

Hydrogenation of the Liquid Organic Hydrogen Carrier Compound Dibenzyltoluene – Reaction Pathway Determination by ^1H -NMR Spectroscopy

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Supporting Information

Predicted Data

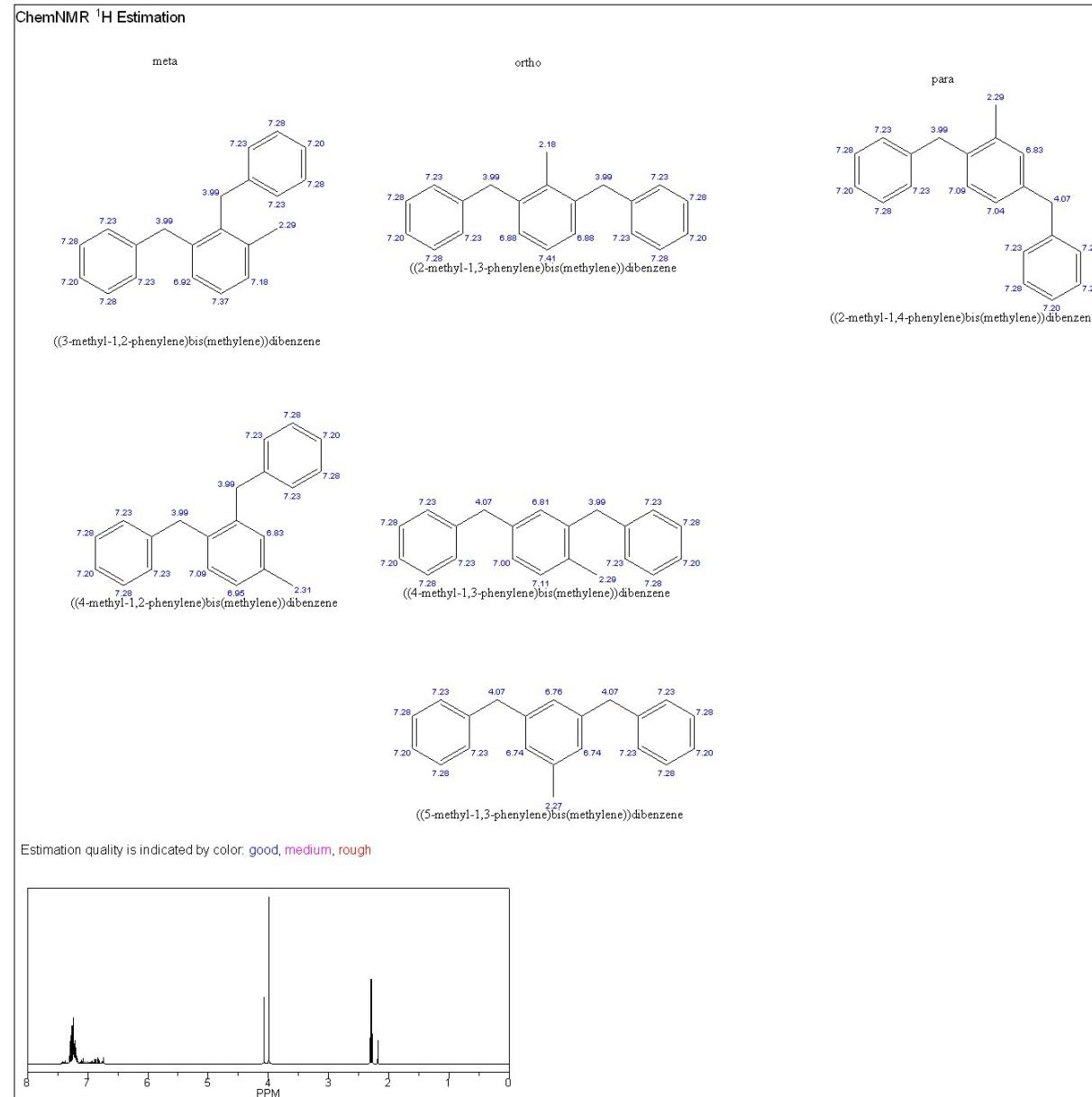
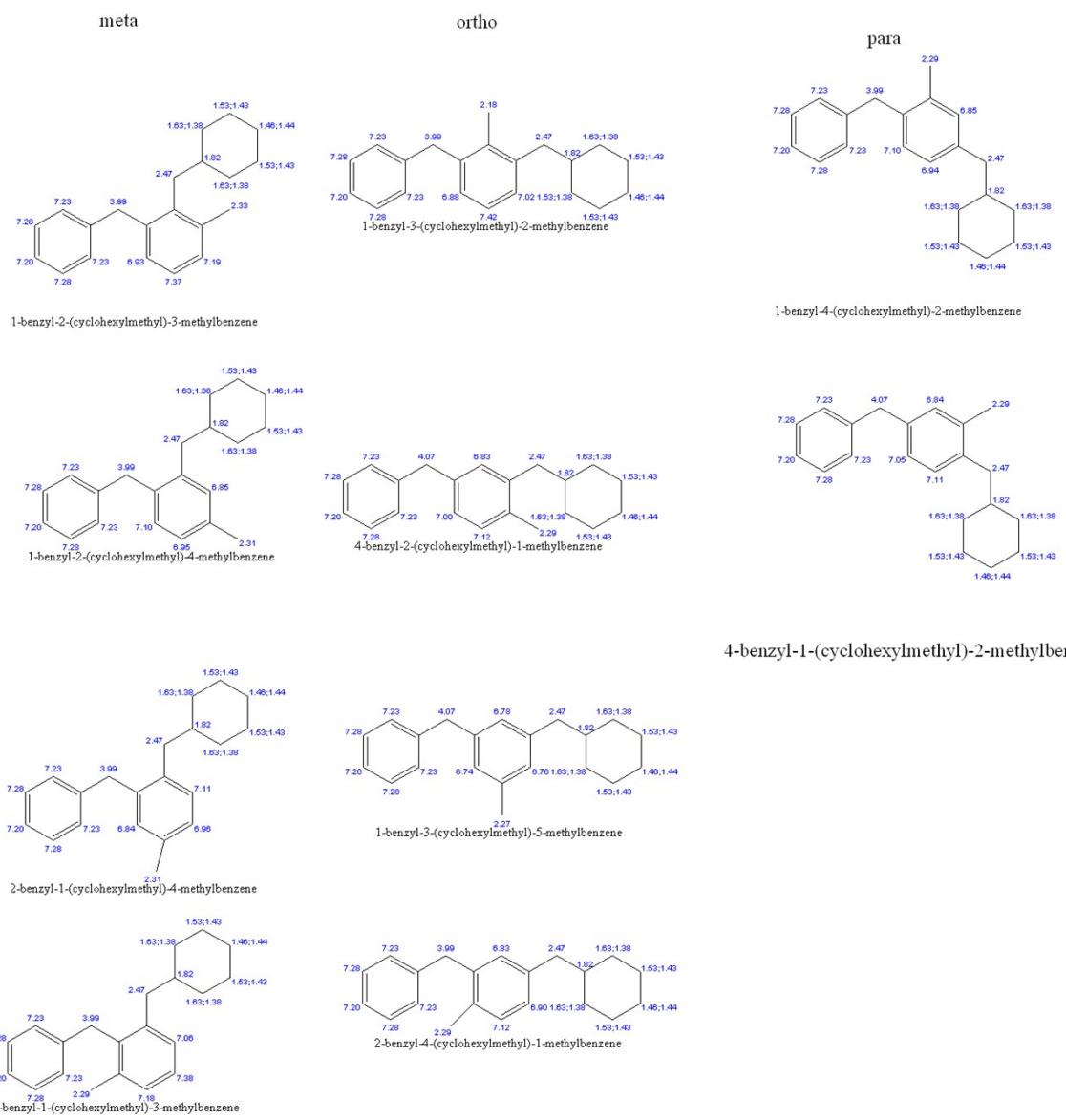


Figure S 1: All H0-DBT₀₀₀ structural isomers with respective predicted chemical shifts of ^1H NMR (combined in spectrum)

ChemNMR ^1H Estimation



Estimation quality is indicated by color: good, medium, rough

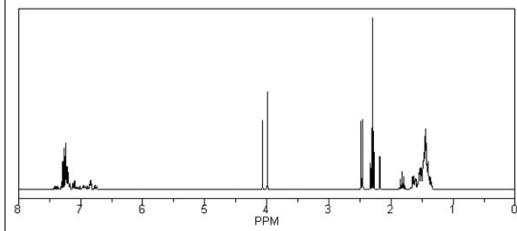
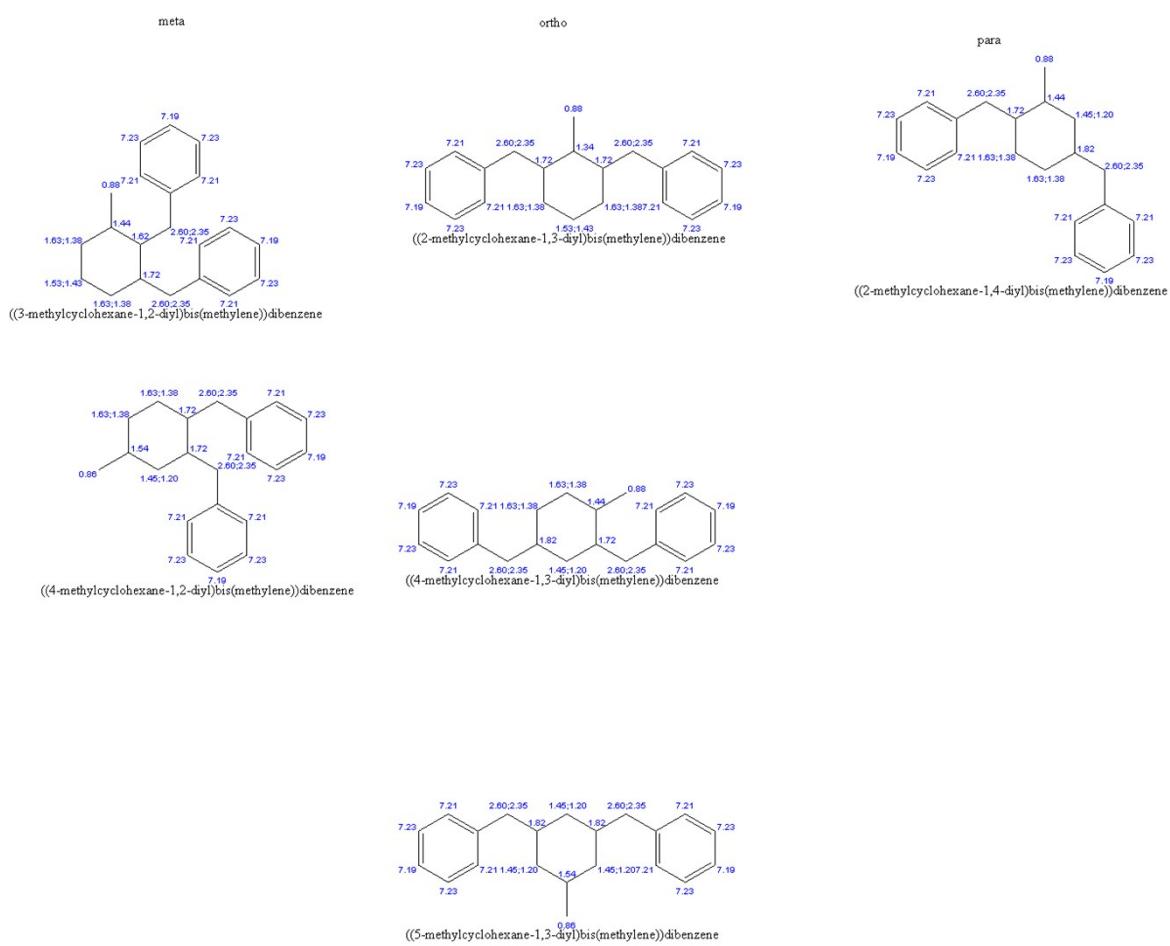


Figure S 2: All H6-DBT_{OO} structural isomers with respective predicted chemical shifts of ¹H NMR (combined in spectrum)

ChemNMR ^1H Estimation



Estimation quality is indicated by color: [good](#), [medium](#), [rough](#)

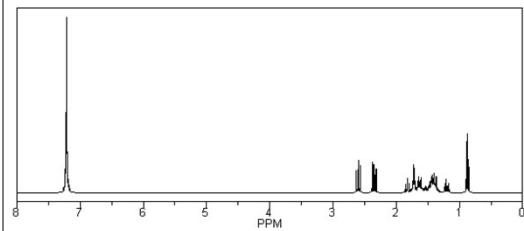
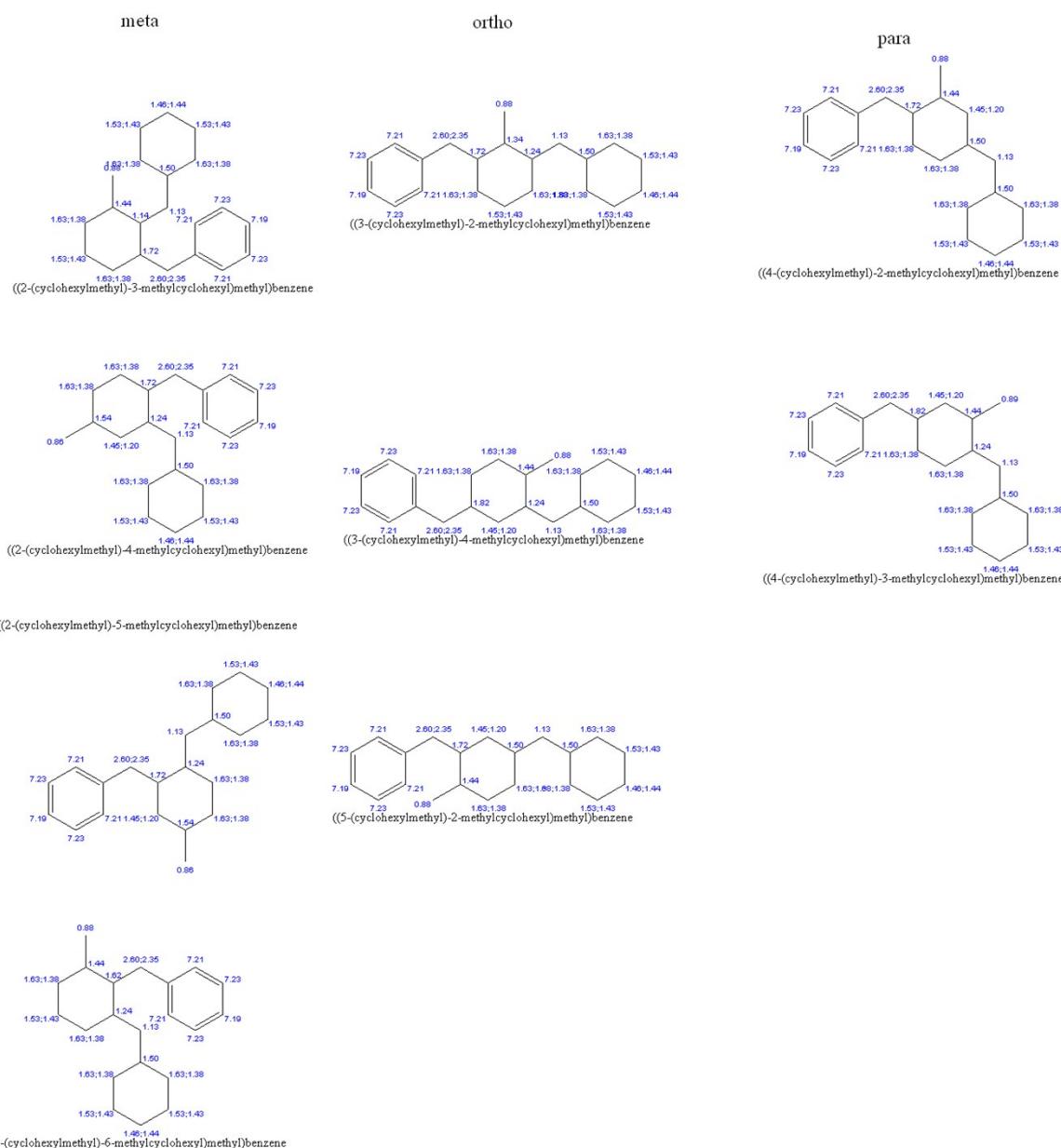


Figure S 3: All H₆-DBT_{OXO} structural isomers with respective predicted chemical shifts of ^1H NMR (combined in spectrum)

ChemNMR ^1H Estimation



Estimation quality is indicated by color: good, medium, rough

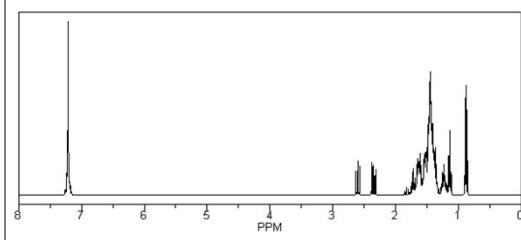


Figure S 4: All H12-DBT_{Ox} structural isomers with respective predicted chemical shifts of ¹H NMR (combined in spectrum)

ChemNMR ^1H Estimation

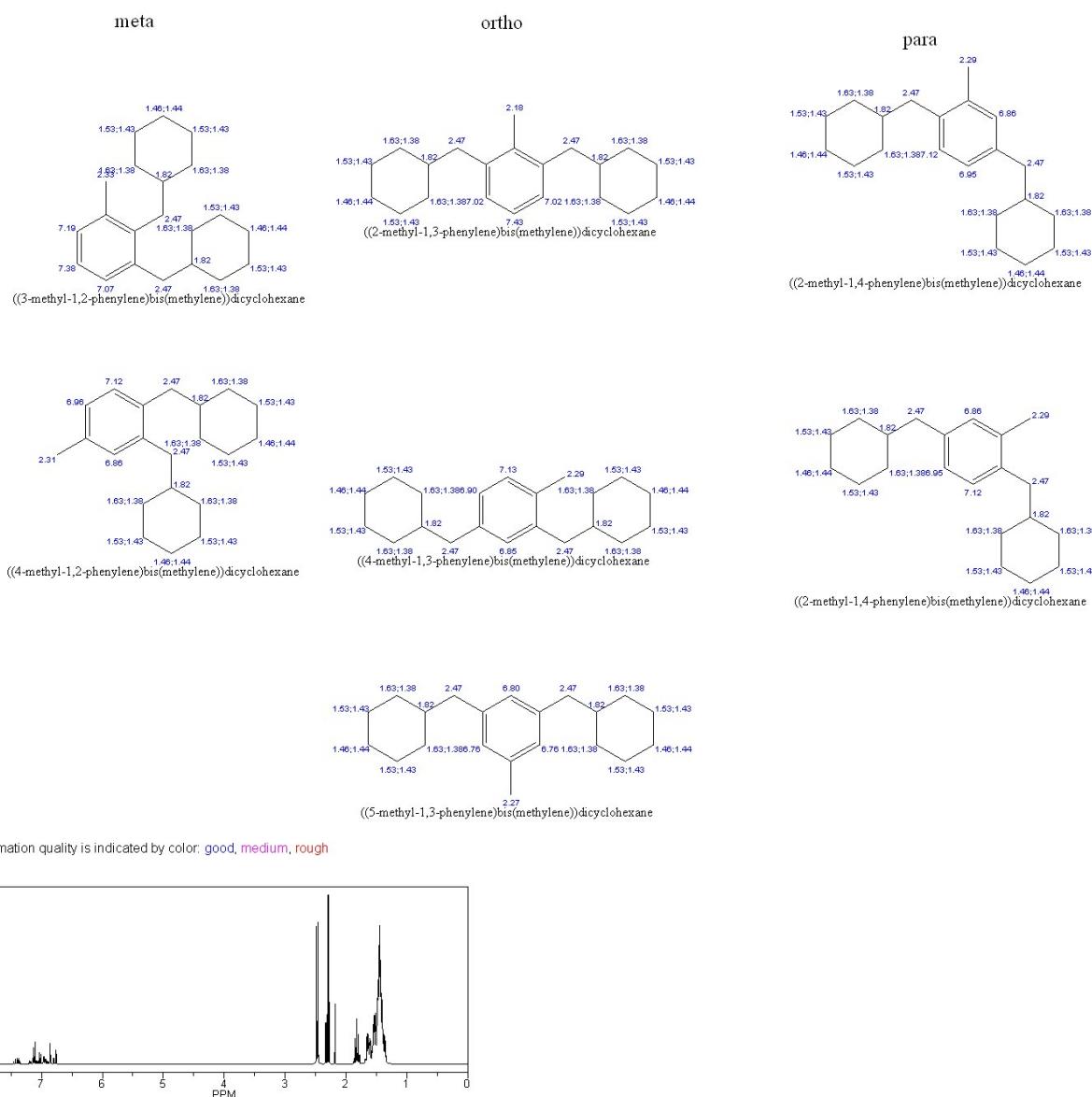


Figure S 5: All H12-DBT_{XOX} structural isomers with respective predicted chemical shifts of ^1H NMR (combined in spectrum)

ChemNMR ^1H Estimation

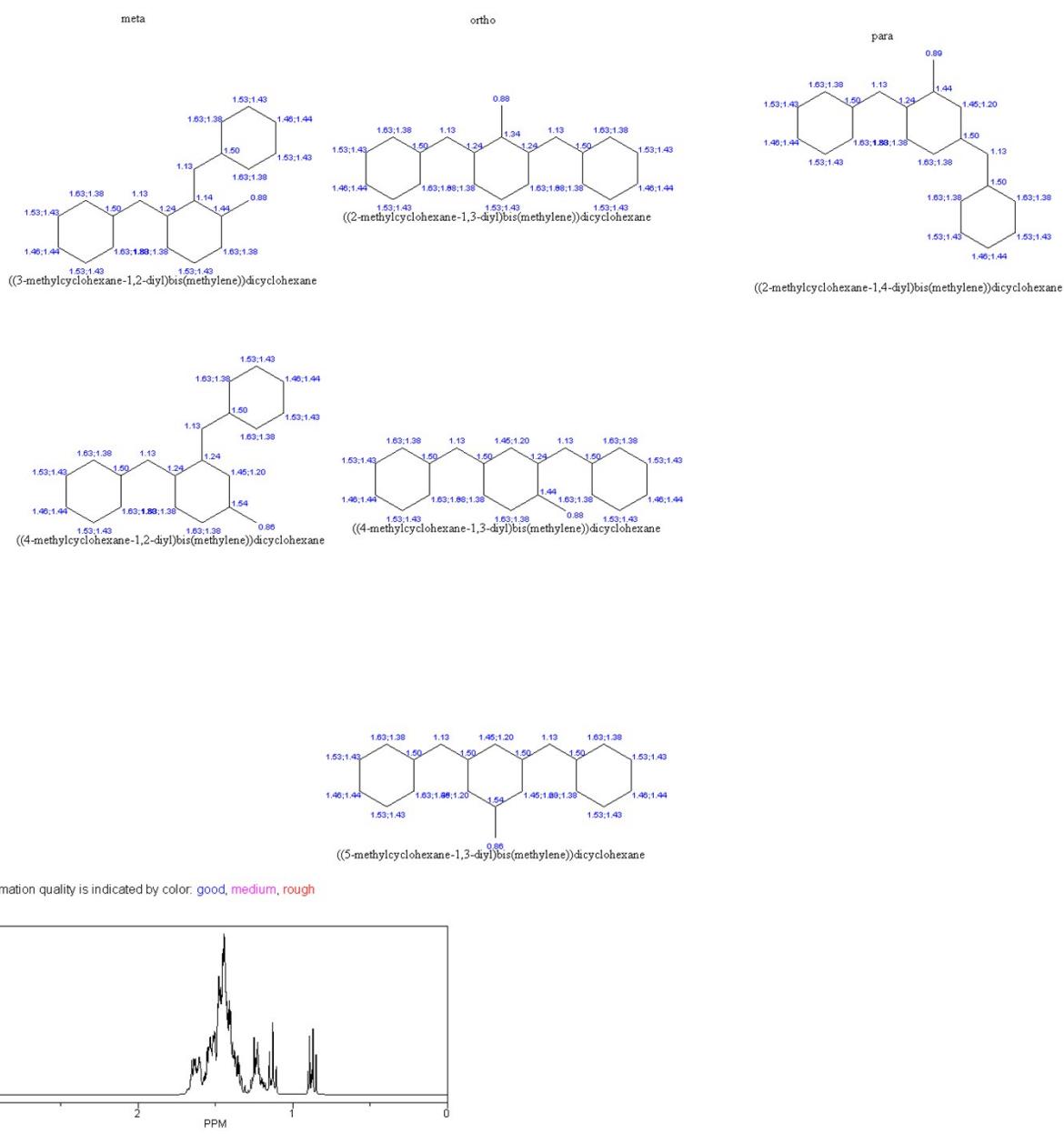


Figure S 6: All H12-DBT_{XXX} structural isomers with respective predicted chemical shifts of ^1H NMR (combined in spectrum)

