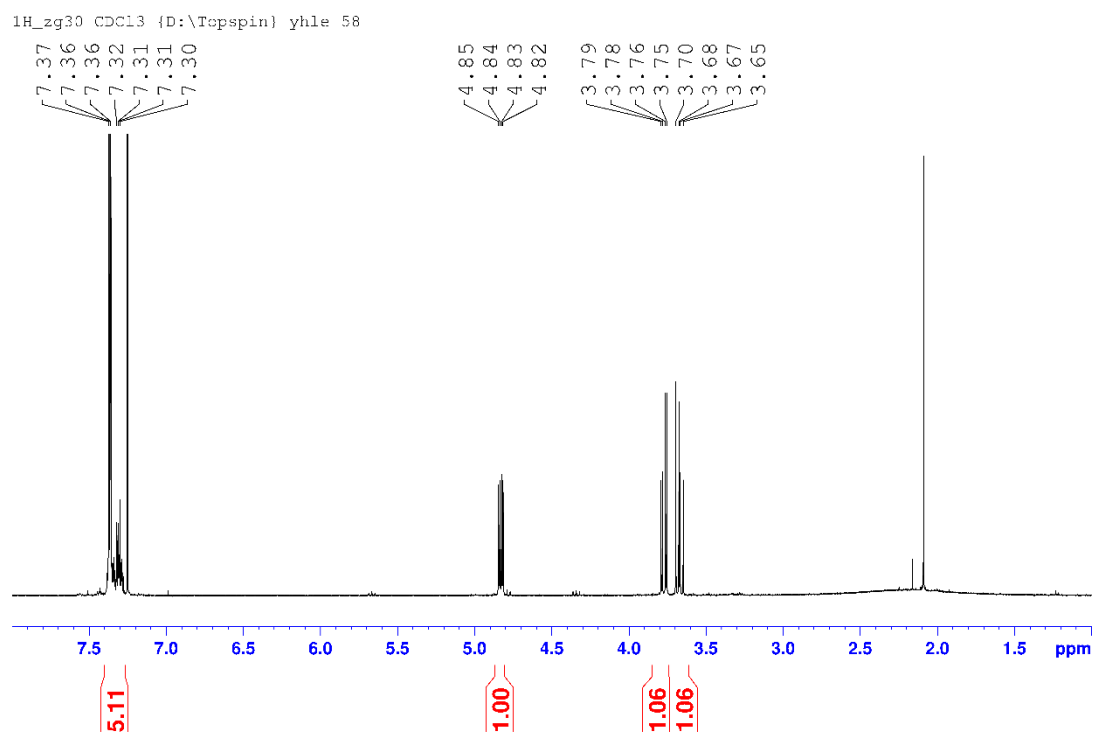
**Dimethyl carbonate, 0.80 mol % catalyst loading**