Experimental Data

T = 120 °C ; P = 50 bar

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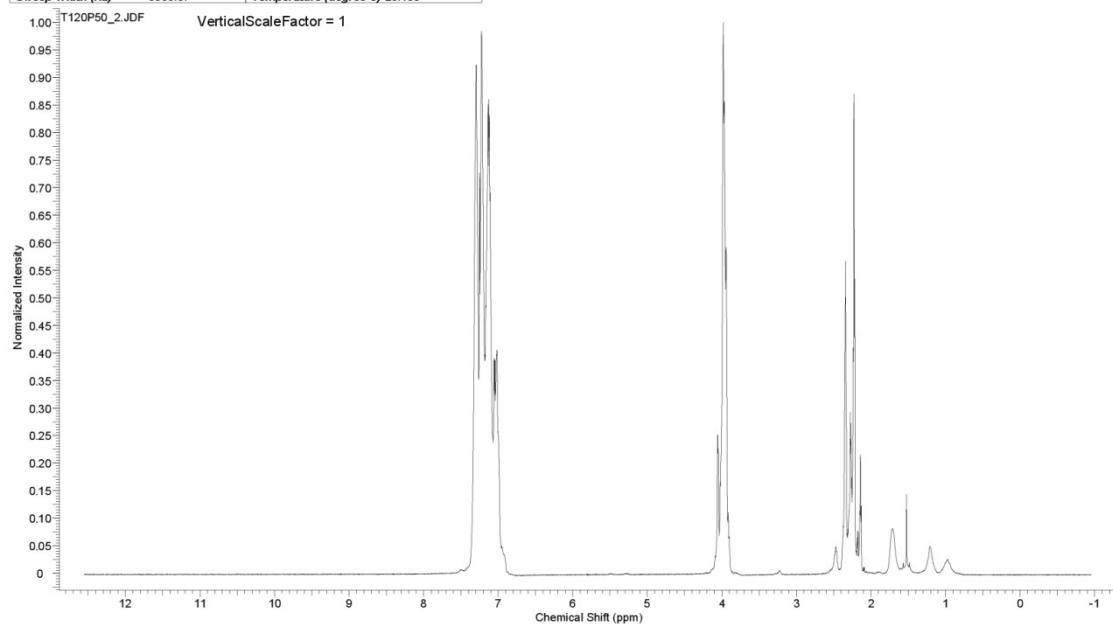


Figure S 7: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 2 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/Al₂O₃; m[H0-DBT] = 150 g; n_{Ru}/n_{Al₂O₃} = 0.25 mol%)

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03.01.2016 20:41:21

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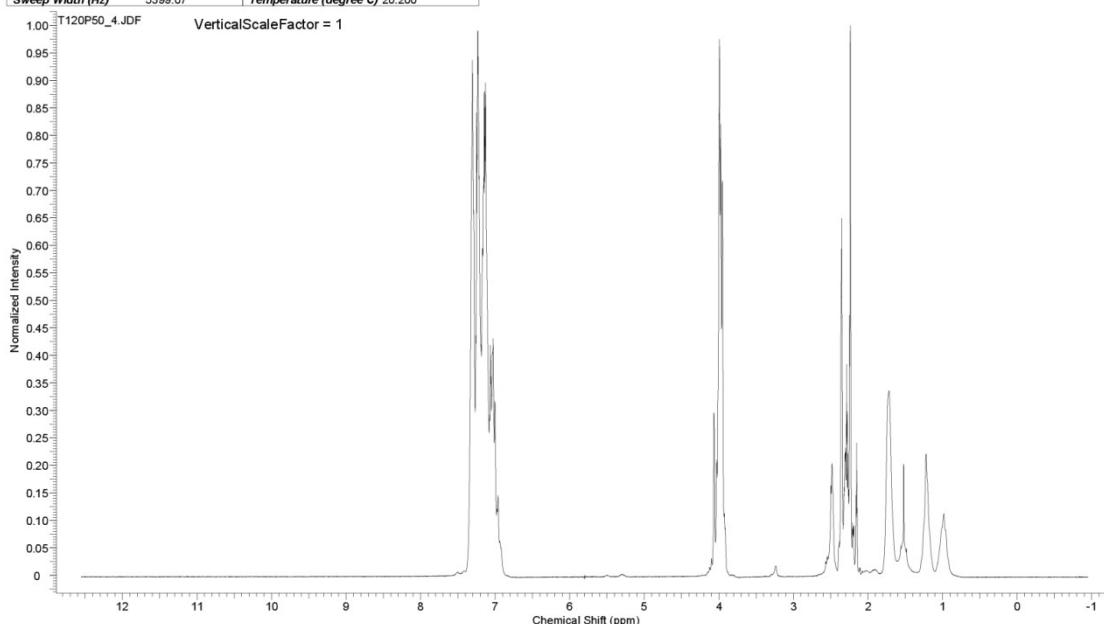


Figure S 8: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 4 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}] = 150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3} = 0.25 \text{ mol\%}$)

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Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	34.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.100	Spectrum Type	STANDARD

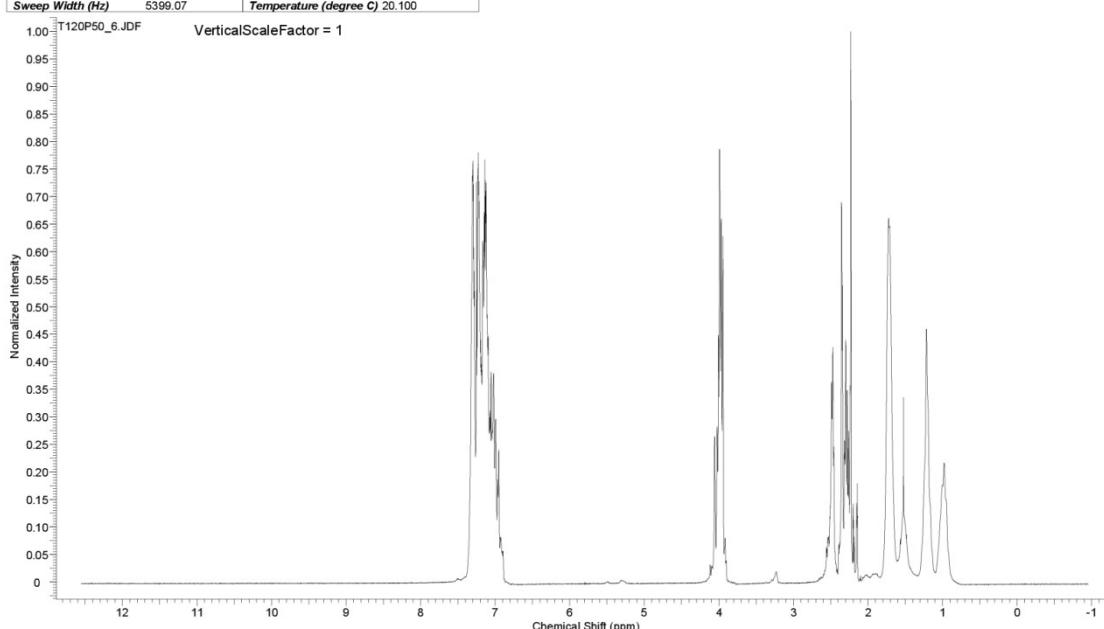


Figure S 9: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 6 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}] = 150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3} = 0.25 \text{ mol\%}$)

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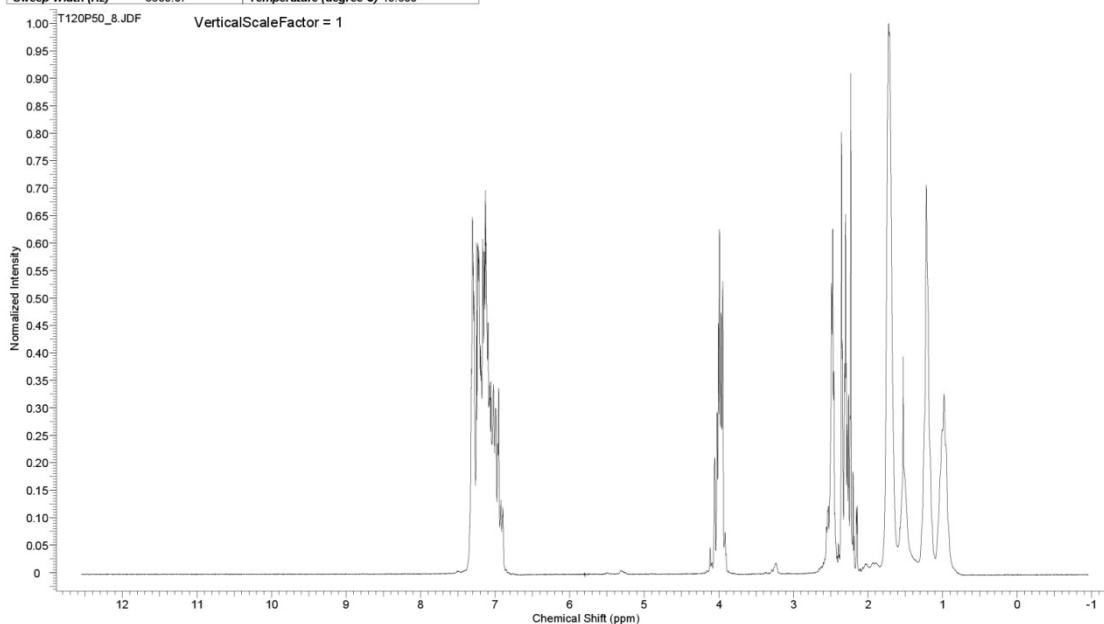


Figure S 10: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 8 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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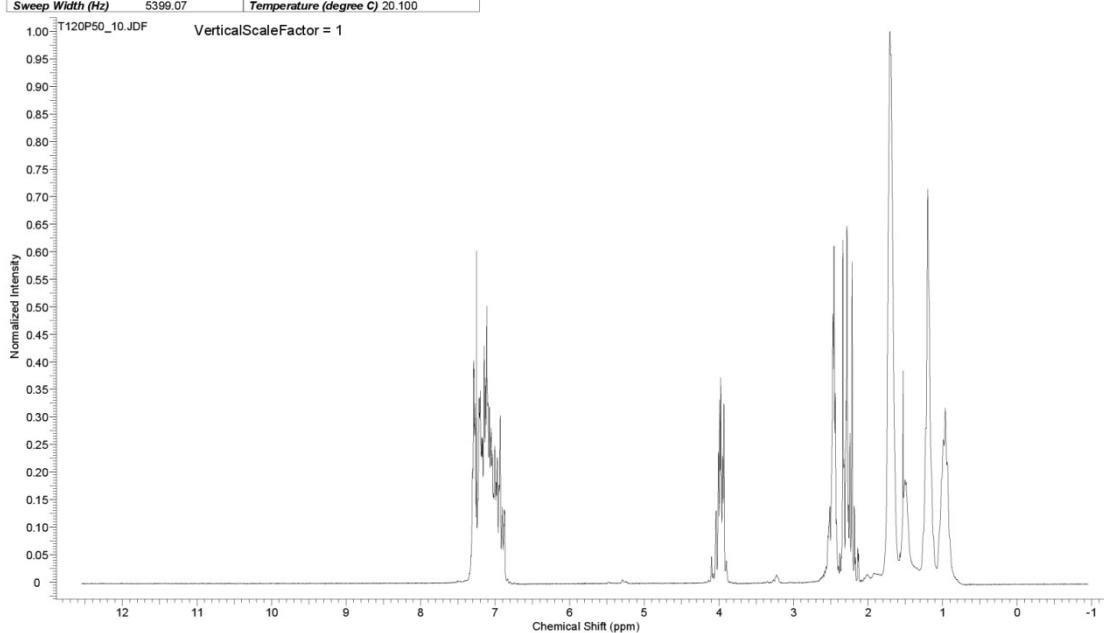


Figure S 11: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 10 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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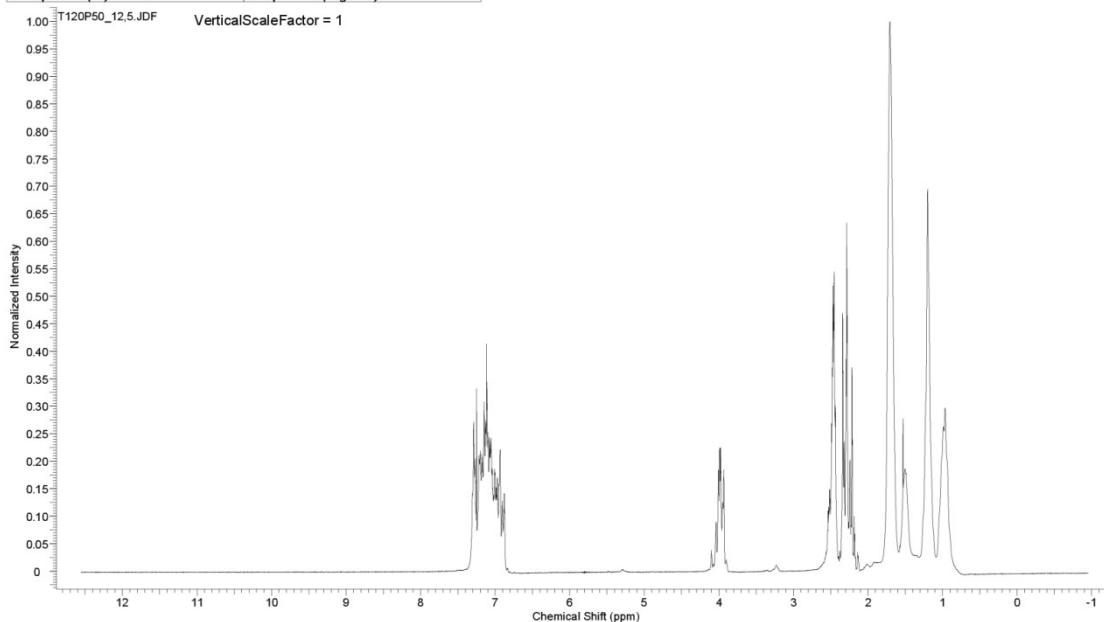


Figure S 12: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 12.5 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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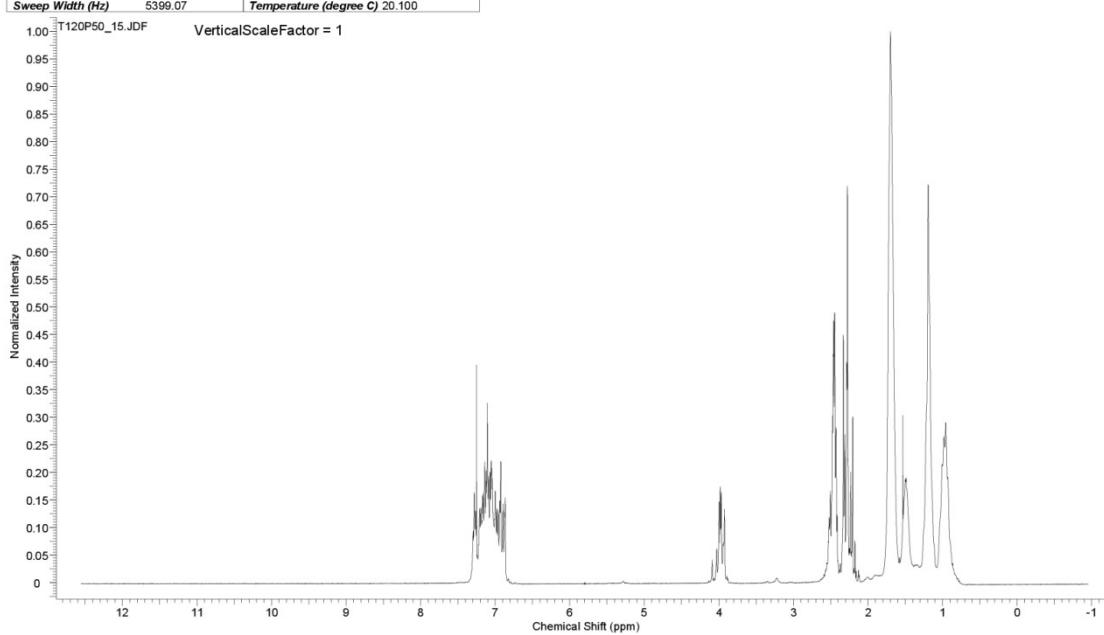


Figure S 13: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 15 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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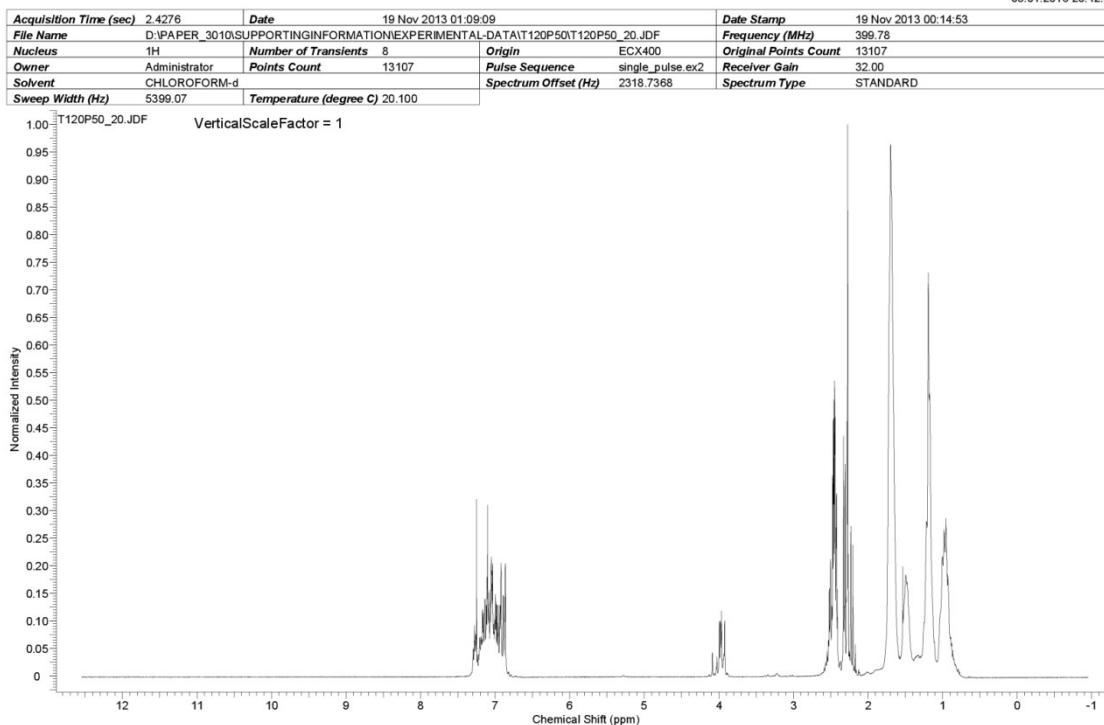


Figure S 14: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 20 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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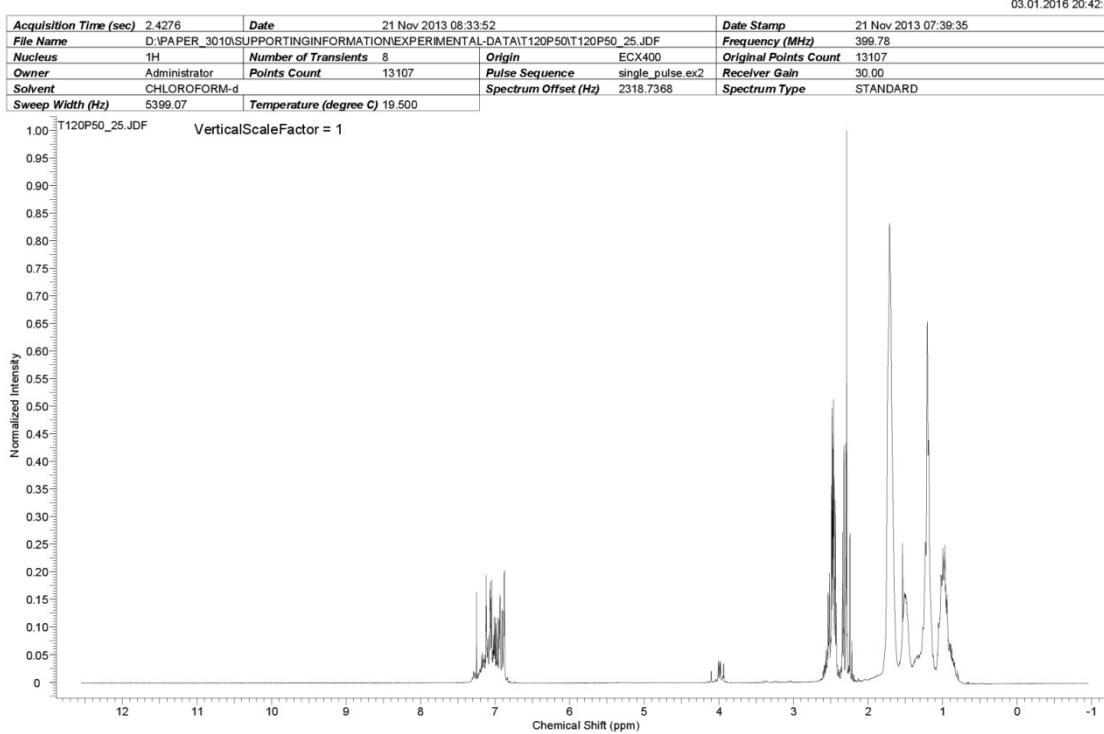