**Figure S20.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 0 °C. For reaction conditions Table 1.

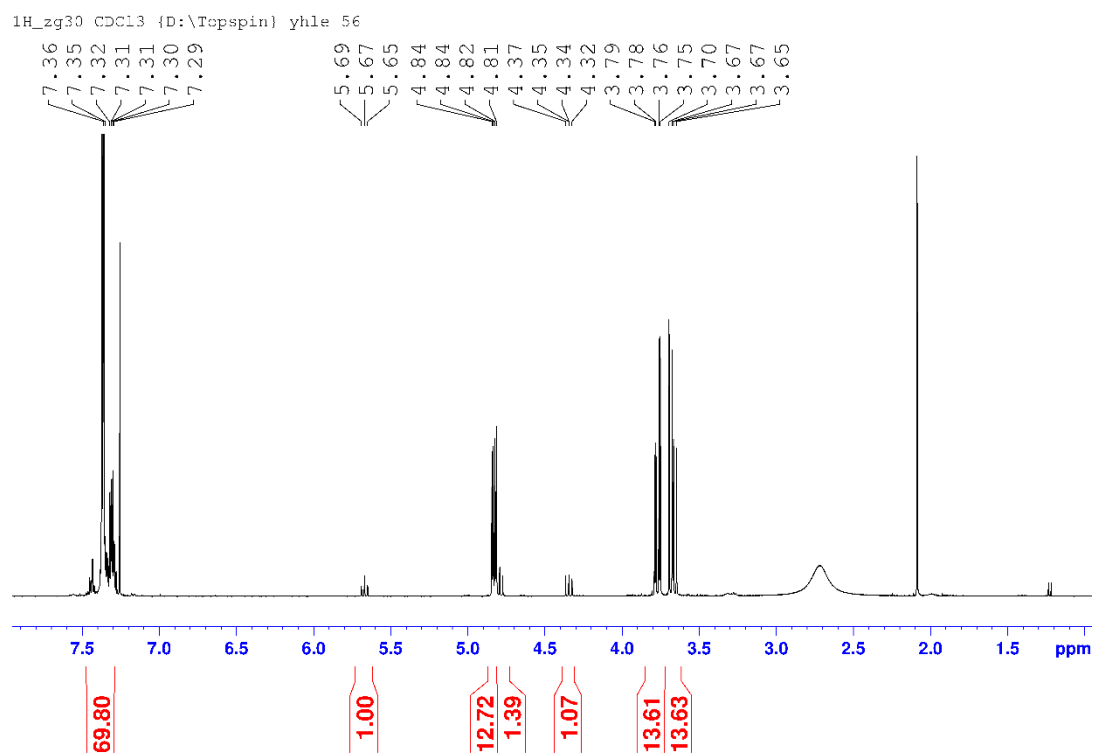


**Figure S21.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 10 °C. For reaction conditions Table 1.

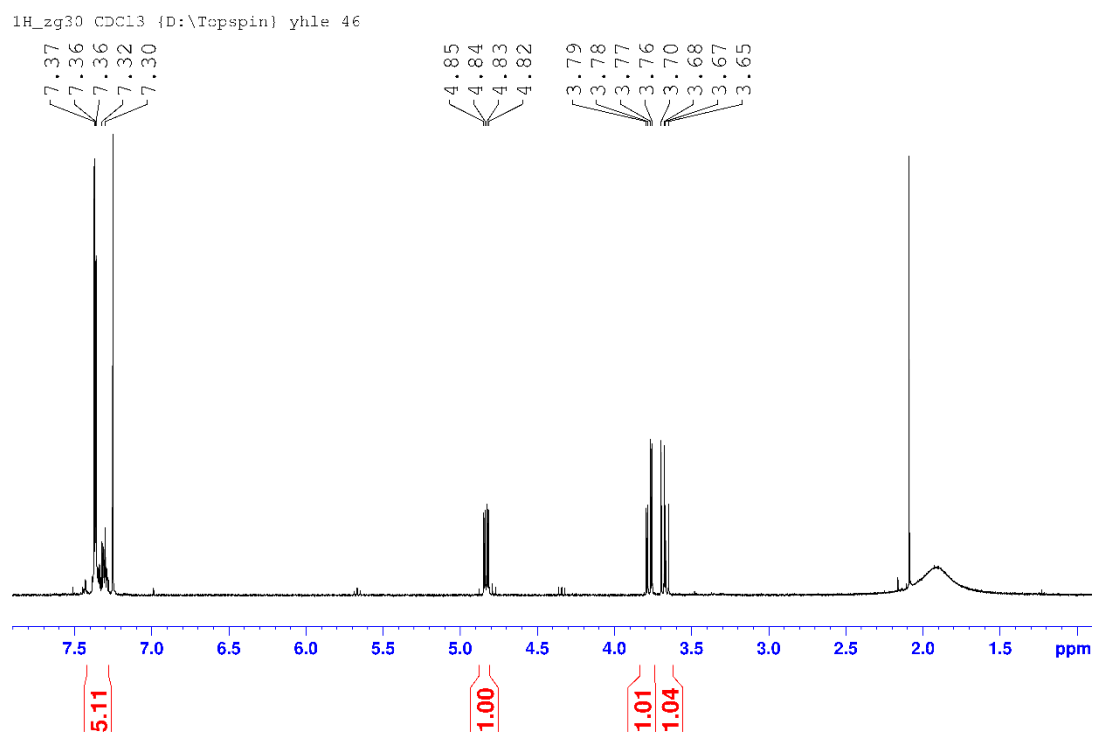