Figure S 15: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 25 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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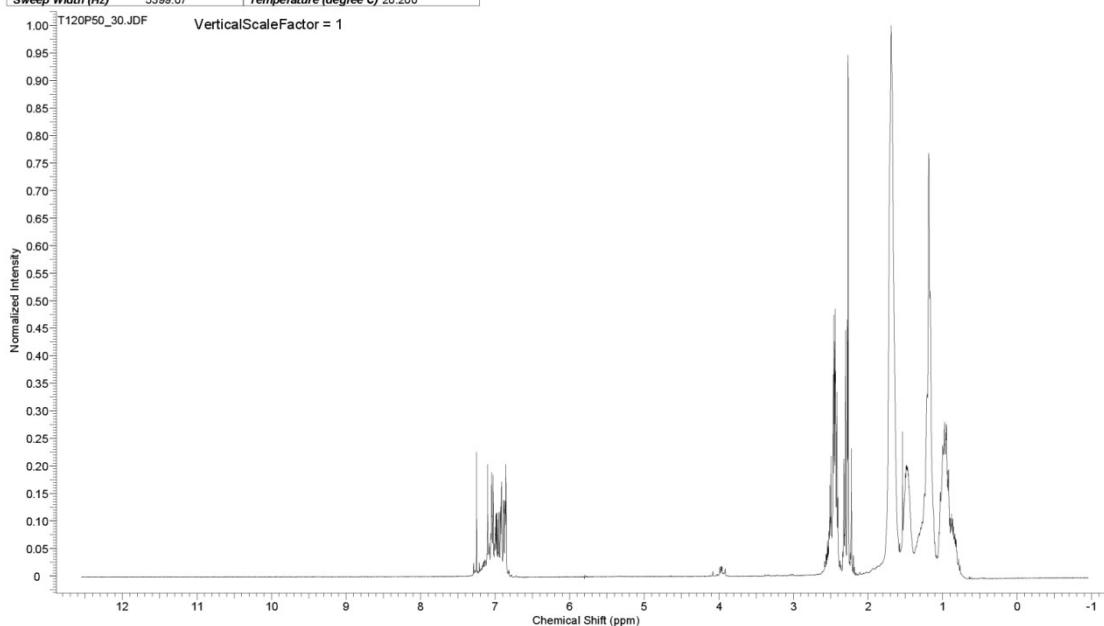


Figure S 16: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 30 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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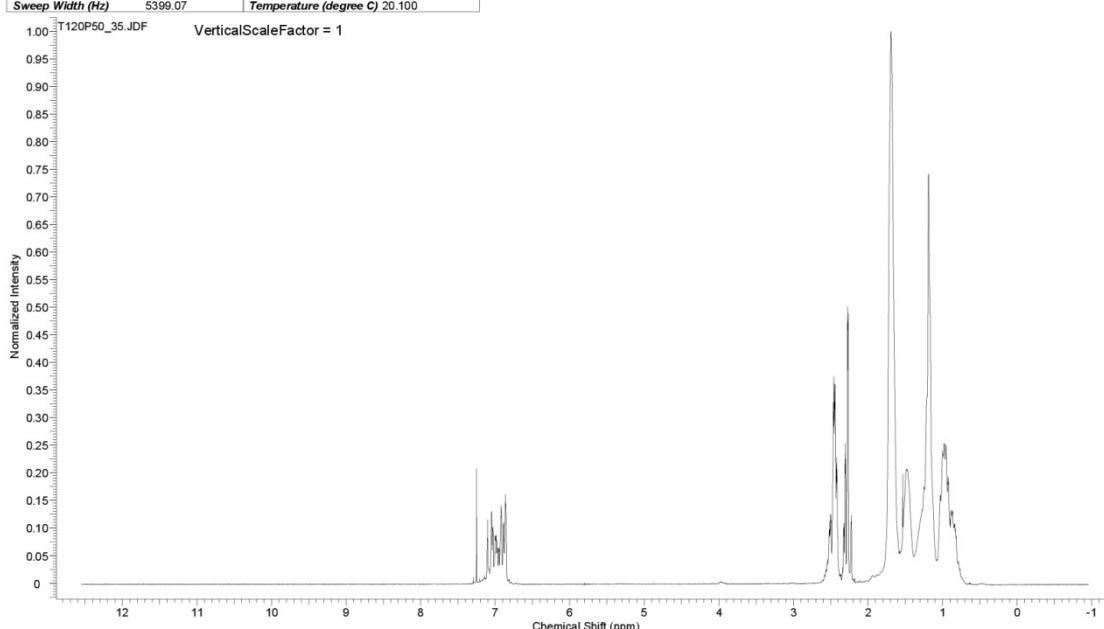


Figure S 17: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 35 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc

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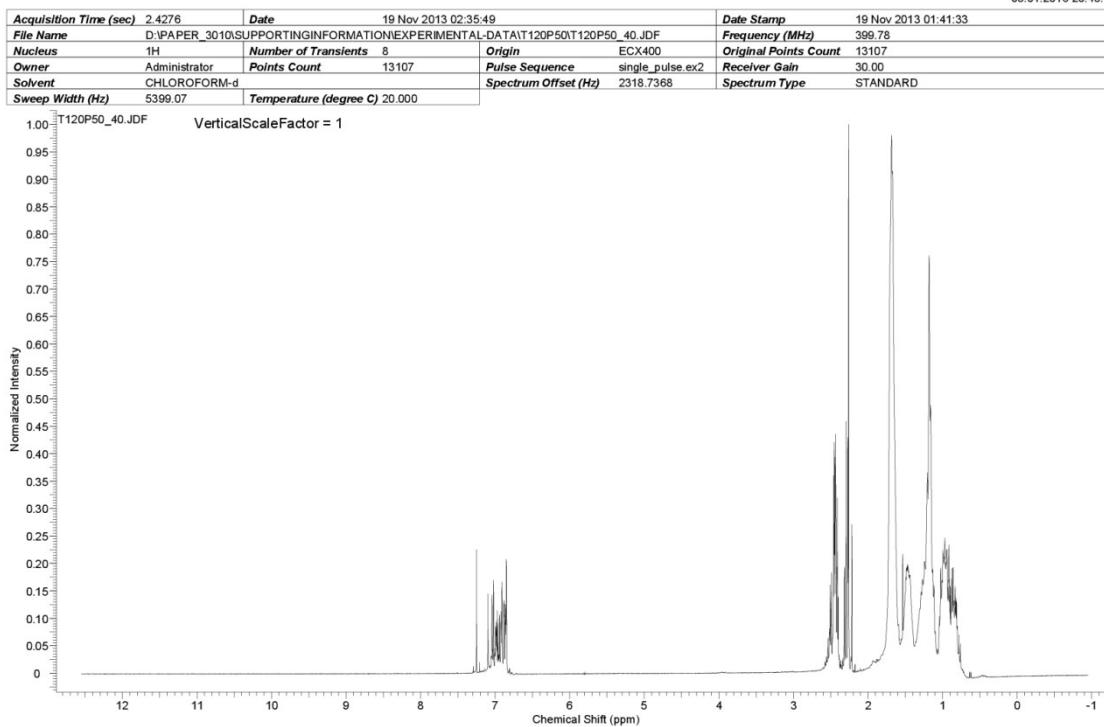


Figure S 18: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 40 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc

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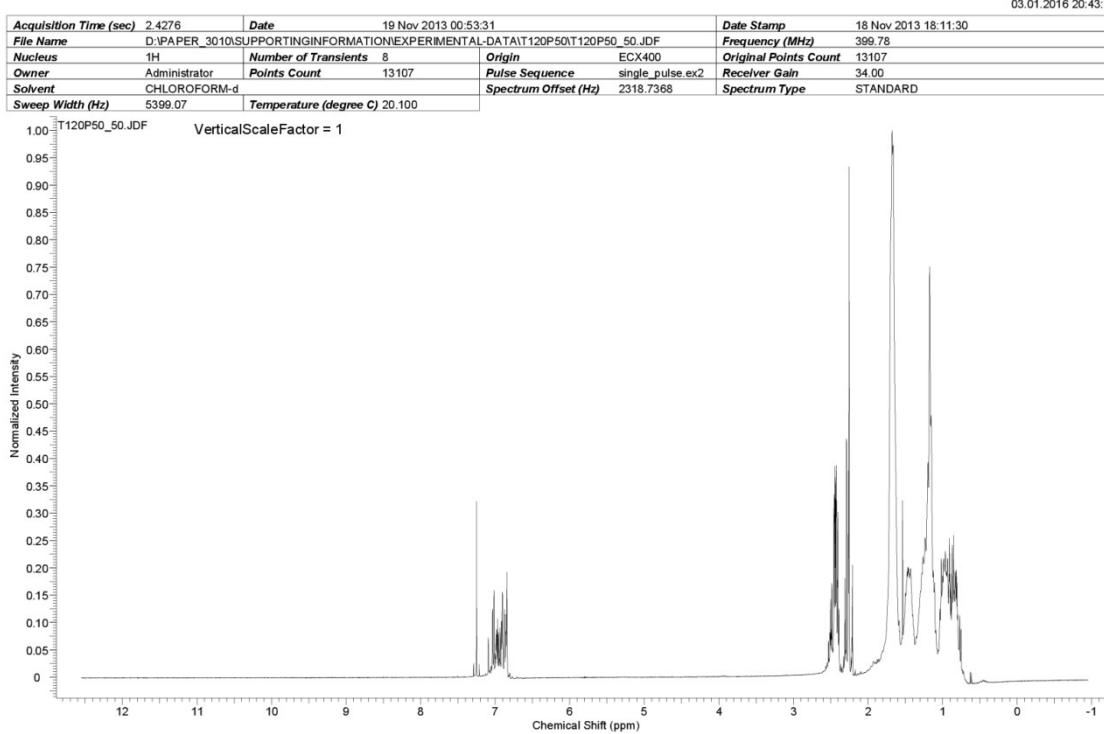


Figure S 19: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 50 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

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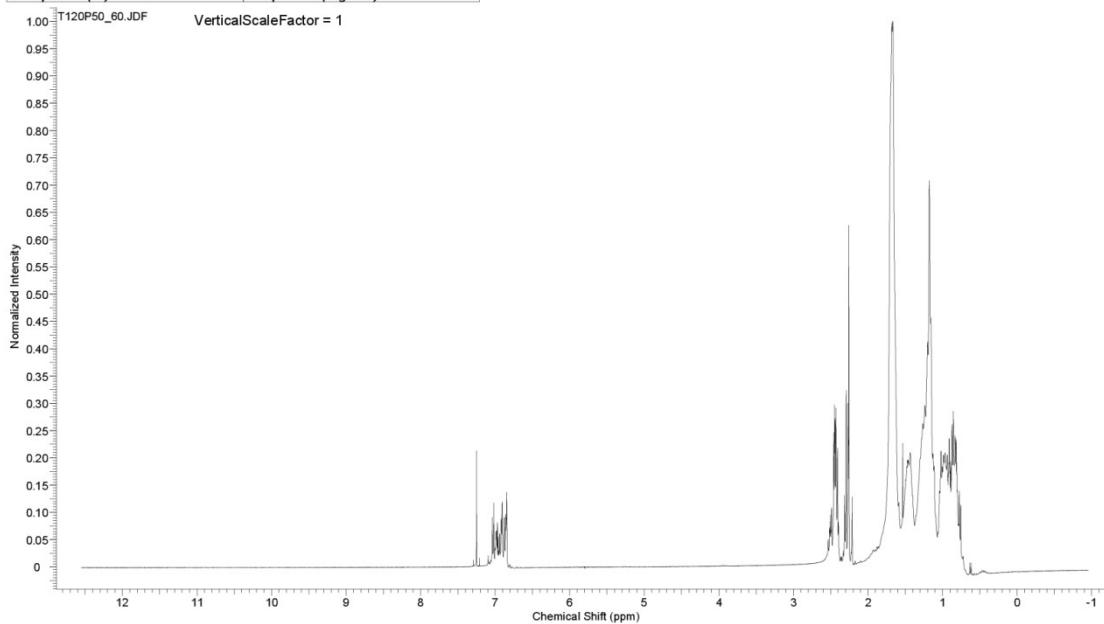


Figure S 20: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 60 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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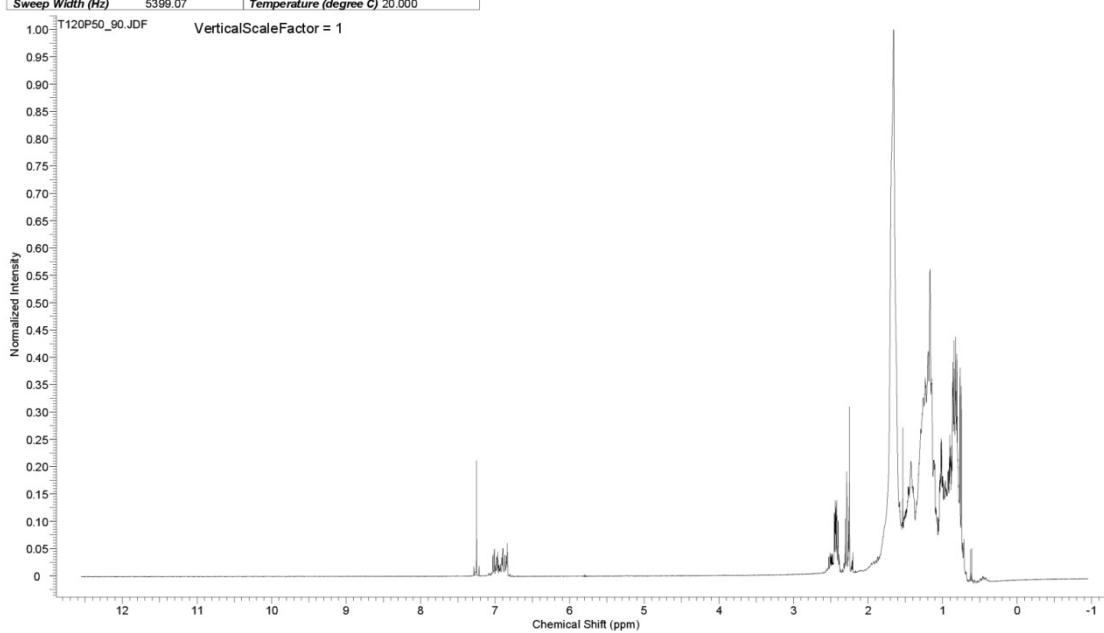


Figure S 21: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 90 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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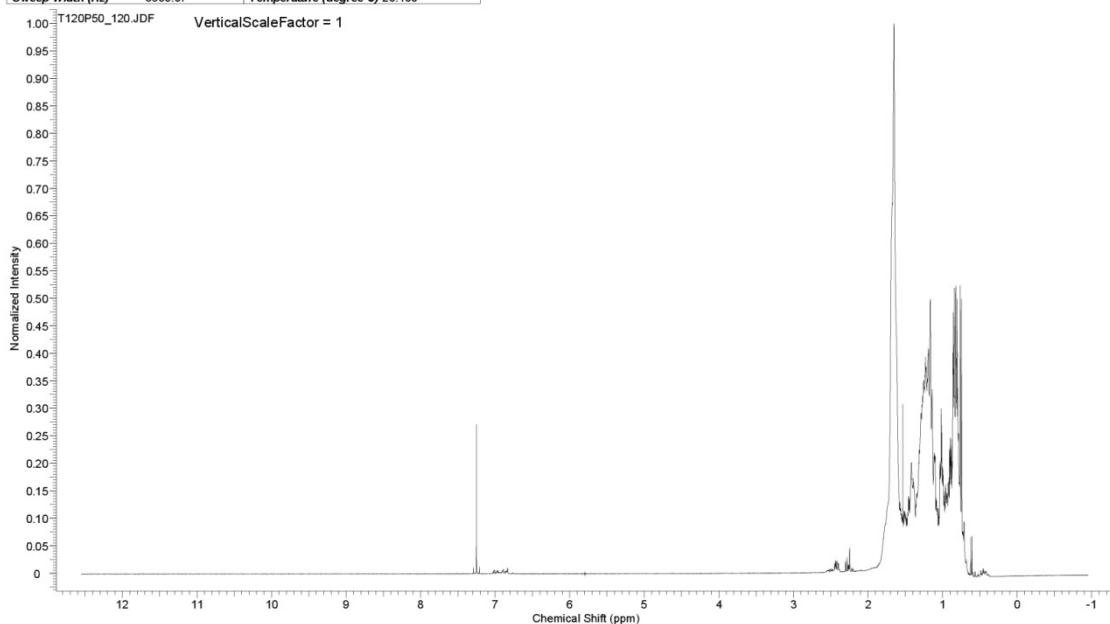


Figure S 22: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 120 \text{ min}$ ($T=120^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

T = 140 °C ; P = 50 bar

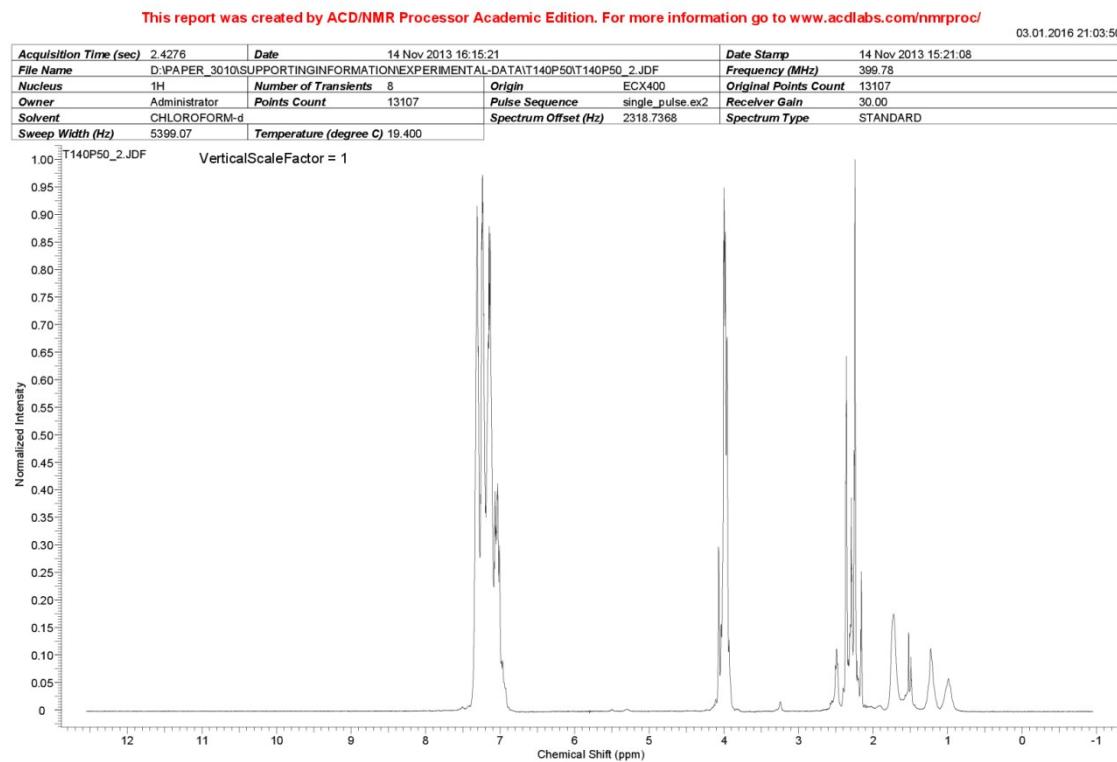


Figure S 23: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 2 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

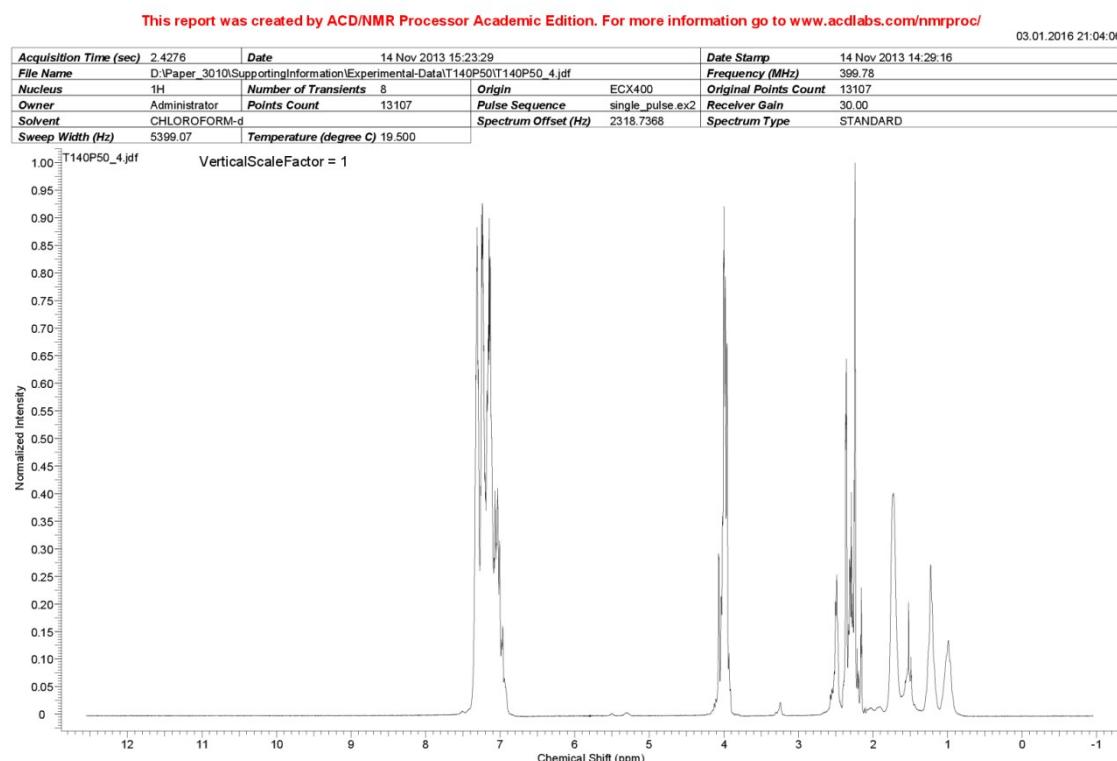


Figure S 24: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 4 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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Sweep Width (Hz)	5399.07	Temperature (degree C)	19.300	Spectrum Type	STANDARD