**Figure S22:**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 20 °C. For reaction conditions Table 1.

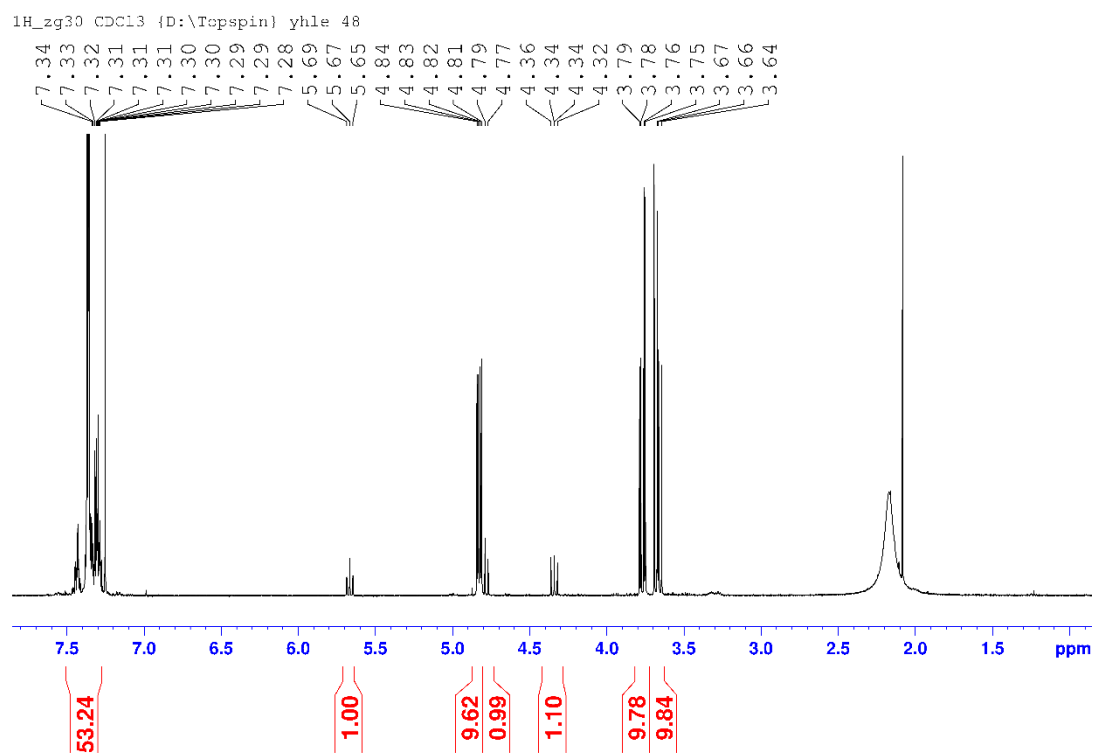




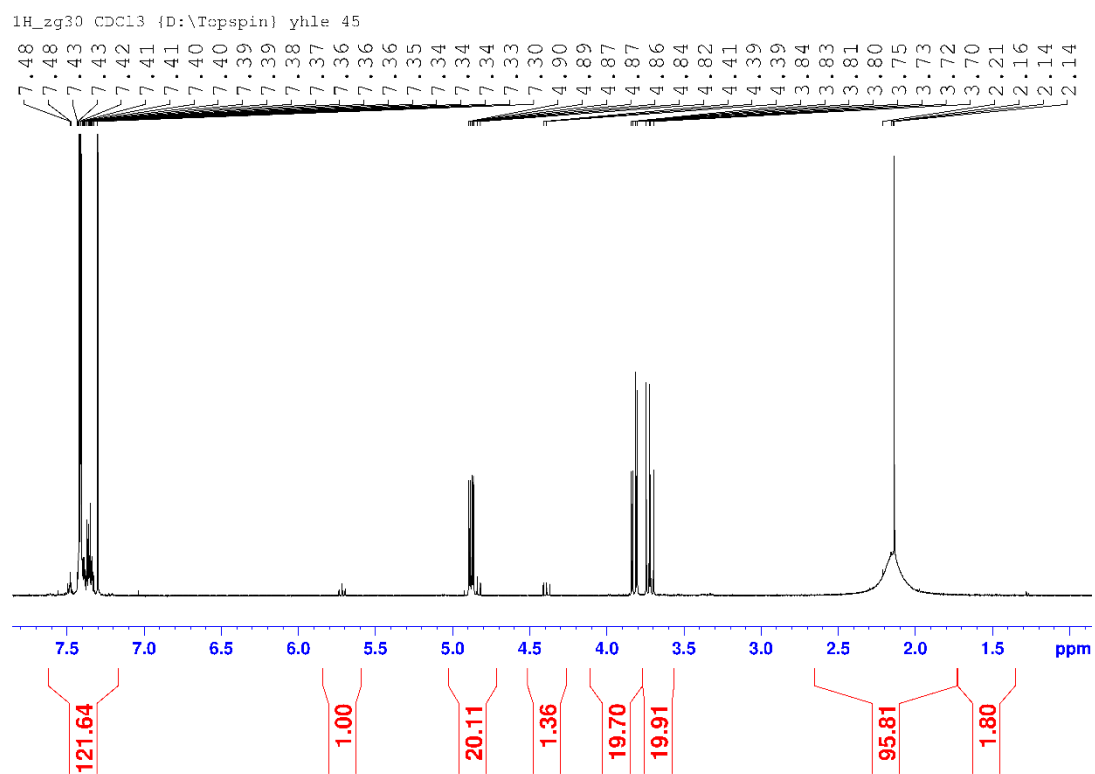
**Figure S23.** <sup>1</sup>H-NMR spectrum in deuterated chloroform at a reaction temperature of 30 °C. For reaction conditions Table 1.