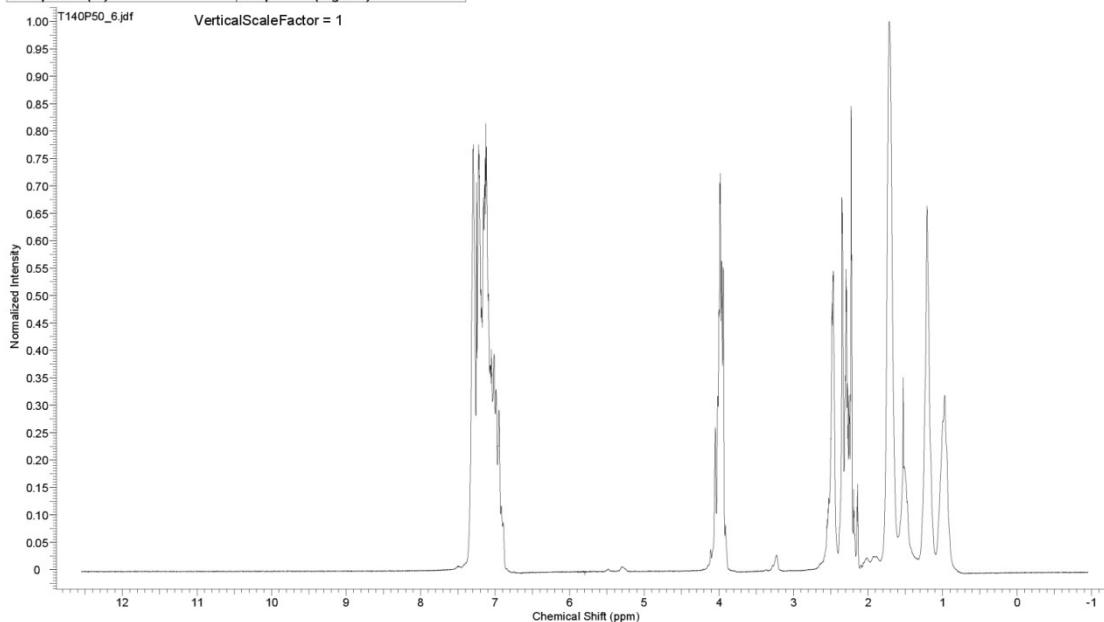


Figure S 25: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 6 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:04:25

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 15:28:43	Date Stamp	14 Nov 2013 14:34:30
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.400	Spectrum Type	STANDARD

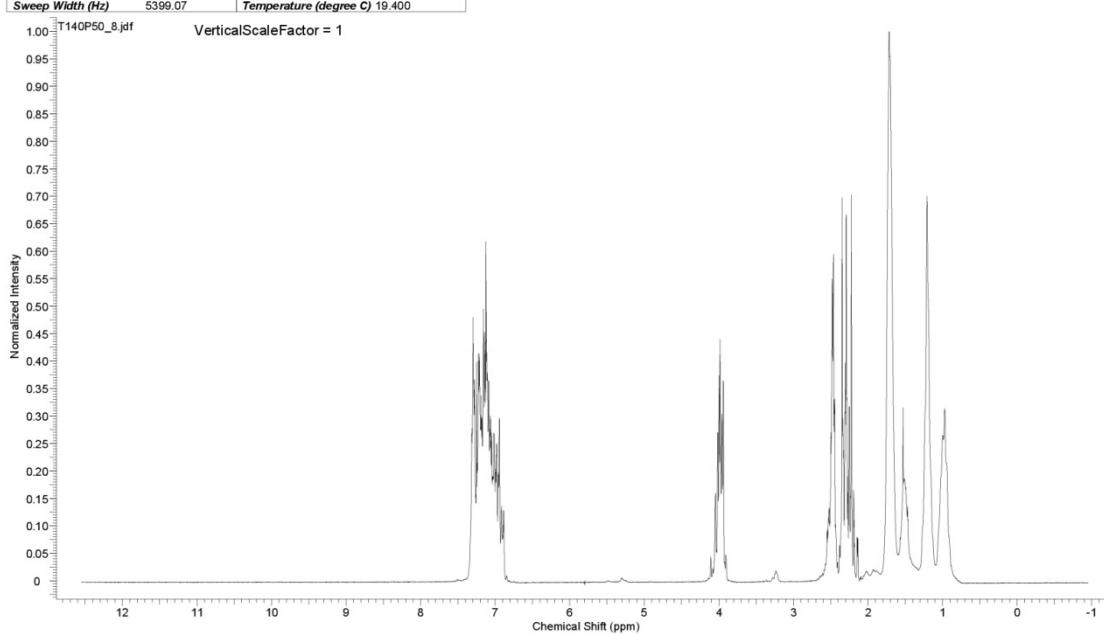


Figure S 26: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 8 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:04:34

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 15:49:40	Date Stamp	14 Nov 2013 14:55:27
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Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

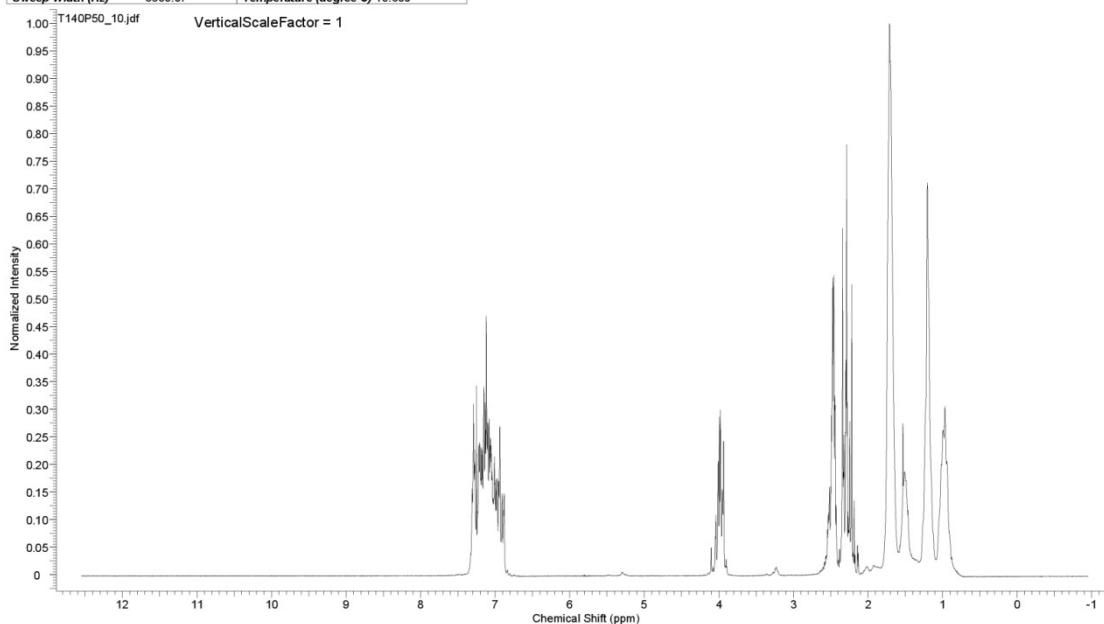


Figure S 27: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 10 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:04:42

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 16:10:12	Date Stamp	14 Nov 2013 15:15:59
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Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

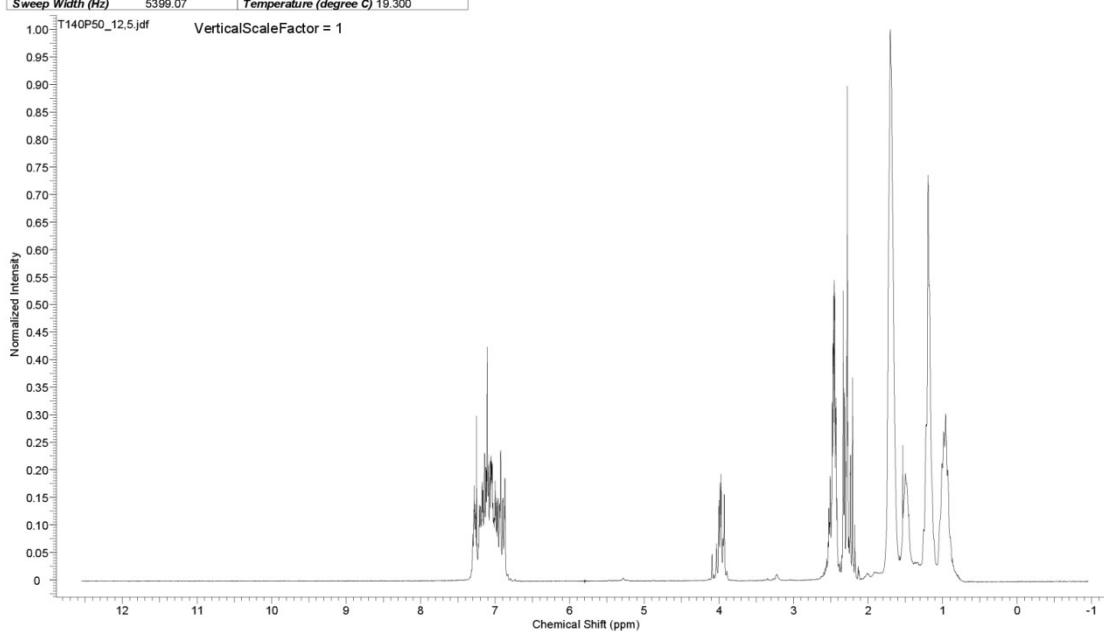


Figure S 28: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 12.5 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:04:56

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 15:39:26	Date Stamp	14 Nov 2013 14:45:13
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T140P50\T140P50_15.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	1H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.400	Spectrum Type	STANDARD

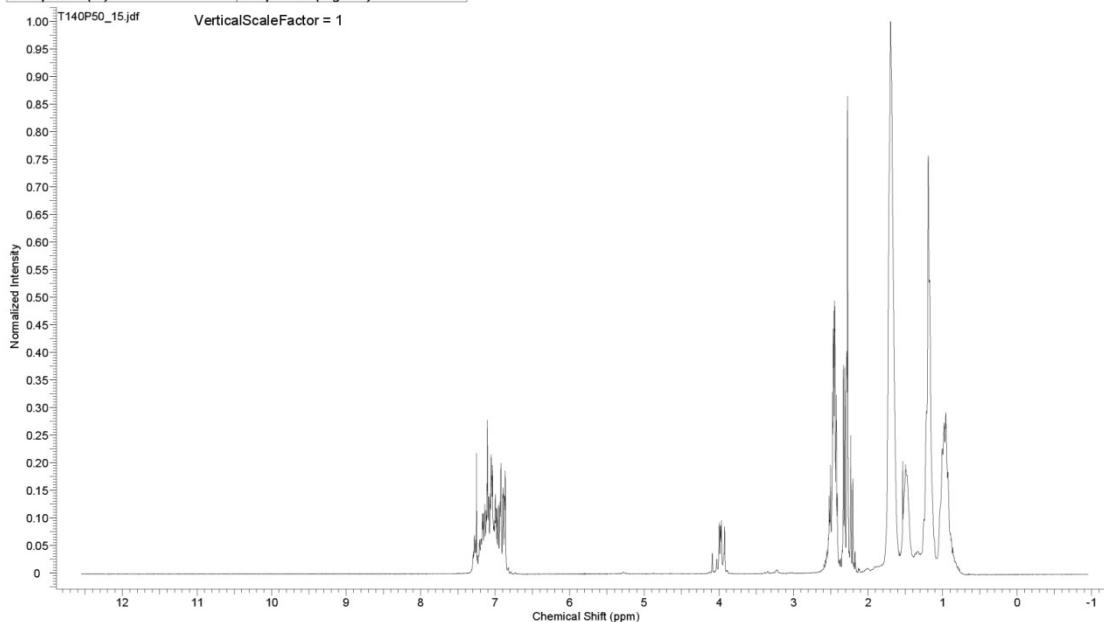


Figure S 29: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 15 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:07

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 16:04:52	Date Stamp	14 Nov 2013 15:10:39
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T140P50\T140P50_20.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	1H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.500	Spectrum Type	STANDARD

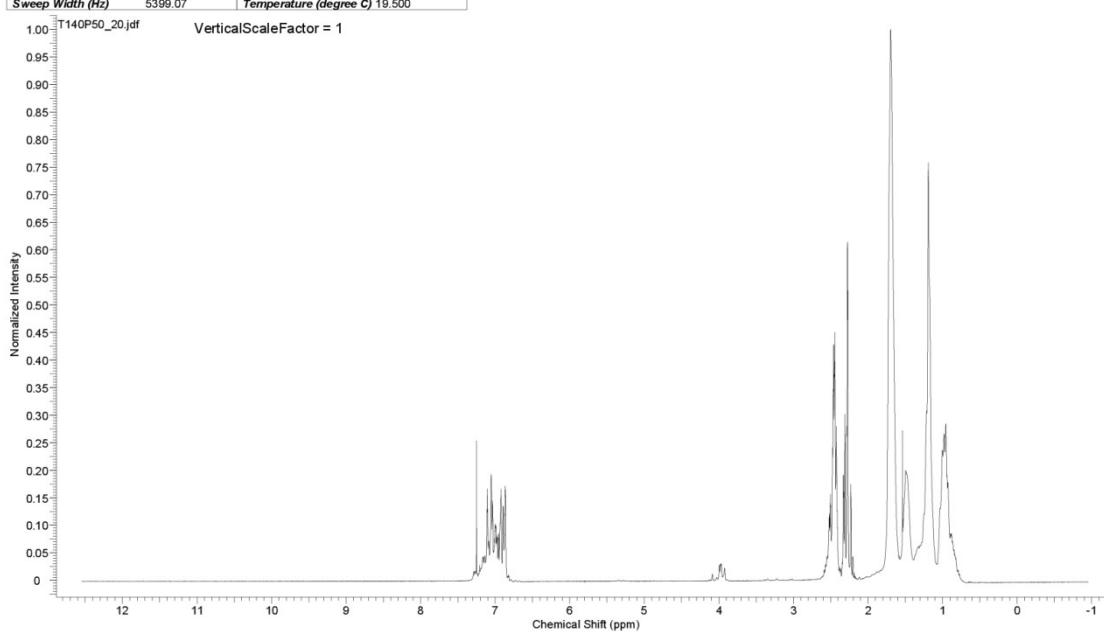


Figure S 30: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 20 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:22

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.500	Spectrum Type	STANDARD

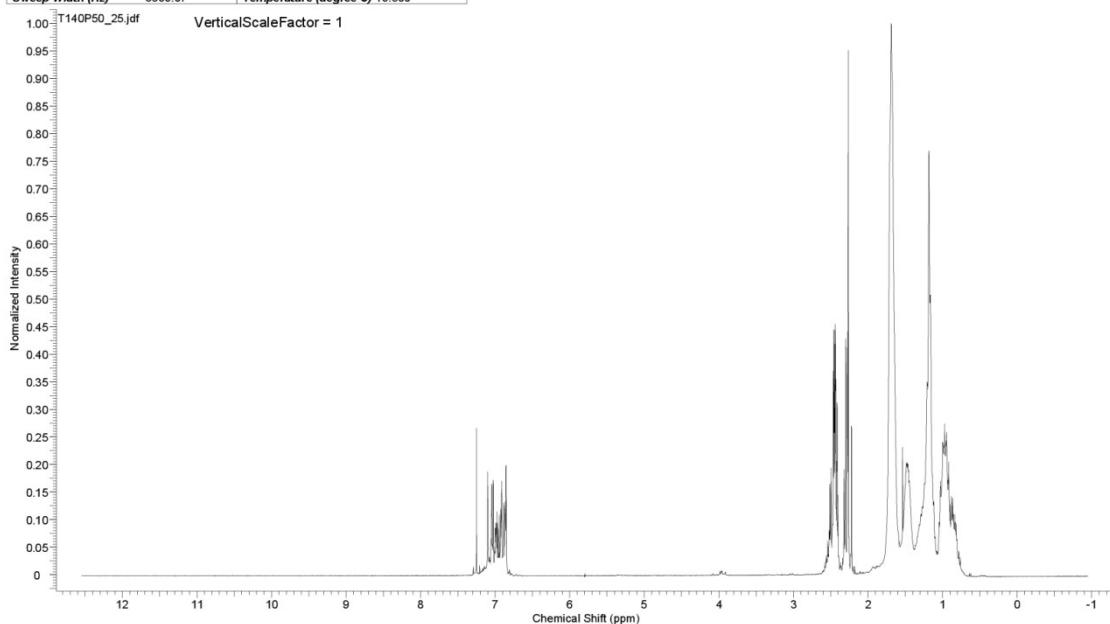


Figure S 31: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 25 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:32

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.300	Spectrum Type	STANDARD

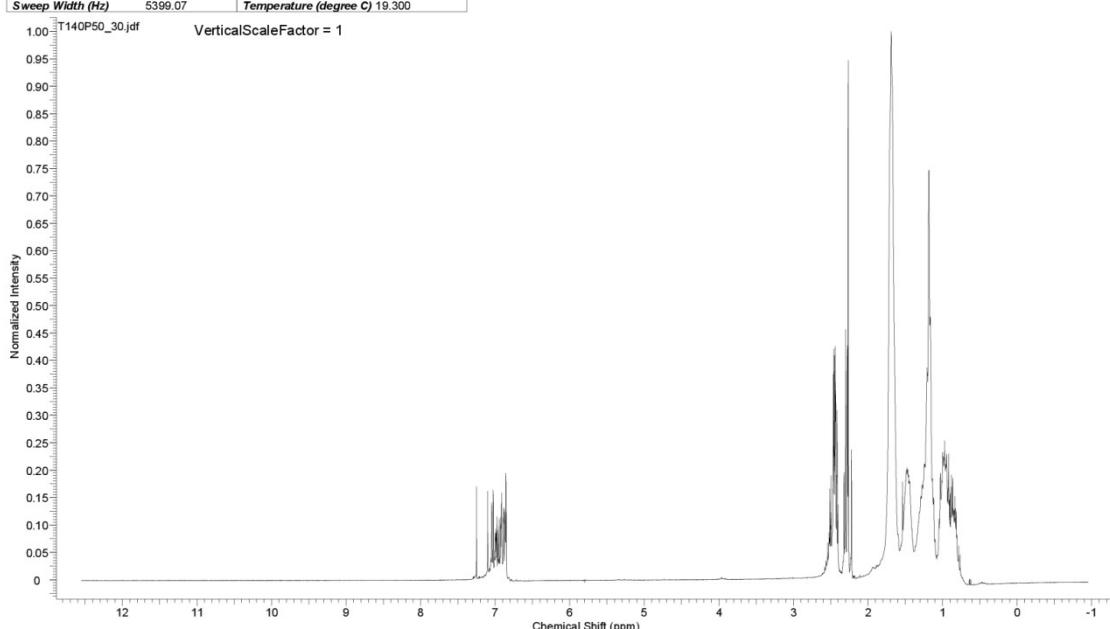


Figure S 32: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 30 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:40

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Nucleus	1H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.400	Spectrum Type	STANDARD

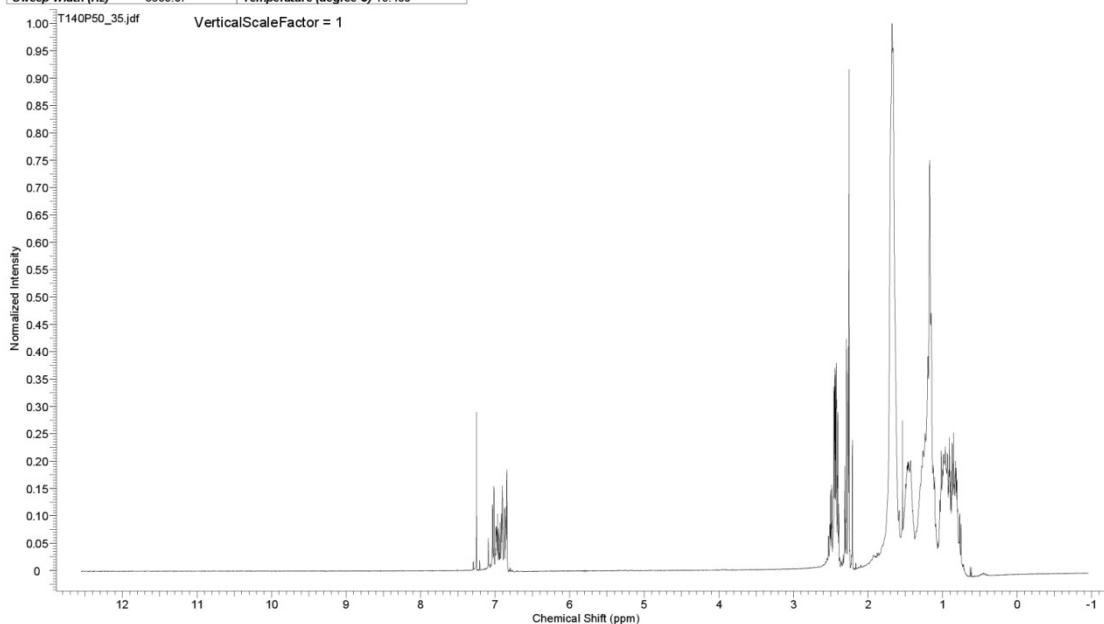


Figure S 33: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 35 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:47

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.400	Spectrum Type	STANDARD

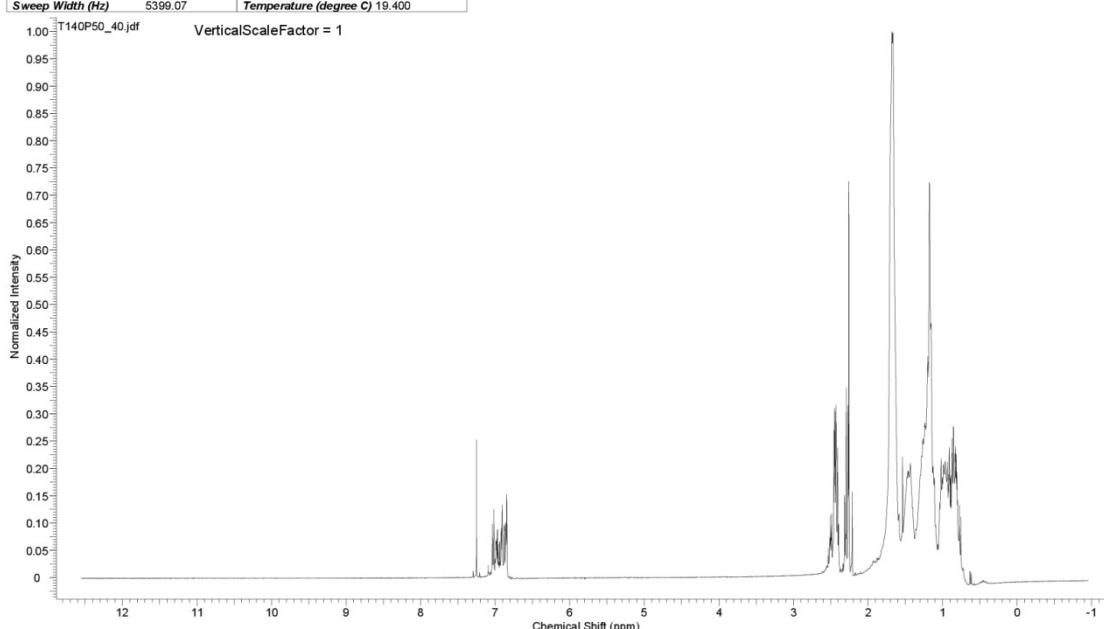


Figure S 34: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 40 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:05:55

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.300	Spectrum Type	STANDARD

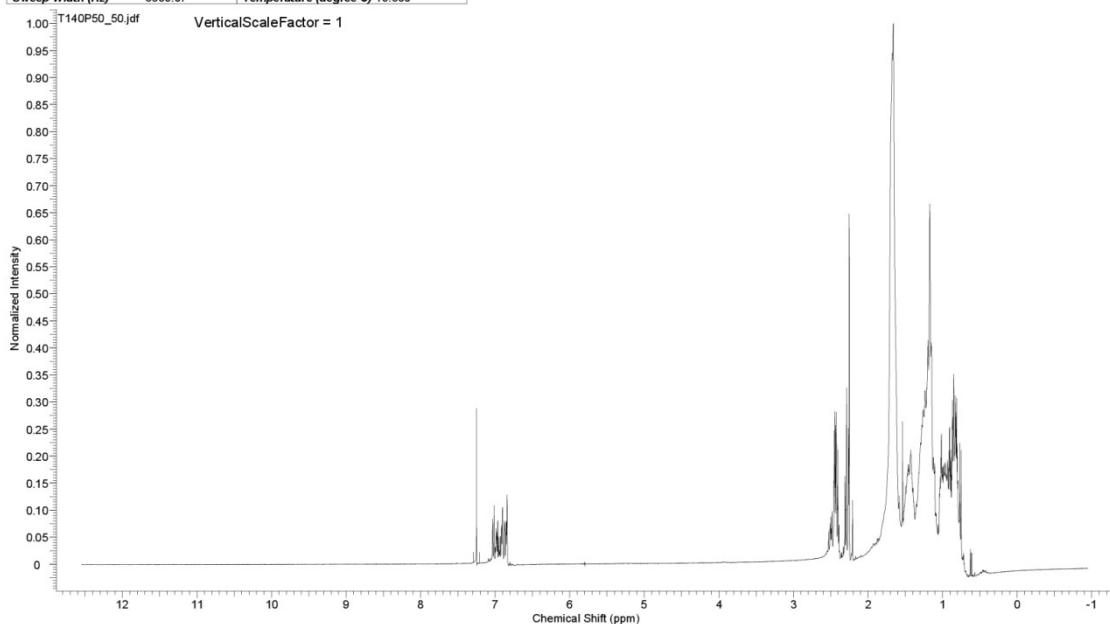


Figure S 35: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 50 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:06:03

Acquisition Time (sec)	2.4276	Date	14 Nov 2013 15:12:46	Date Stamp	14 Nov 2013 14:18:33
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T140P50\T140P50_60.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	1H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	28.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.500	Spectrum Type	STANDARD

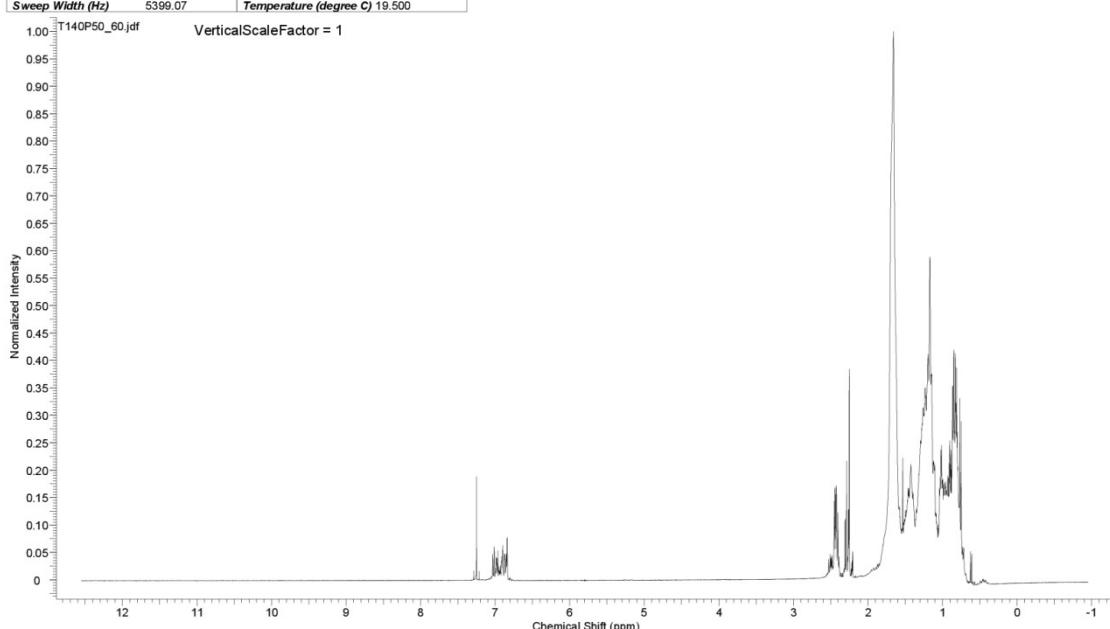


Figure S 36: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 60 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:06:10

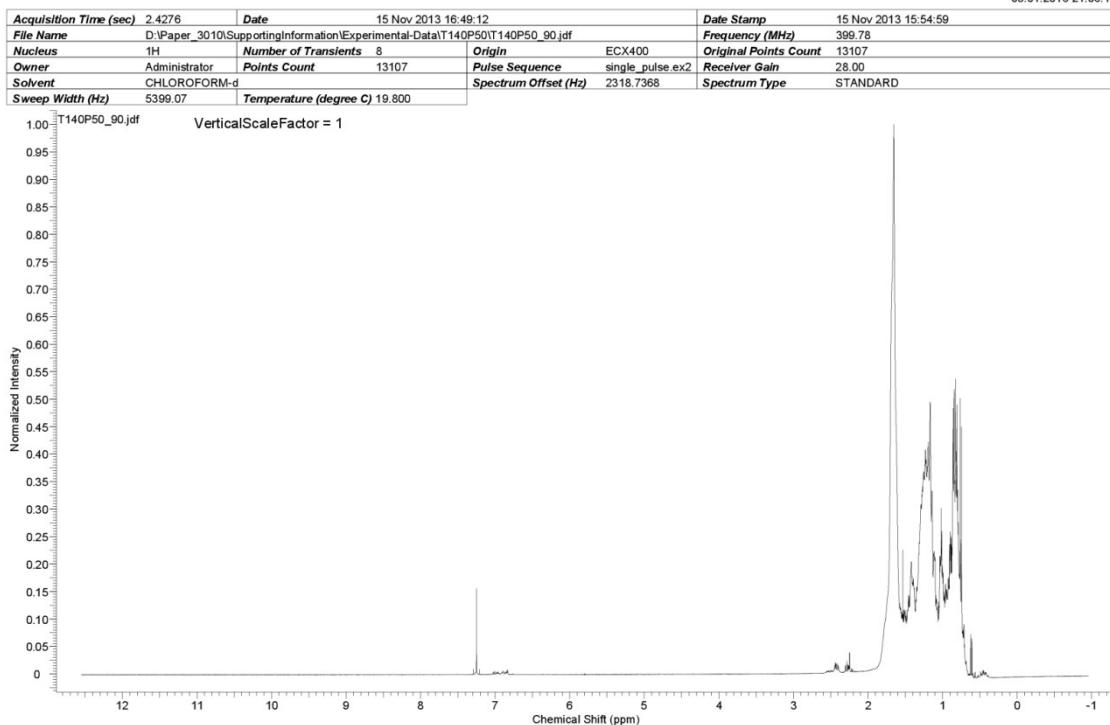


Figure S 37: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 90 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:06:27

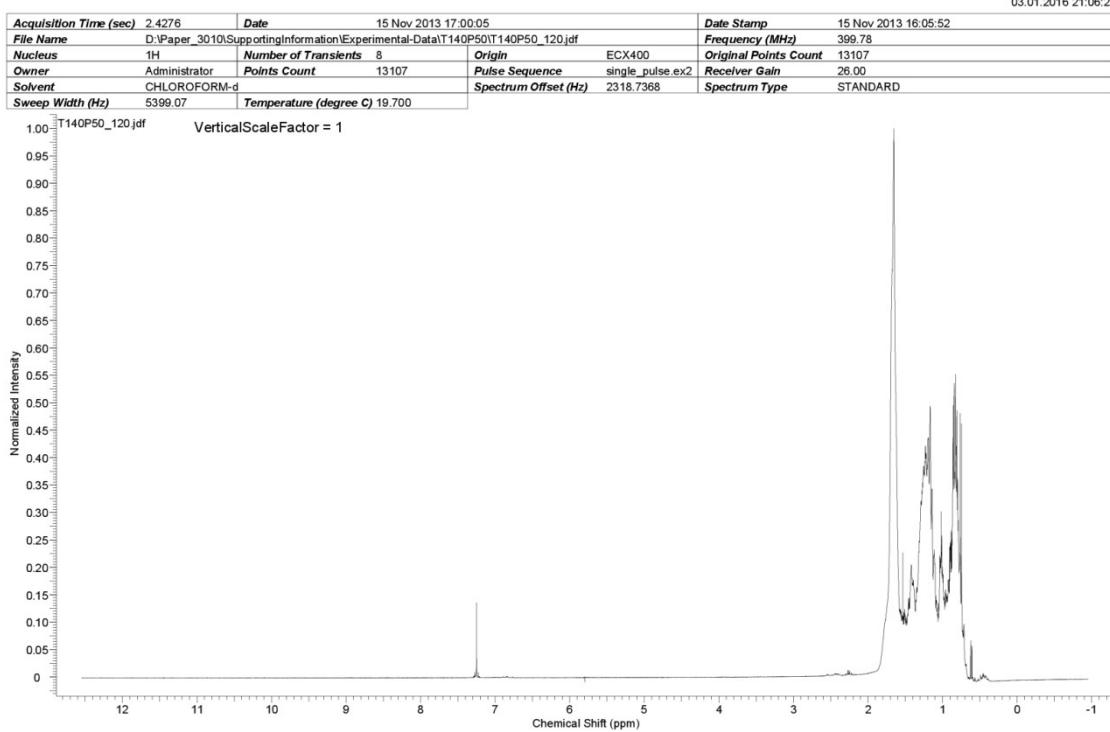


Figure S 38: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 120 \text{ min}$ ($T=140^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

T = 160 °C ; P = 50 bar

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03.01.2016 21:08:57

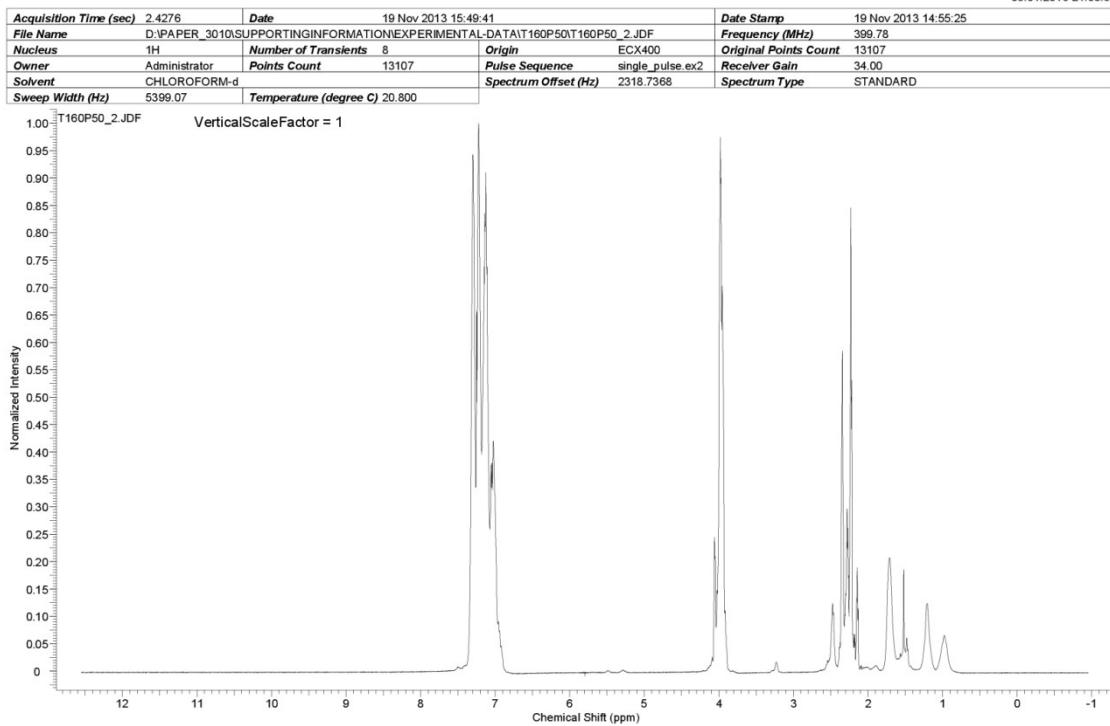


Figure S 39: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 2 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:51

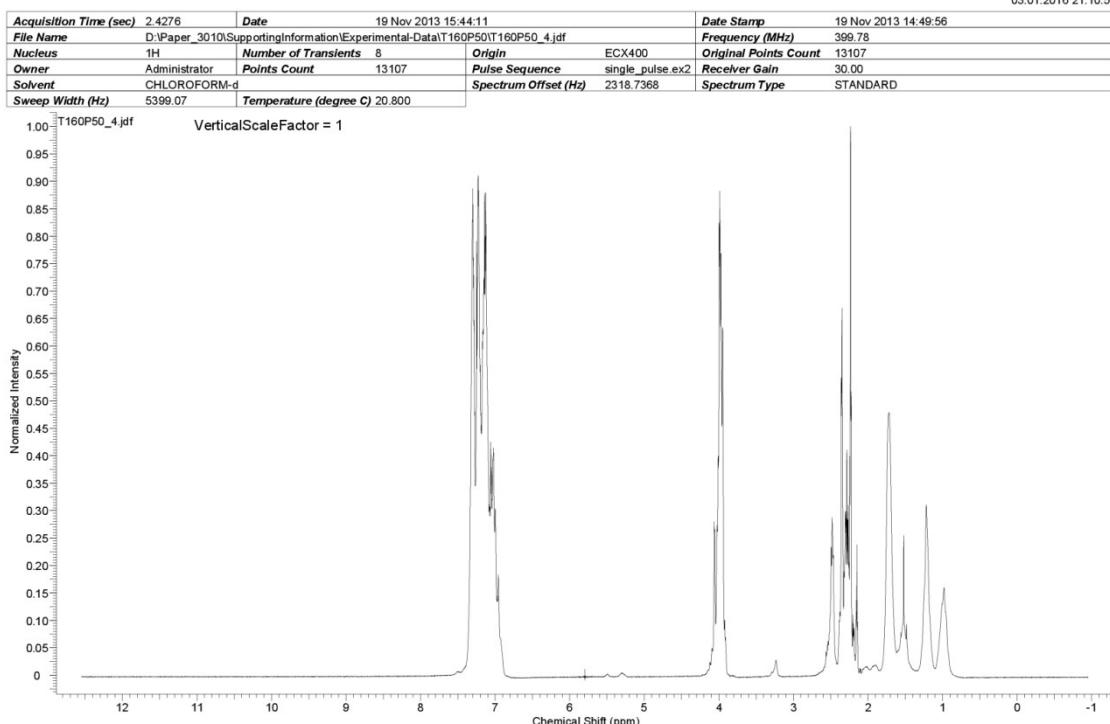


Figure S 40: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 4 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:11:00

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
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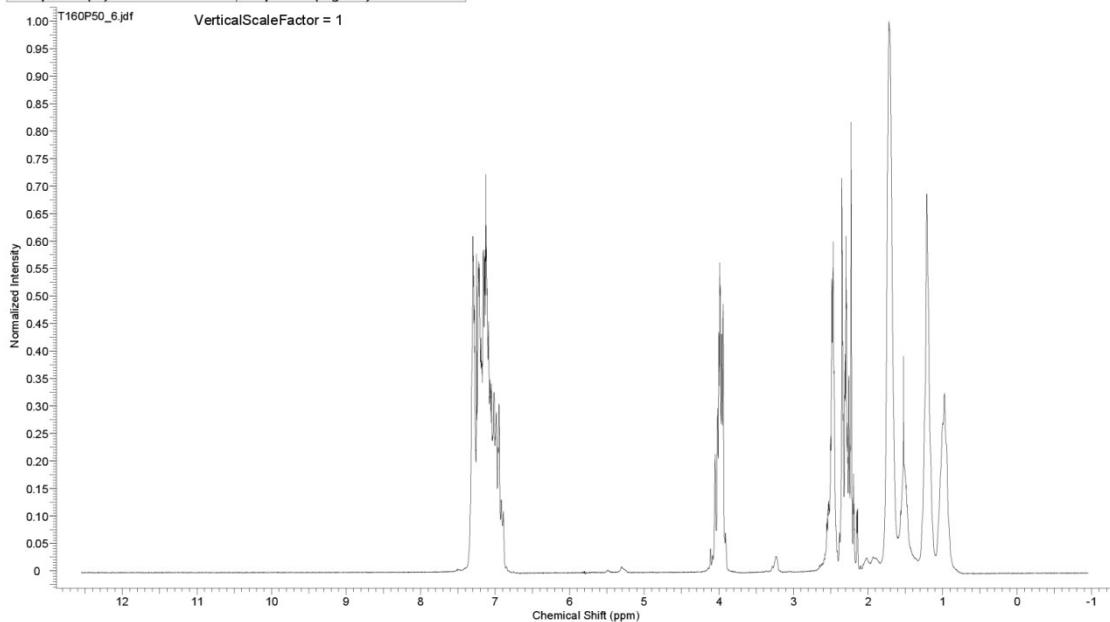


Figure S 41: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 6 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:11:08

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	21.000	Spectrum Type	STANDARD

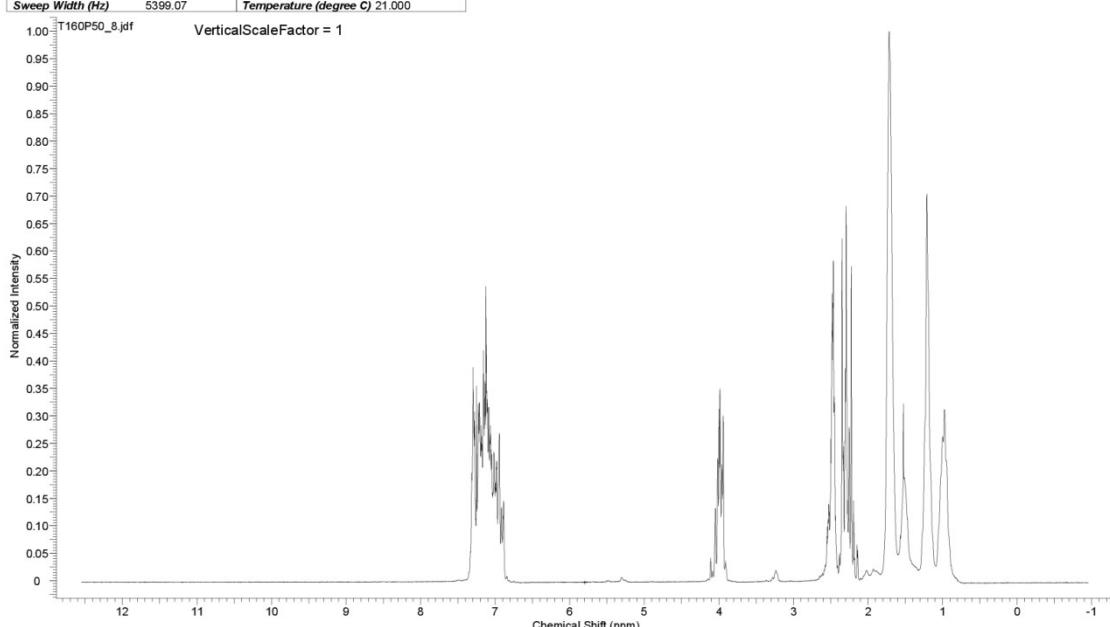


Figure S 42: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 8 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:09:09

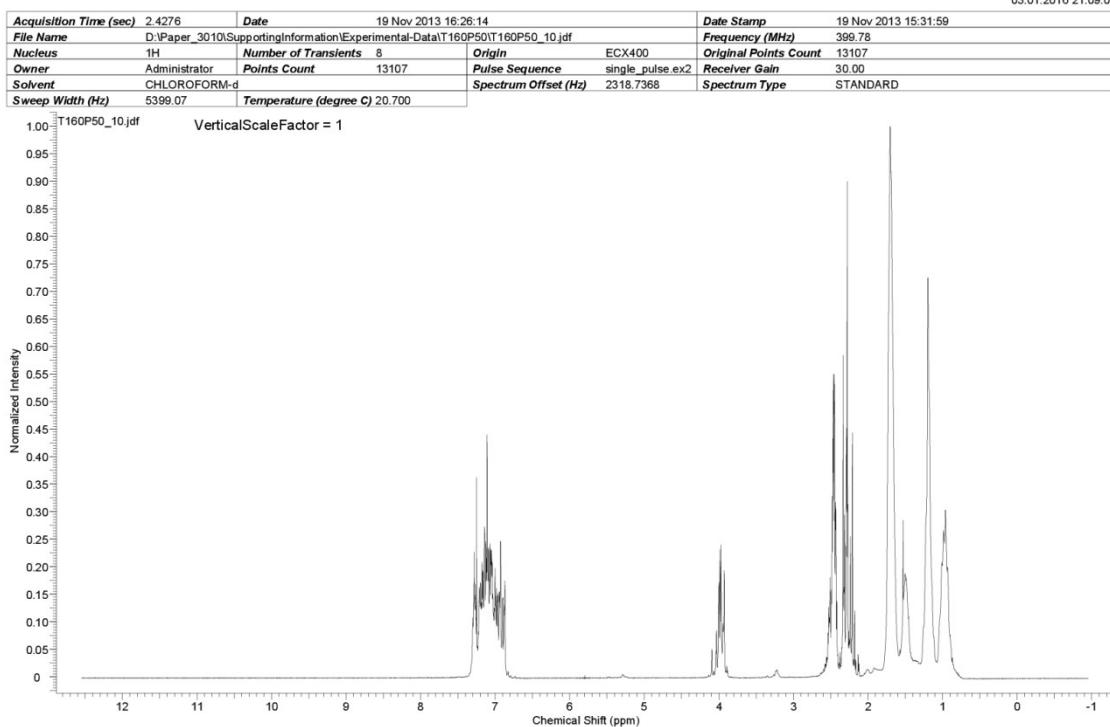


Figure S 43: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 10 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:09:18