**Figure S24.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 40 °C. For reaction conditions Table 1.

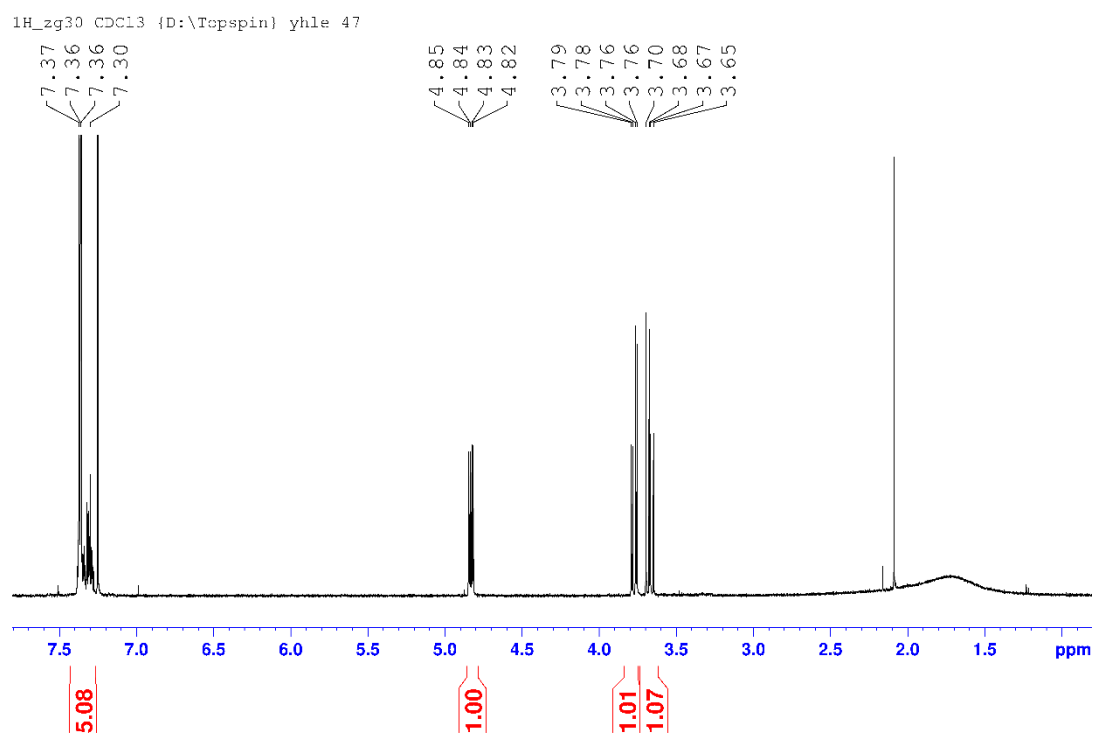


**Figure S25.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 50  $^\circ\text{C}$ . For reaction conditions Table 1.