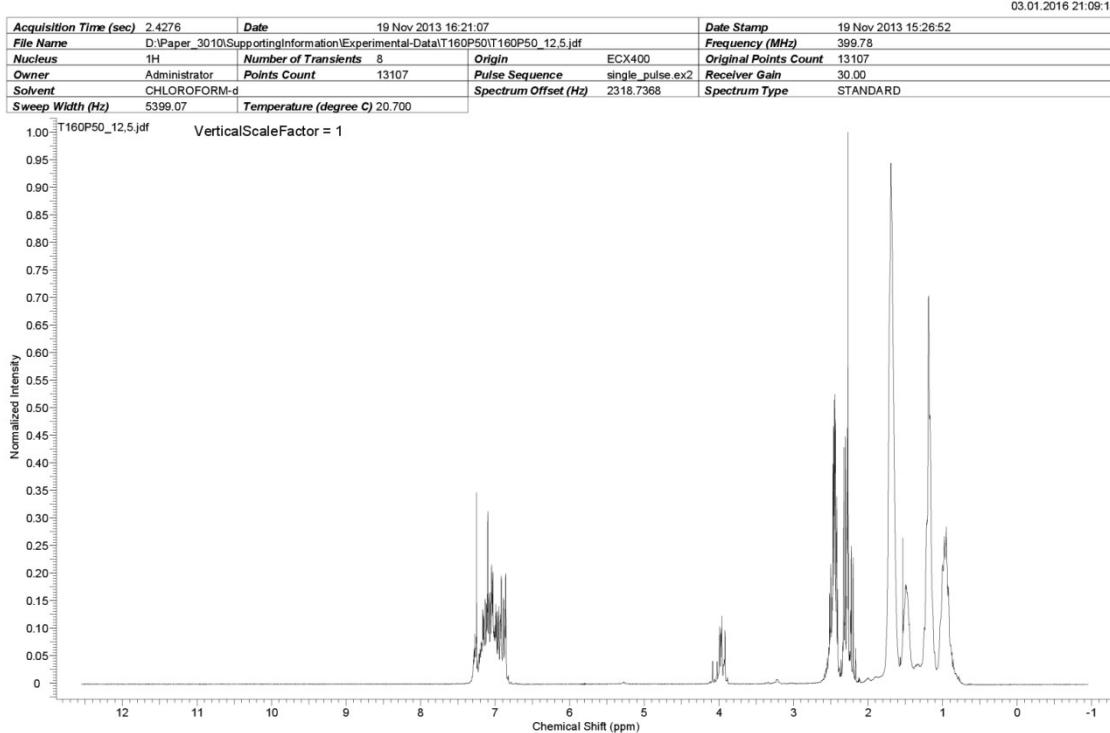


Figure S 44: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 12.5 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:09:27

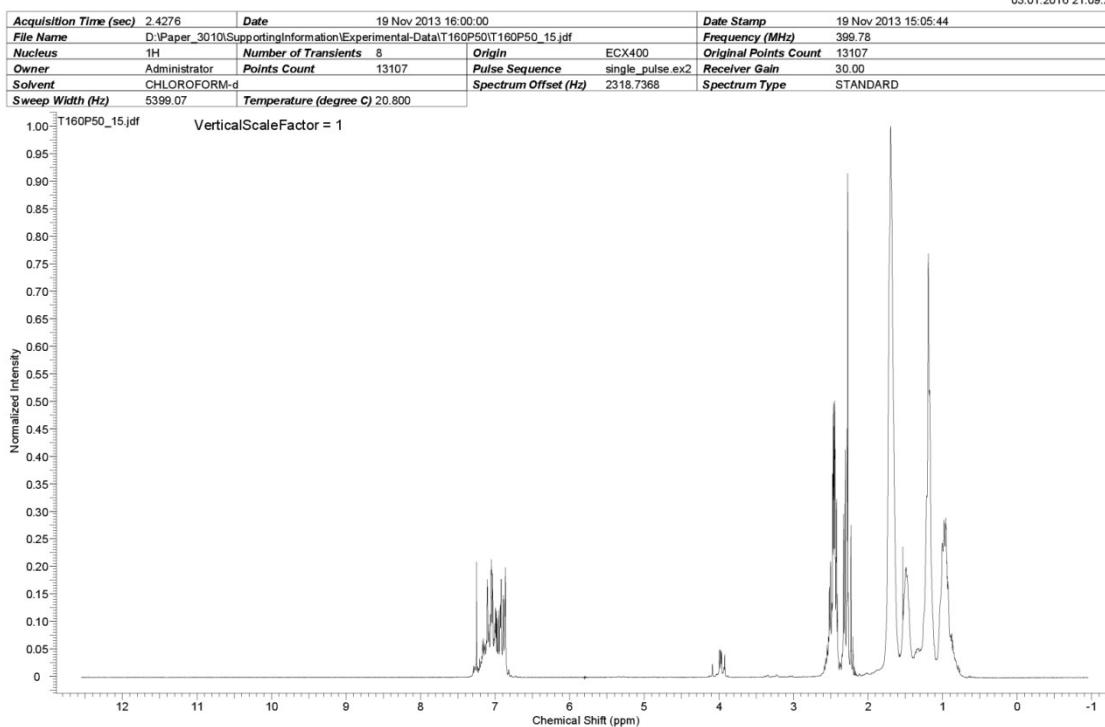


Figure S 45: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 15 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:09:36

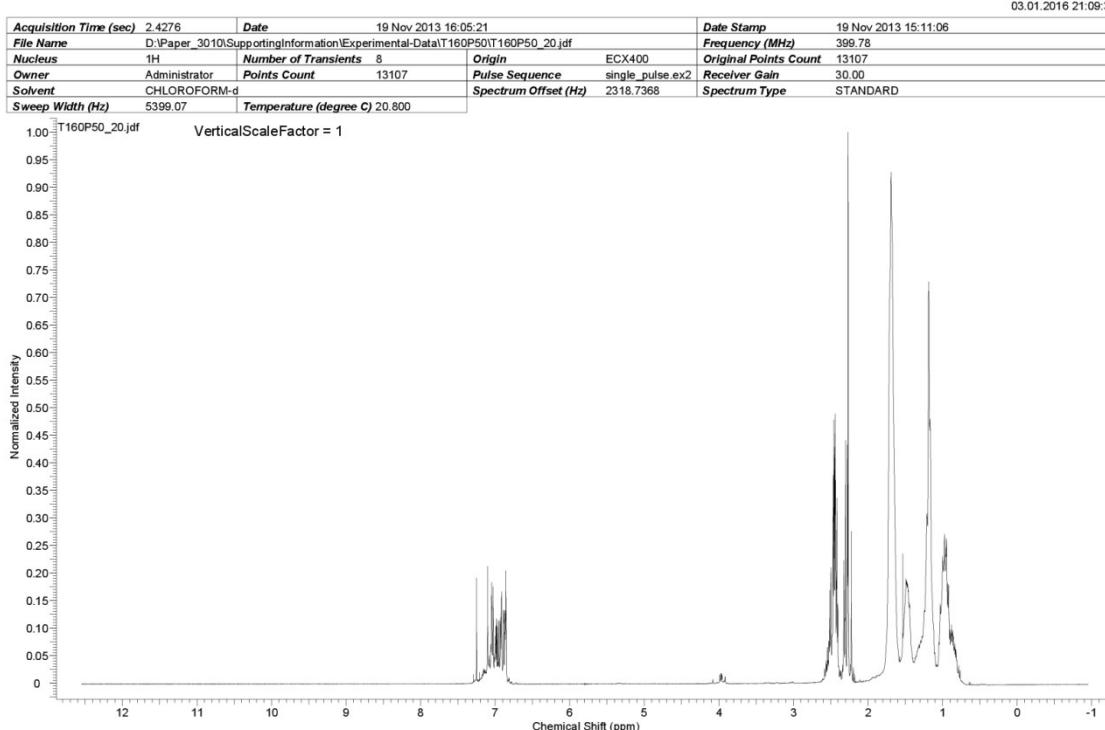


Figure S 46: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 20 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:09:45

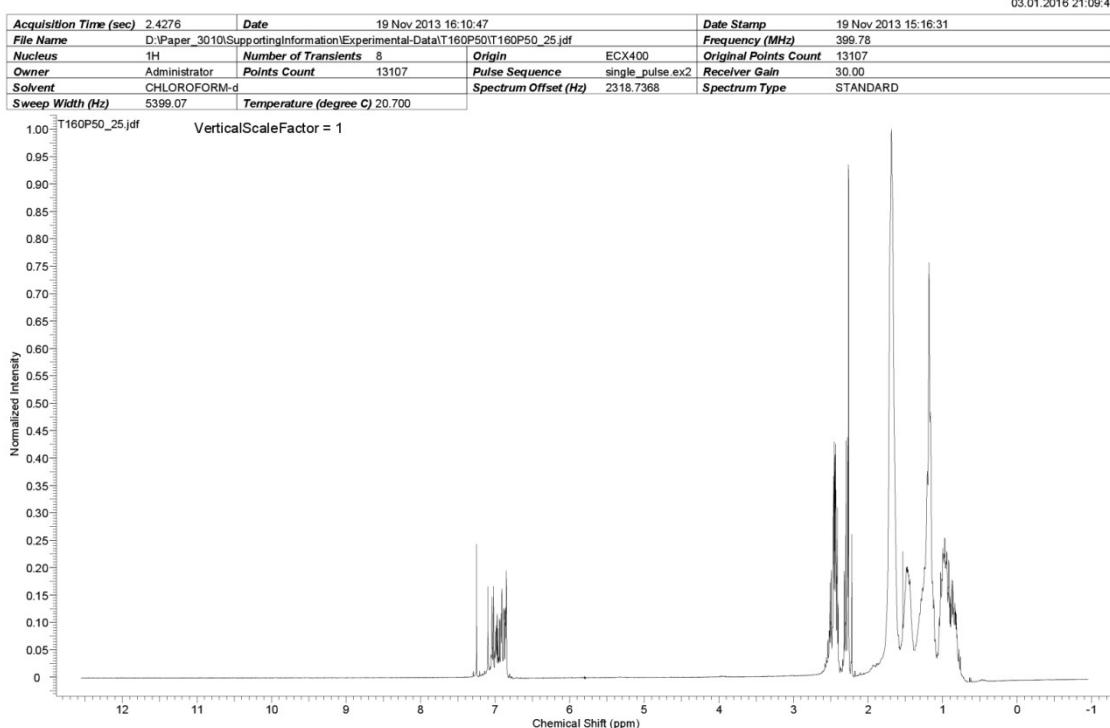


Figure S 47: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 25 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:09:53

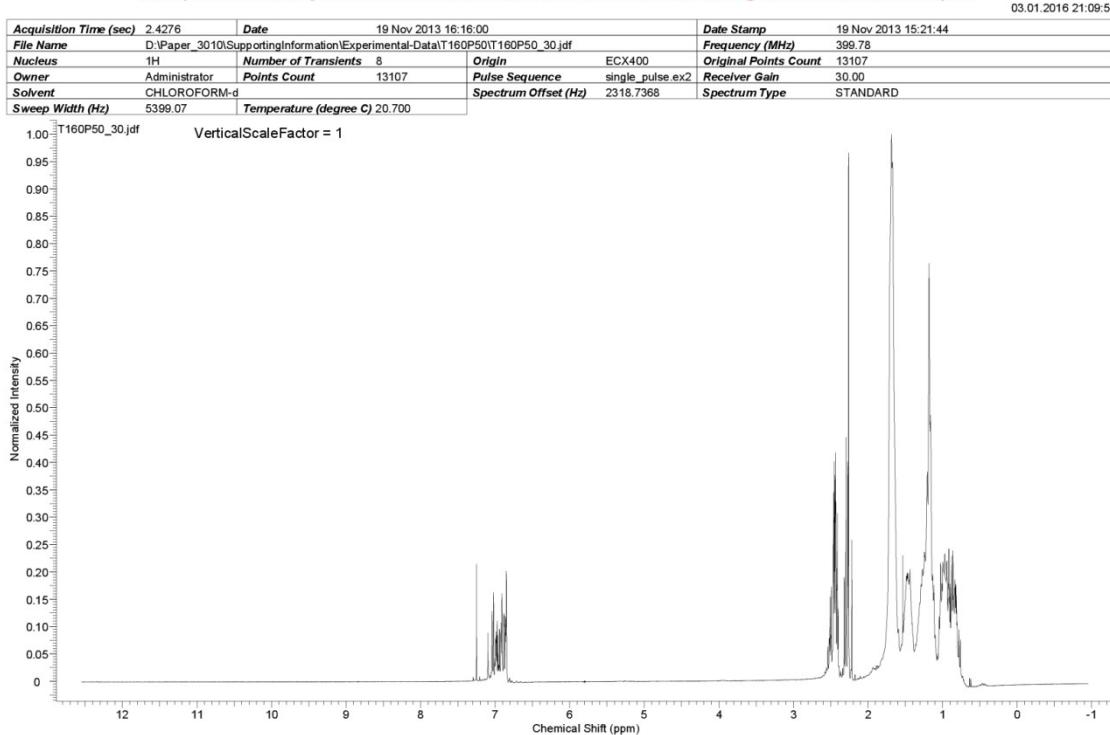


Figure S 48: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 30 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:00

Acquisition Time (sec)	2.4276	Date	19 Nov 2013 15:23:45	Date Stamp	19 Nov 2013 14:29:30
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	21.100	Spectrum Type	STANDARD

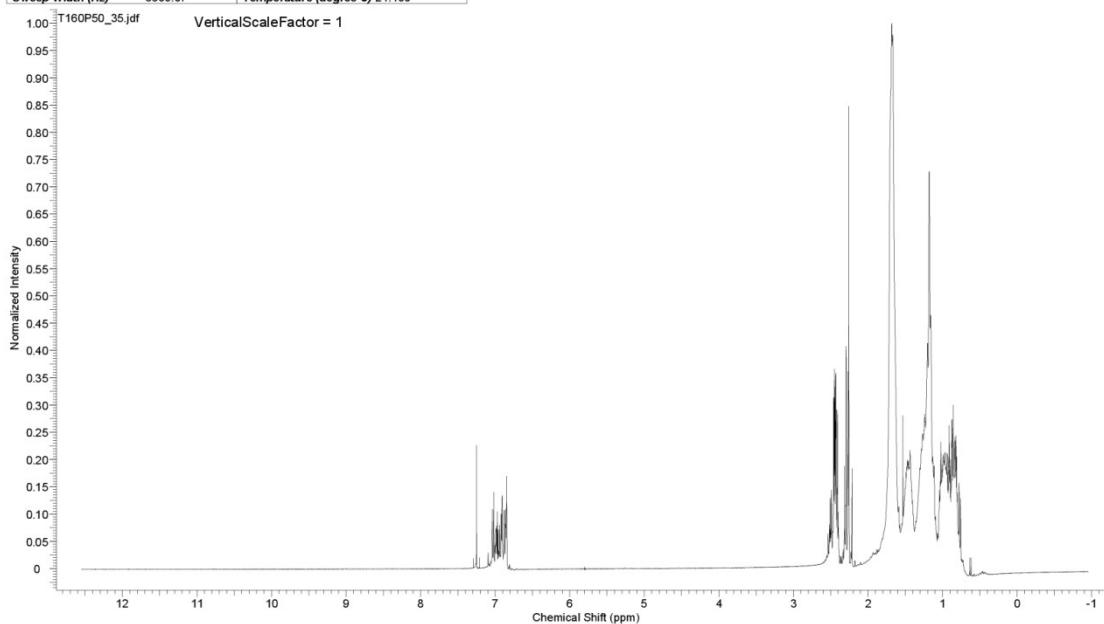


Figure S 49: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 35 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:12

Acquisition Time (sec)	2.4276	Date	19 Nov 2013 16:34:54	Date Stamp	19 Nov 2013 15:40:38
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Nucleus	¹ H	Number of Transients	8	Original Points Count	13107
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.700	Spectrum Type	STANDARD

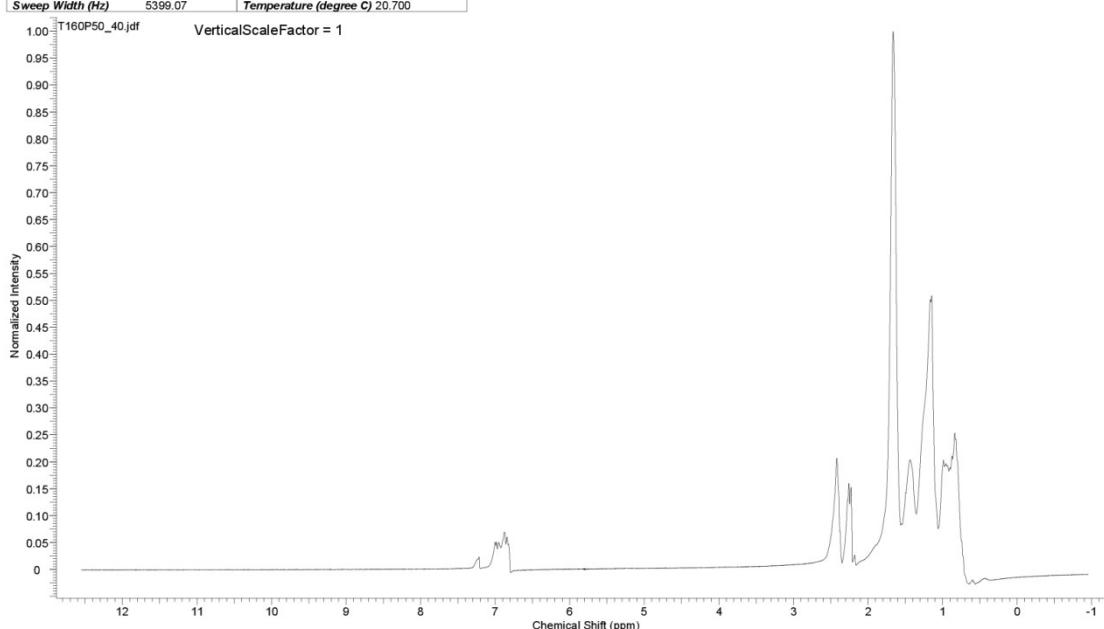


Figure S 50: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 40 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:20

Acquisition Time (sec)	2.4276	Date	19 Nov 2013 15:39:03	Date Stamp	19 Nov 2013 14:44:48
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T160P50\T160P50_50.jdf	Frequency (MHz)	399.78		
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.900	Spectrum Type	STANDARD

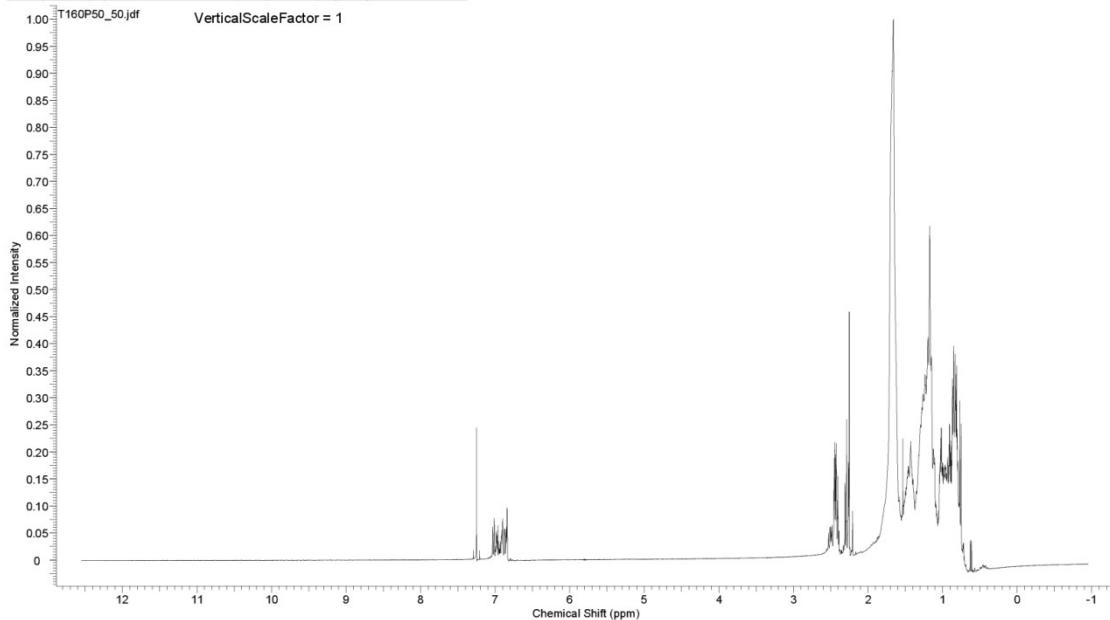


Figure S 51: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 50 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:27

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.700	Spectrum Type	STANDARD

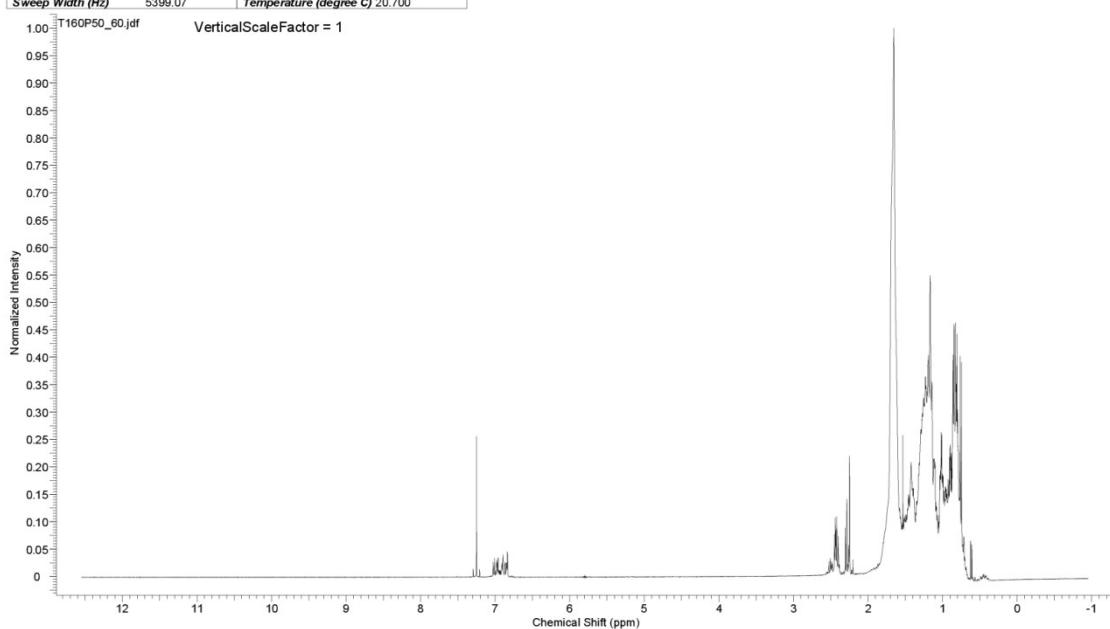


Figure S 52: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 60 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:34

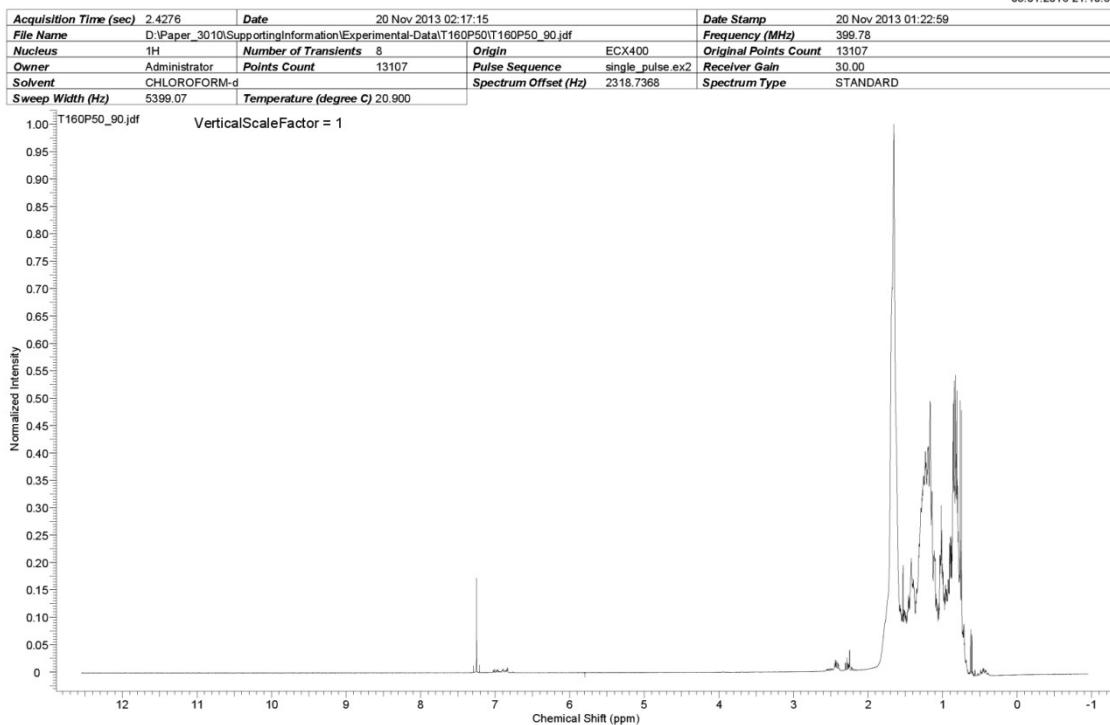


Figure S 53: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 90 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:10:41

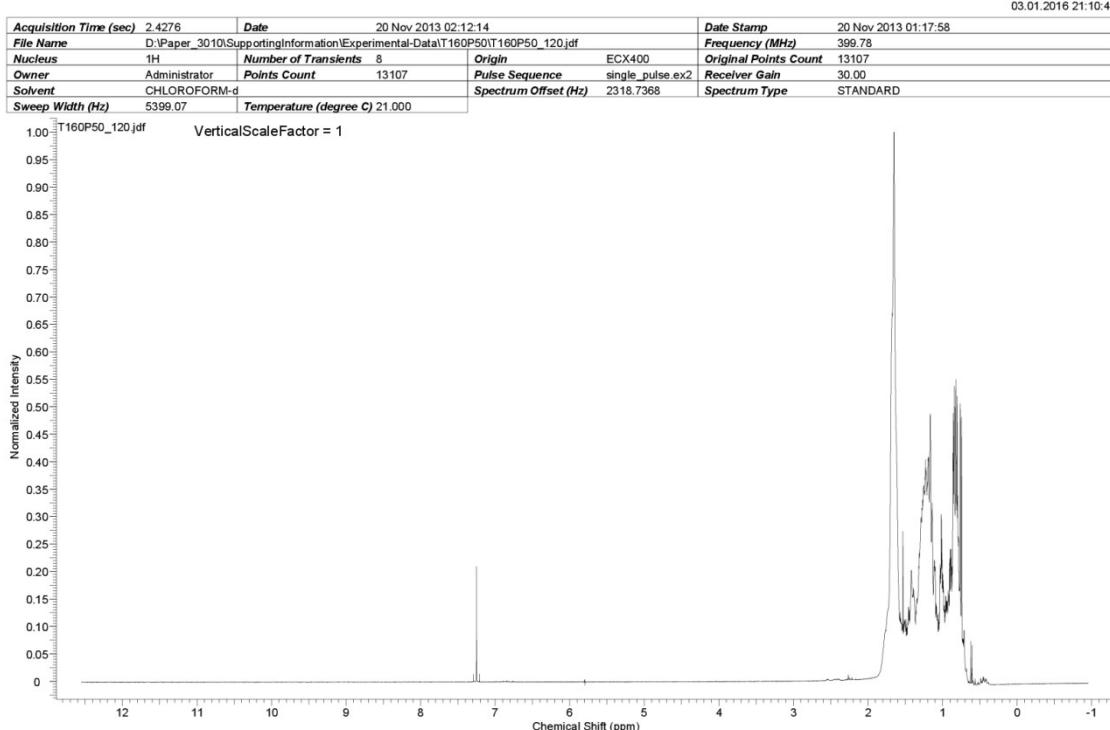


Figure S 54: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 120 \text{ min}$ ($T=160^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

T = 180 °C ; P = 50 bar

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03.01.2016 21:13:58

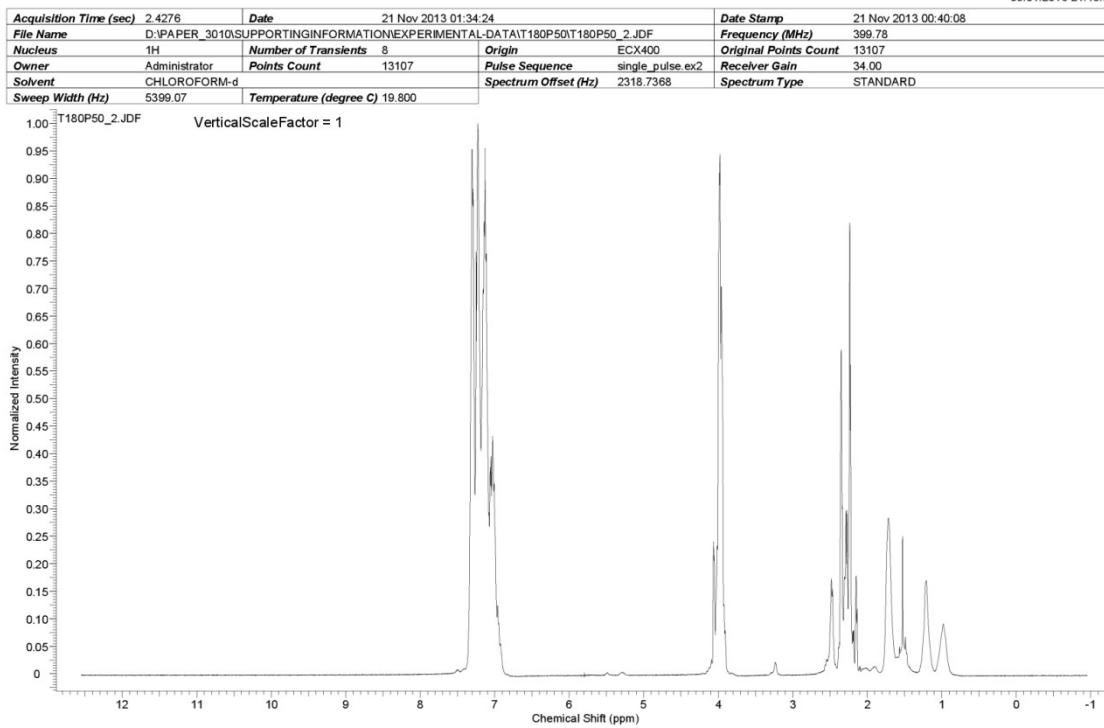


Figure S 55: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 2 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:14:18

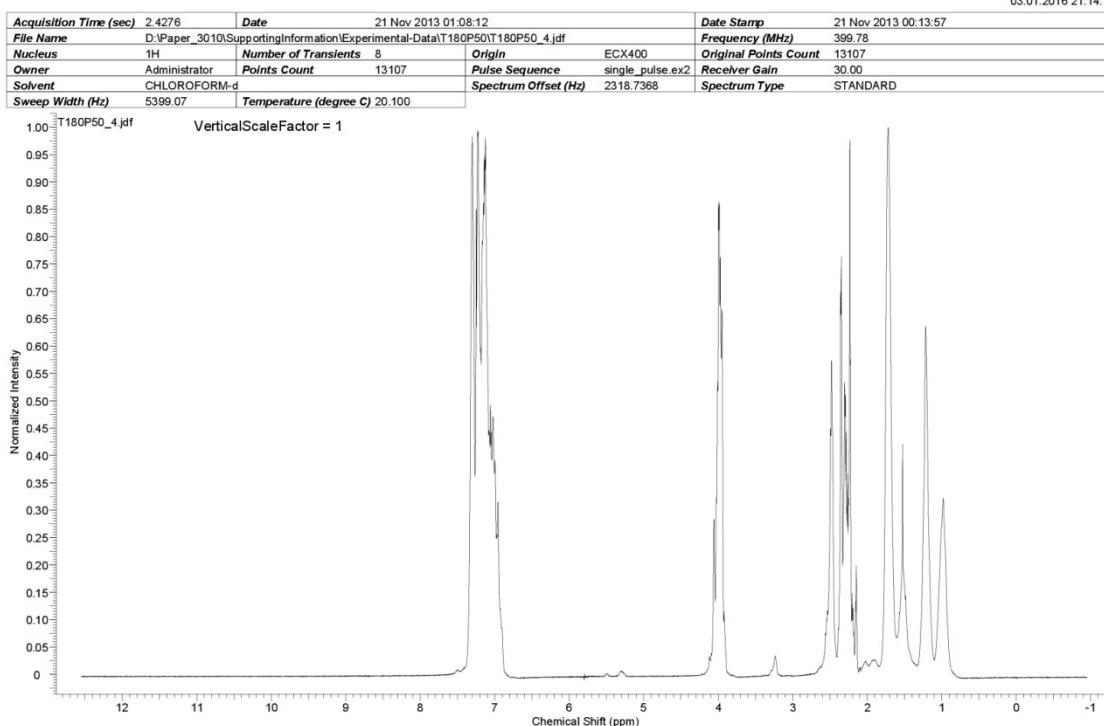


Figure S 56: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 4 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:14:26

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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	32.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.200	Spectrum Type	STANDARD

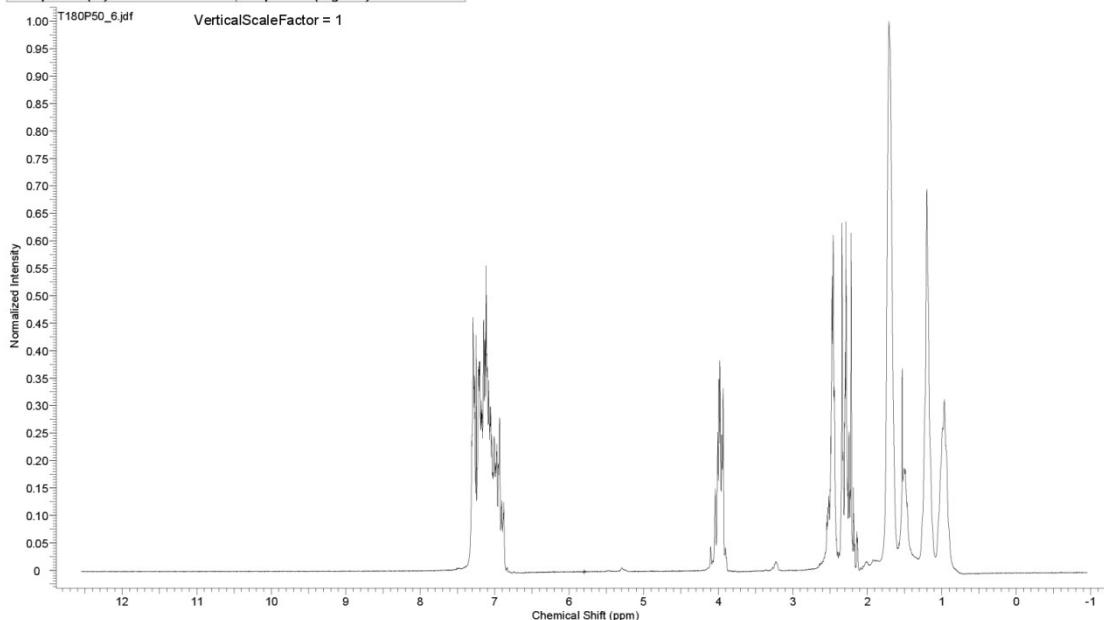


Figure S 57: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 6 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:14:37

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 01:18:11	Date Stamp	21 Nov 2013 00:23:55
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Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.000	Spectrum Type	STANDARD

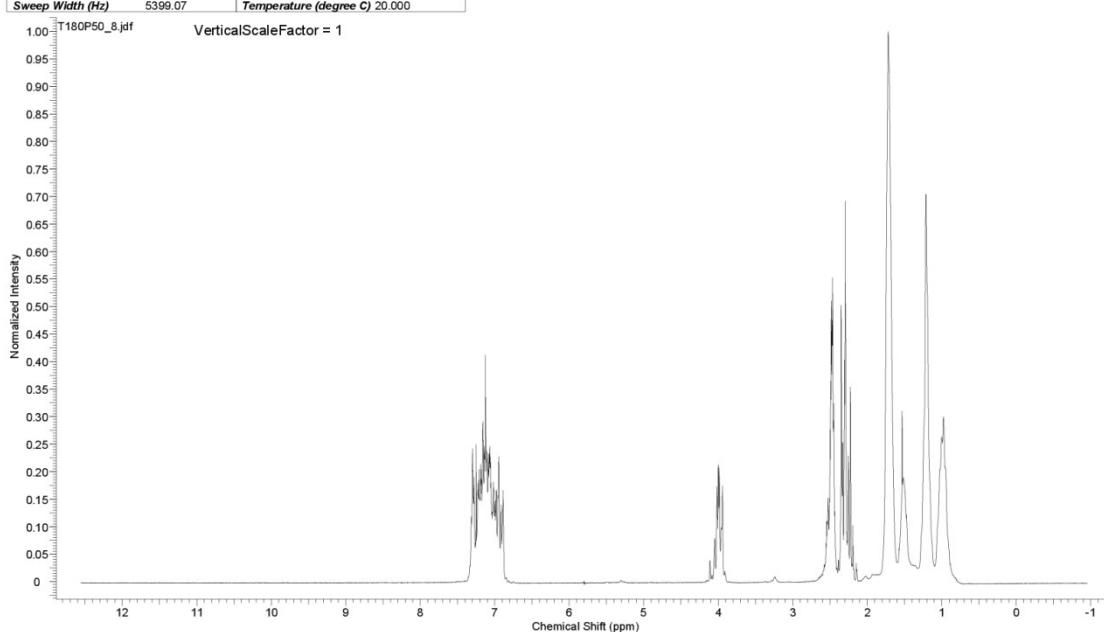


Figure S 58: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 8 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:14:45

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Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

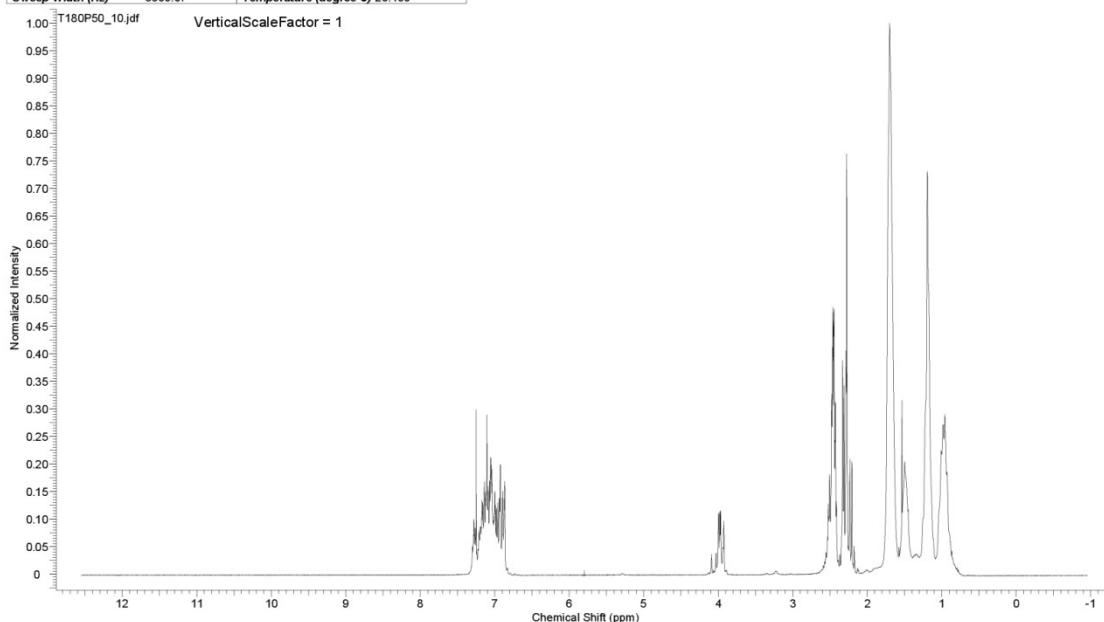


Figure S 59: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 10 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:14:51

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 00:42:07	Date Stamp	20 Nov 2013 18:00:06
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Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

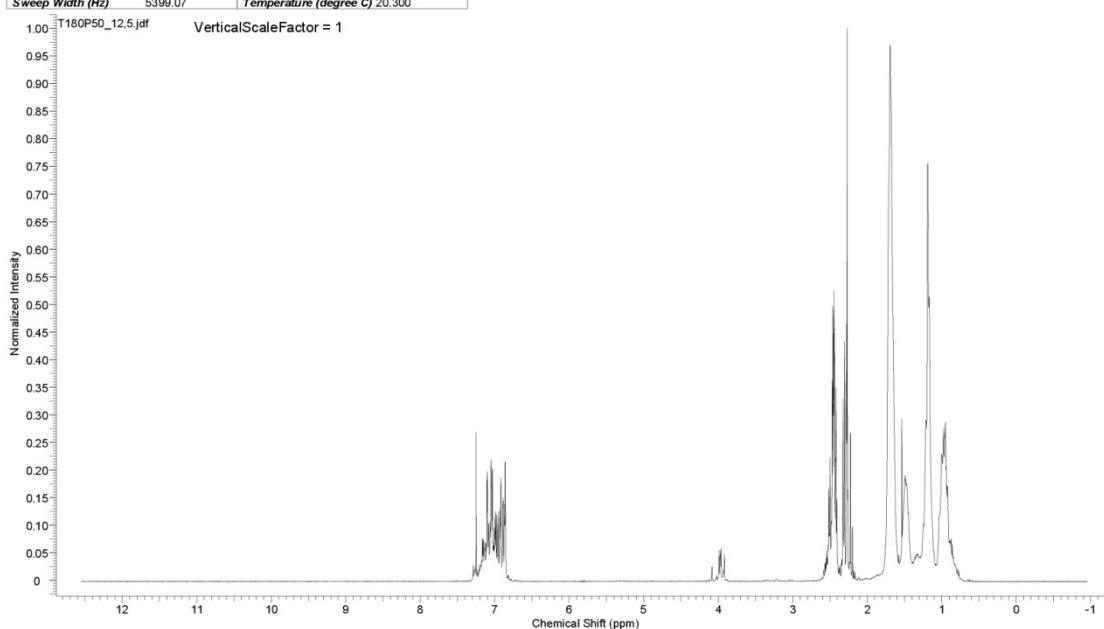


Figure S 60: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 12.5 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:14:59

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 01:23:41	Date Stamp	21 Nov 2013 00:29:25
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.000	Spectrum Type	STANDARD

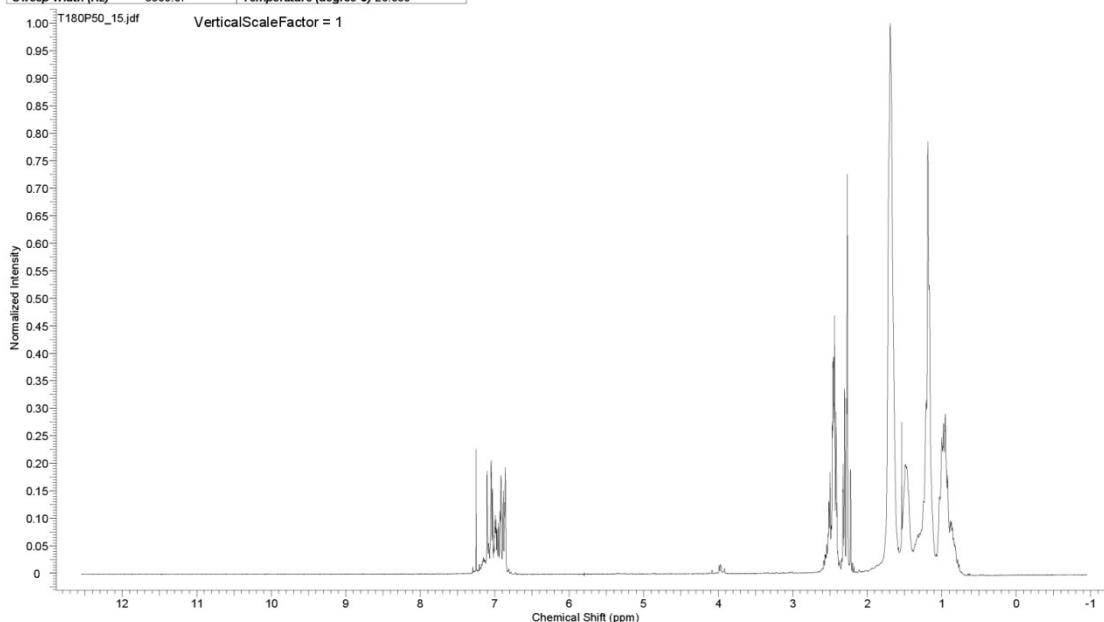


Figure S 61: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 15 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:15:06

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 00:57:53	Date Stamp	21 Nov 2013 00:03:37
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T180P50\T180P50_20.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.200	Spectrum Type	STANDARD

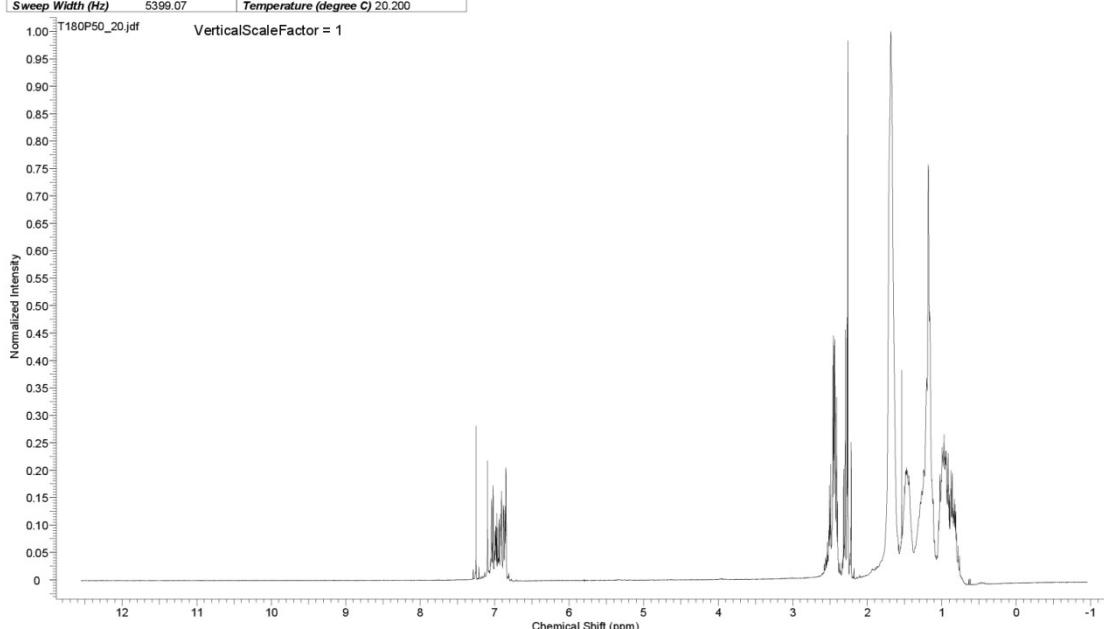


Figure S 62: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 20 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:15:18