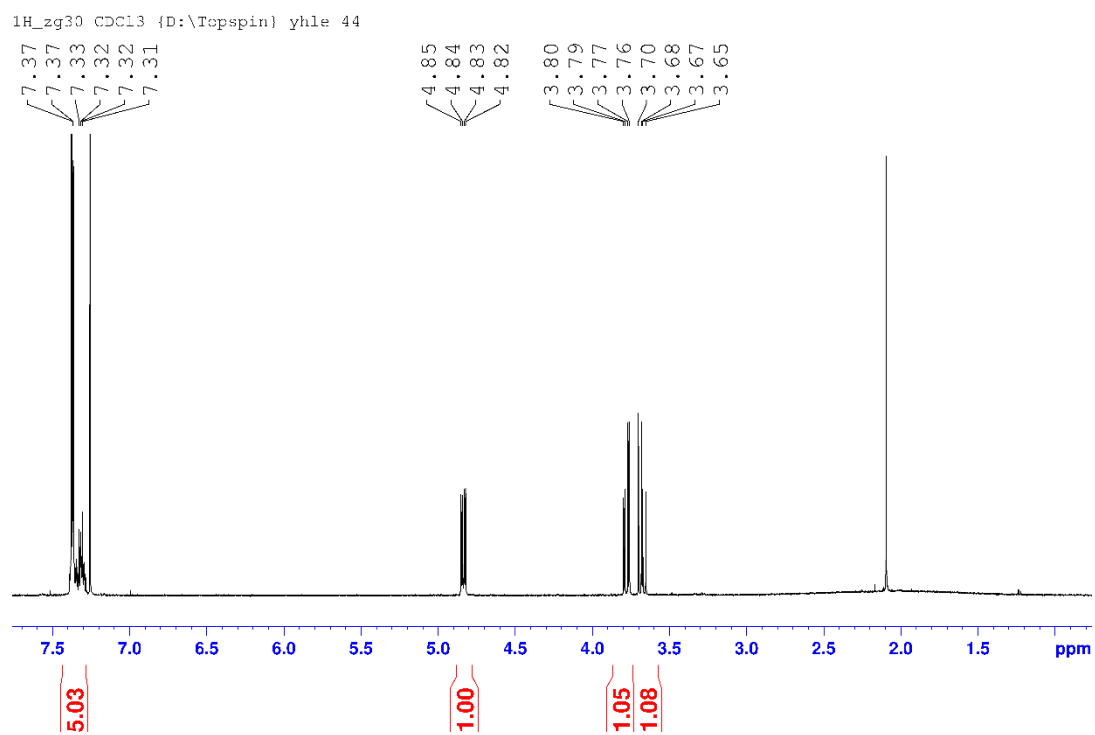


**Figure S26.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 60 °C. For reaction conditions Table 1.

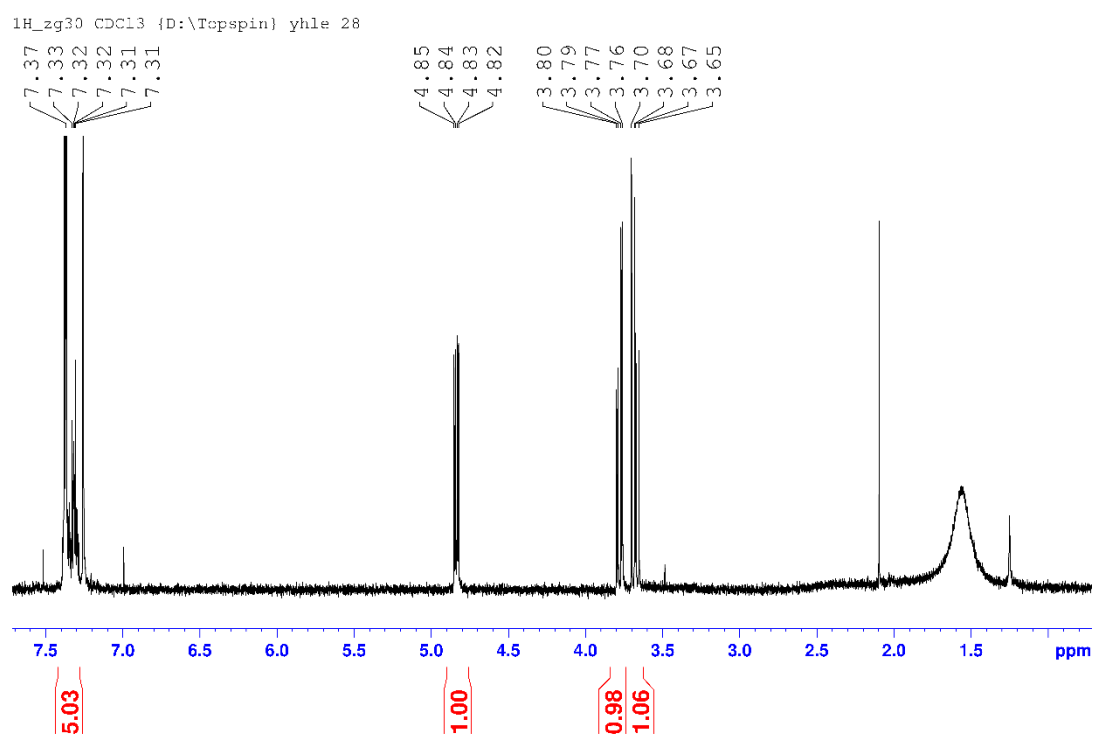
**Dimethyl carbonate, 0.60 mol % catalyst loading**



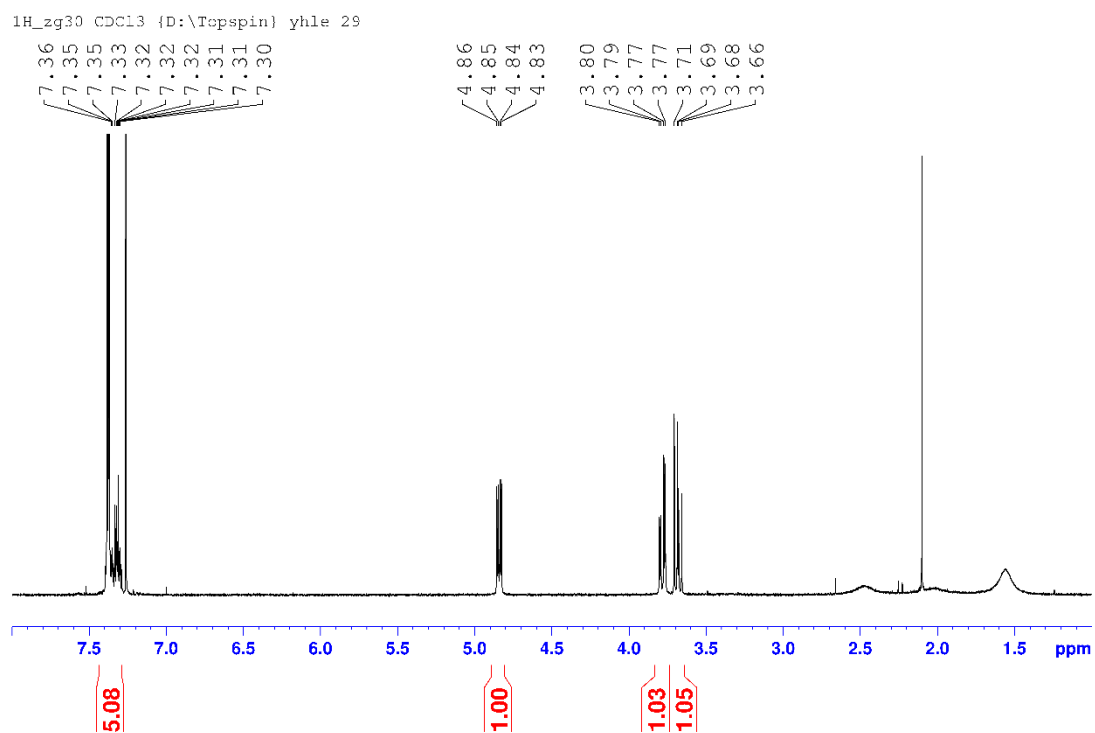
**Figure S27.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 30 °C. For reaction conditions see Table 1.



**Figure S28.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 20 °C. For reaction conditions Table 1.

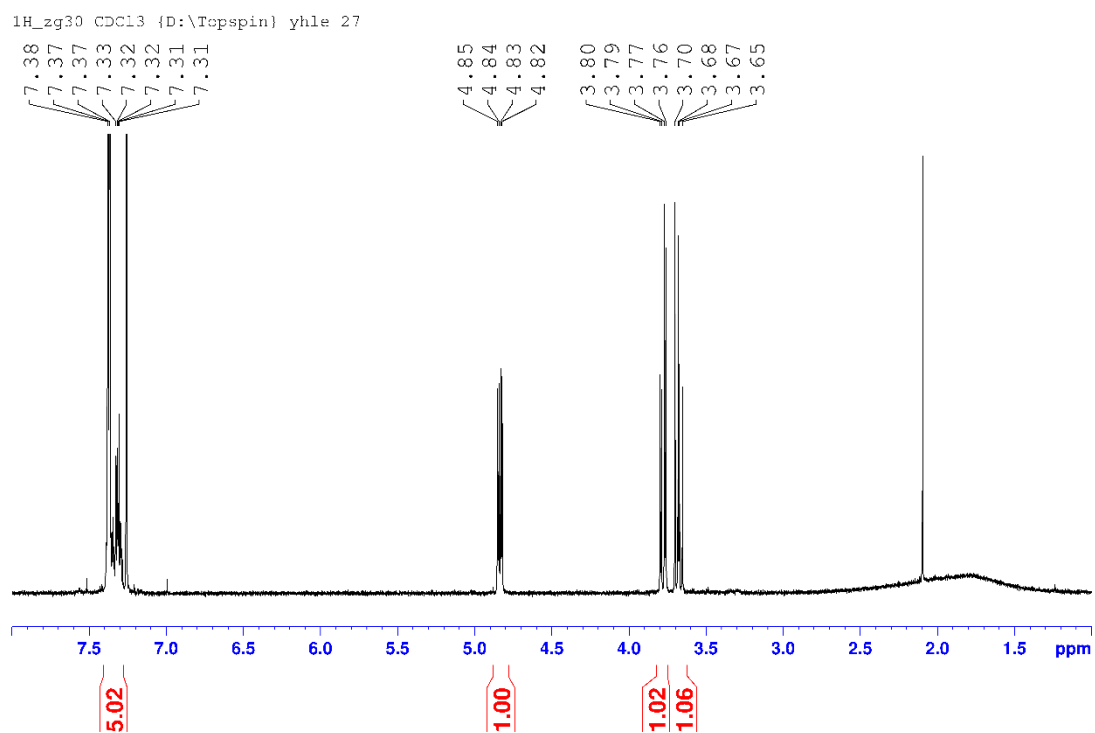


**Figure S29.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 0 °C. For reaction conditions Table 1.

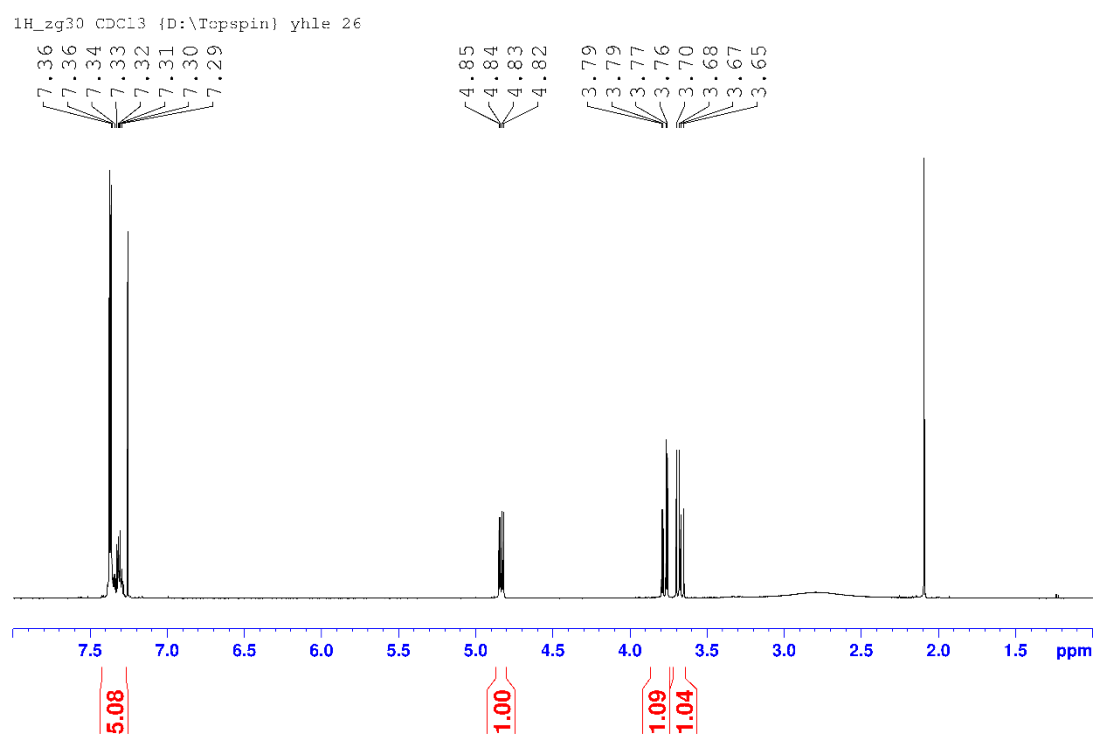


**Figure S30.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 10 °C. For reaction conditions Table 1.

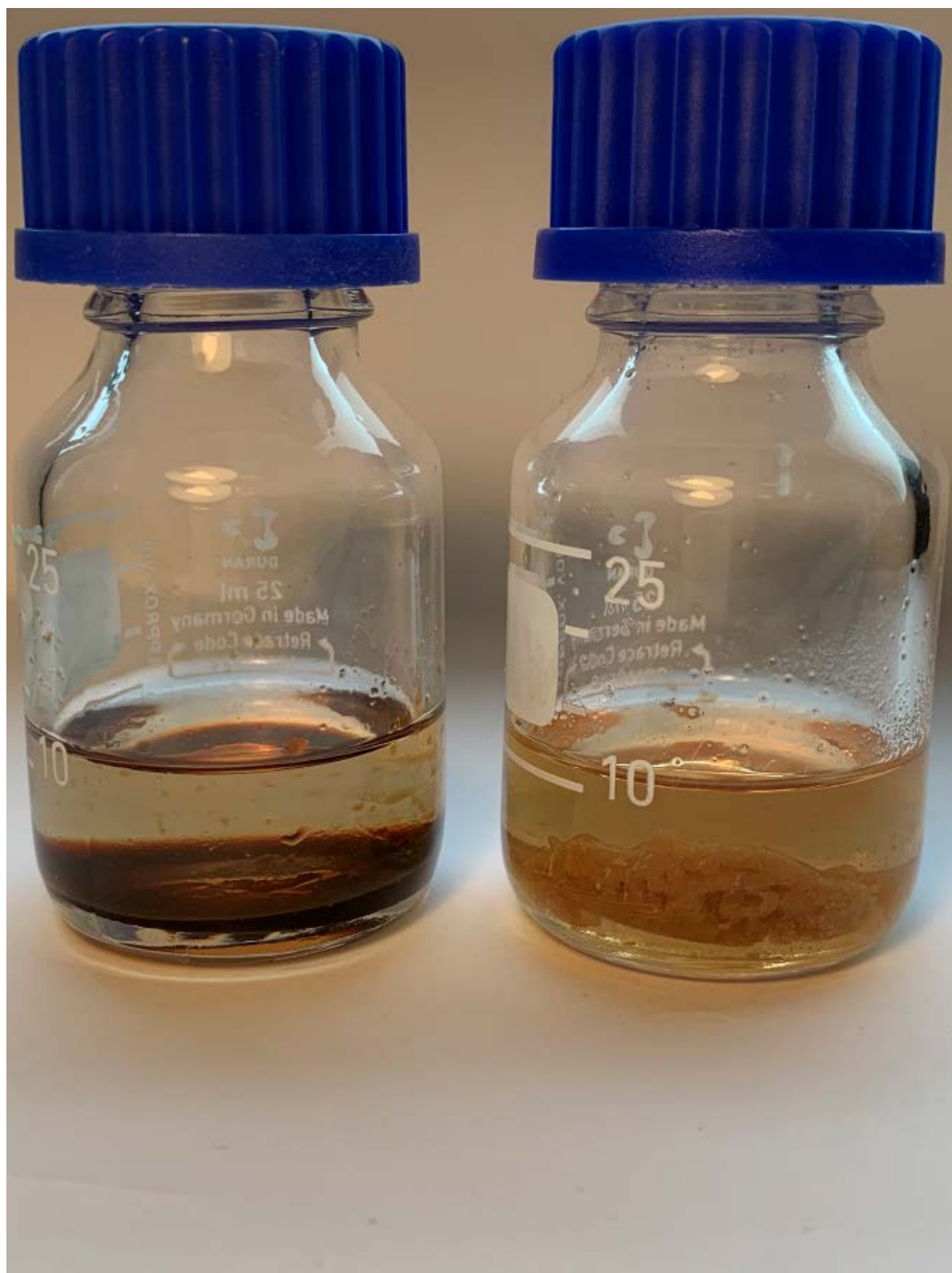




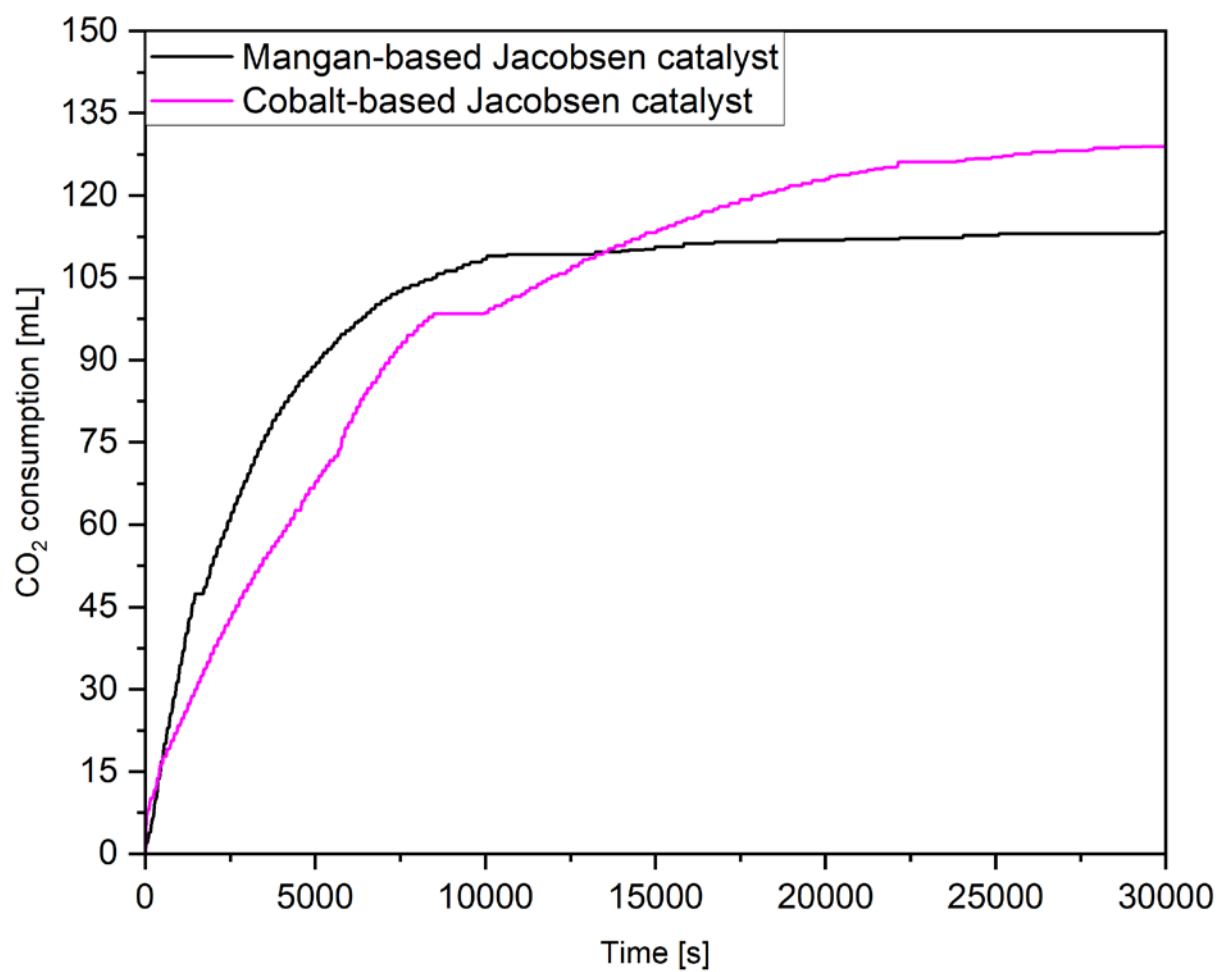
**Figure S31.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 40 °C. For reaction conditions Table 1.



**Figure S32.**  $^1\text{H}$ -NMR spectrum in deuterated chloroform at a reaction temperature of 50 °C. For reaction conditions Table 1.



**Figure S33.** Reaction product for experiment (left) 120°C, 15 bar with a cyclic product and product (right) 130°C, 15 bar with formation of polymer.



**Figure S34.** Comparison of the CO<sub>2</sub> consumption of cobalt-based Jacobsen catalyst (JCC) and mangan-based Jacobsen catalyst (JCM).