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 01:39:41	Date Stamp	21 Nov 2013 00:45:25
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T180P50\T180P50_25.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	32.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.800	Spectrum Type	STANDARD

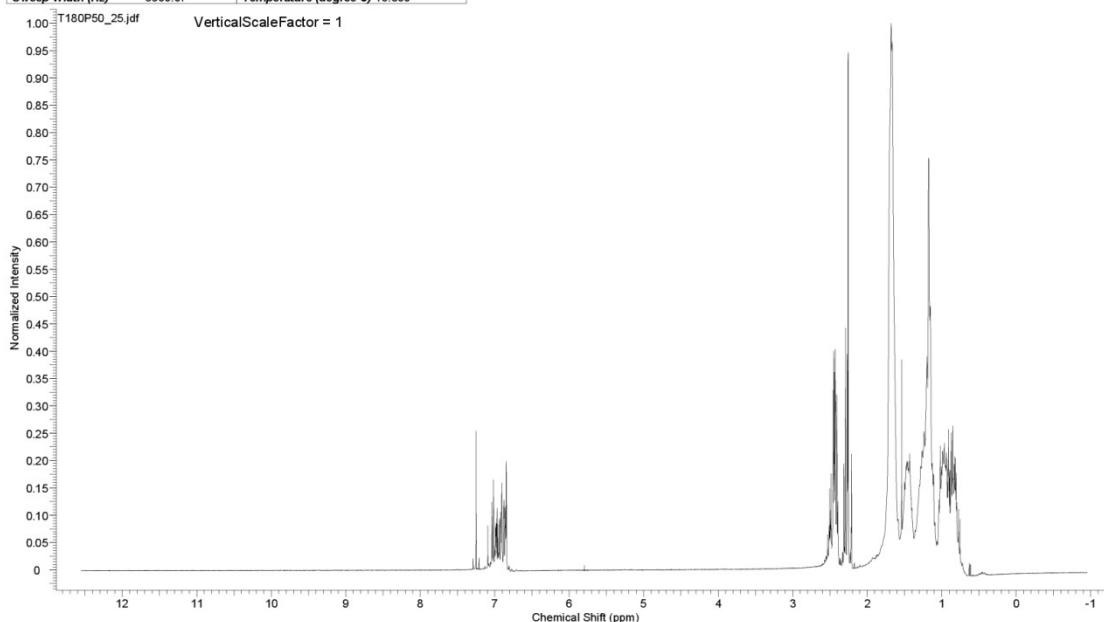


Figure S 63: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 25 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:15:25

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 01:39:02	Date Stamp	21 Nov 2013 00:18:46
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	20.100	Spectrum Type	STANDARD

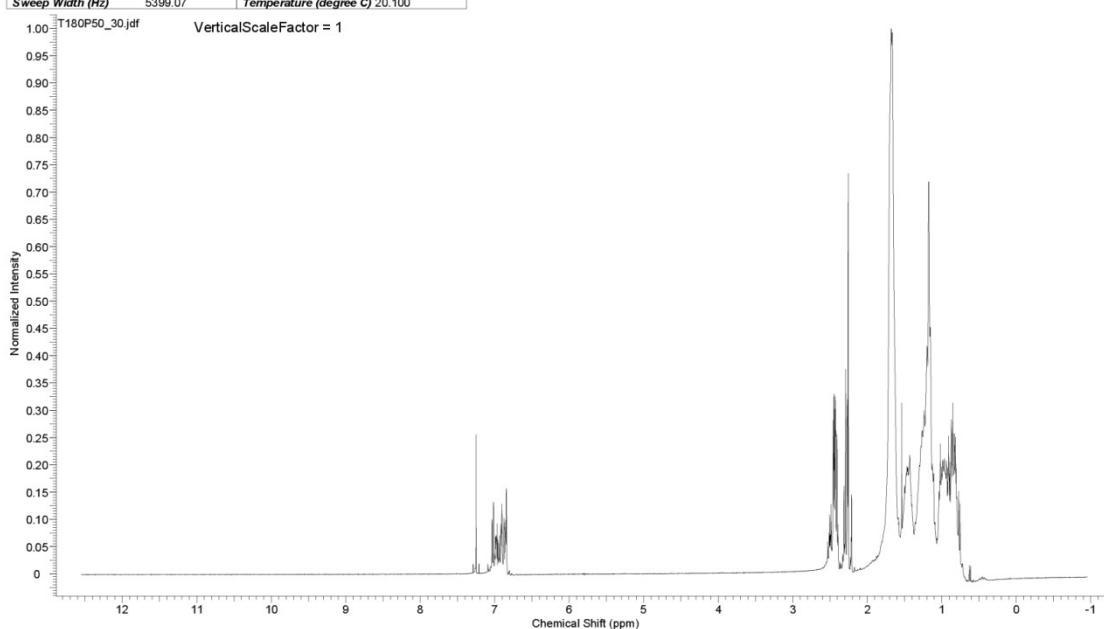


Figure S 64: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 30 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:15:32

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 01:28:57	Date Stamp	21 Nov 2013 00:34:41
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Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

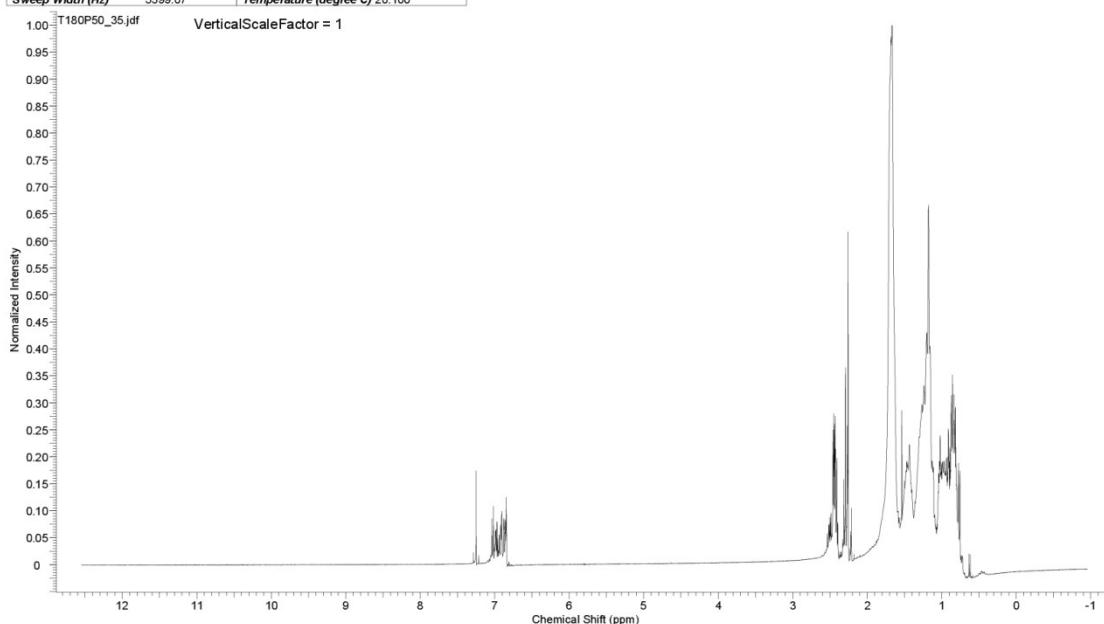


Figure S 65: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 35 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:15:40

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 00:36:48	Date Stamp	20 Nov 2013 17:54:48
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Owner	Administrator	Points Count	13107	Original Points Count	13107
Solvent	CHLOROFORM-d	Pulse Sequence	single_pulse.ex2	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Spectrum Offset (Hz)	2318.7368	Spectrum Type	STANDARD

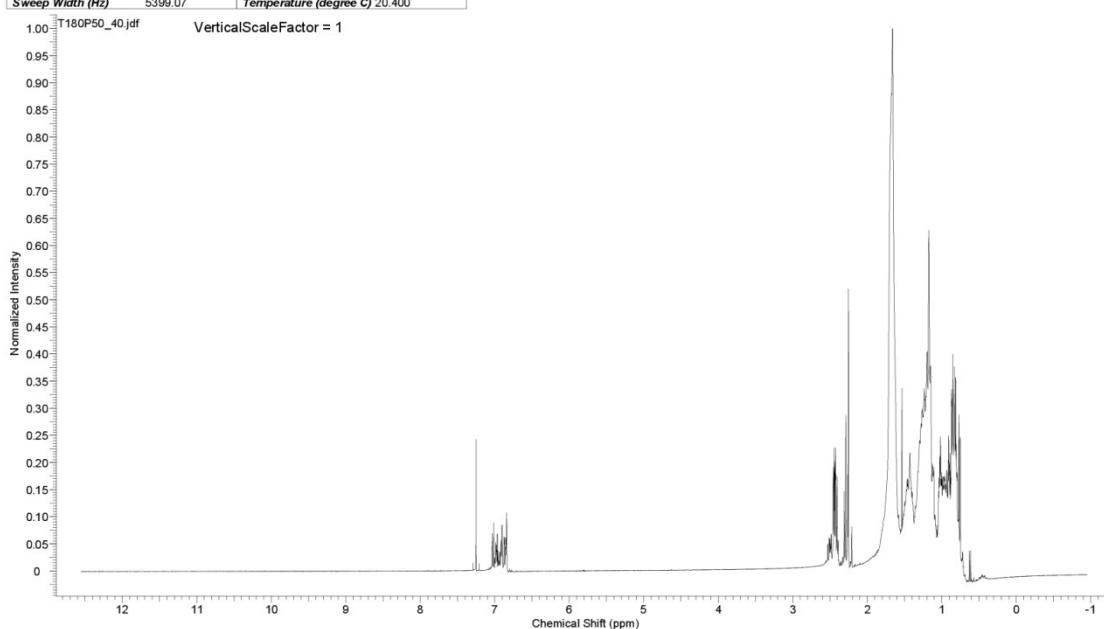


Figure S 66: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 40 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:15:48

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 08:17:31	Date Stamp	21 Nov 2013 07:23:15
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T180P50\T180P50_50.jdf	Frequency (MHz)	399.78	Original Points Count	13107
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.600	Spectrum Type	STANDARD

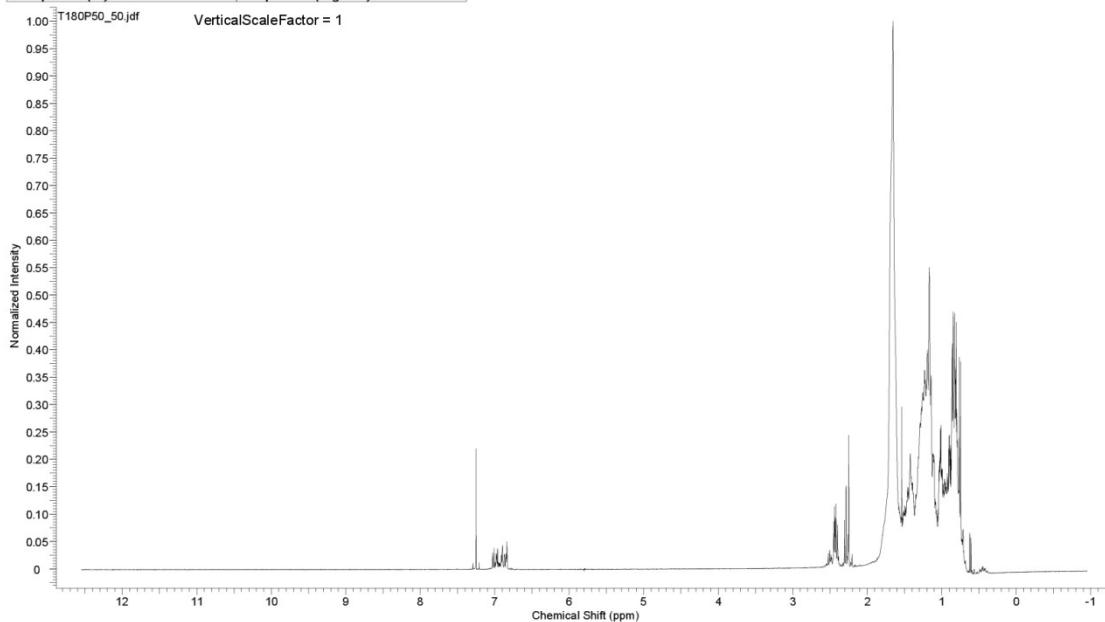


Figure S 67: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 50 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:15:54

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Nucleus	1H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.500	Spectrum Type	STANDARD

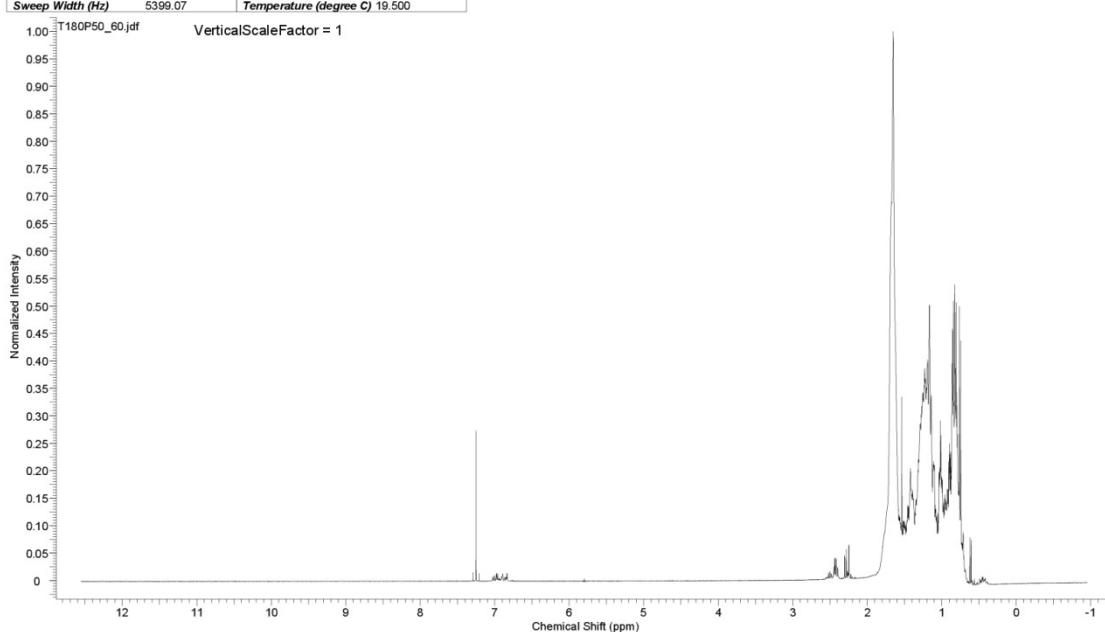


Figure S 68: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 60 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:16:00

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 08:23:01	Date Stamp	21 Nov 2013 07:28:45
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T180P50\T180P50_90.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.400	Spectrum Type	STANDARD

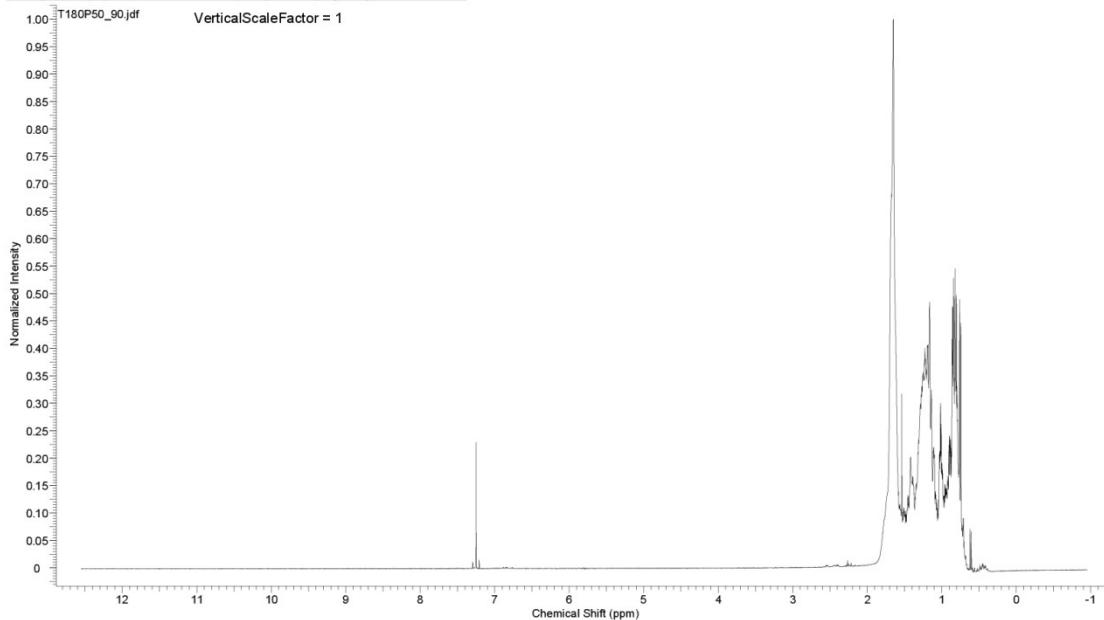


Figure S 69: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 90 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:16:10

Acquisition Time (sec)	2.4276	Date	21 Nov 2013 08:27:22	Date Stamp	21 Nov 2013 07:13:05
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T180P50\T180P50_120.jdf	Frequency (MHz)	399.78	Original Points Count	13107
Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	19.500	Spectrum Type	STANDARD

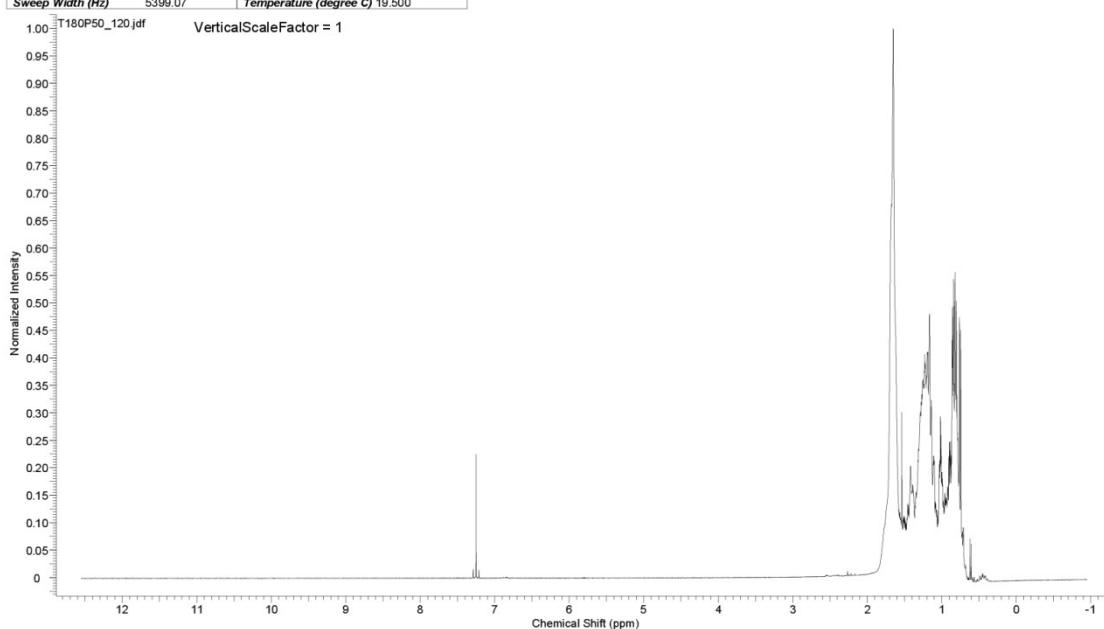


Figure S 70: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 120 \text{ min}$ ($T=180^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

T = 200 °C ; P = 50 bar

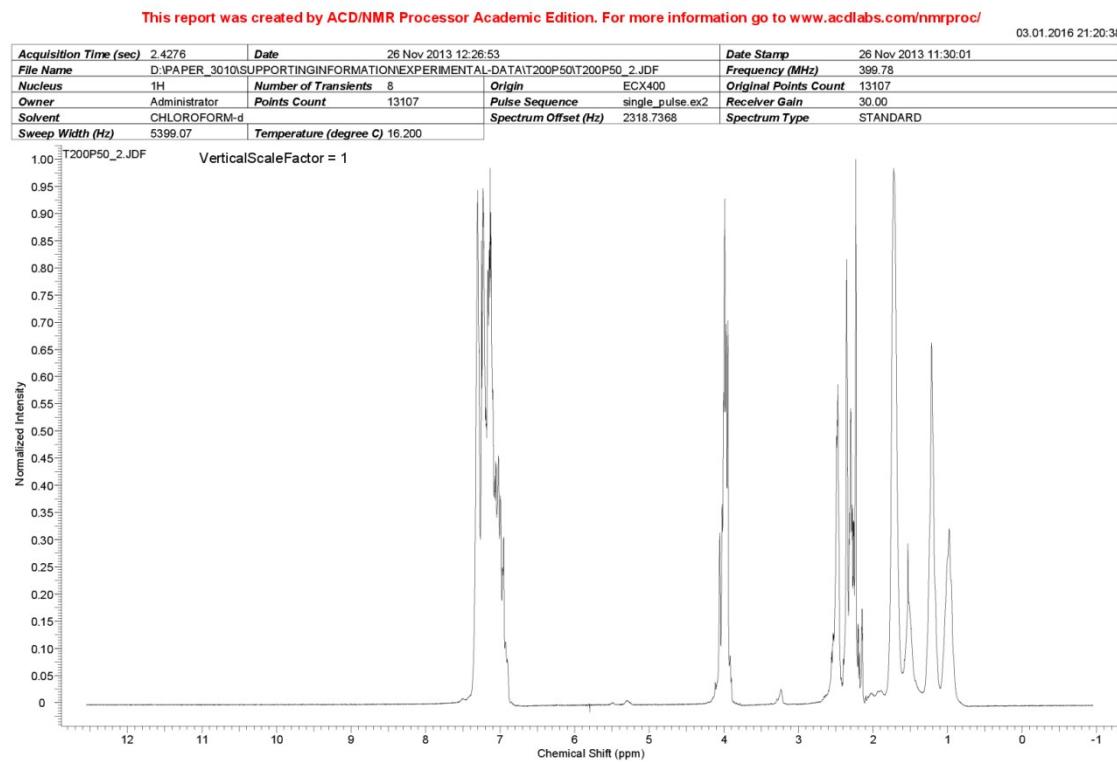


Figure S 71: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 2 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

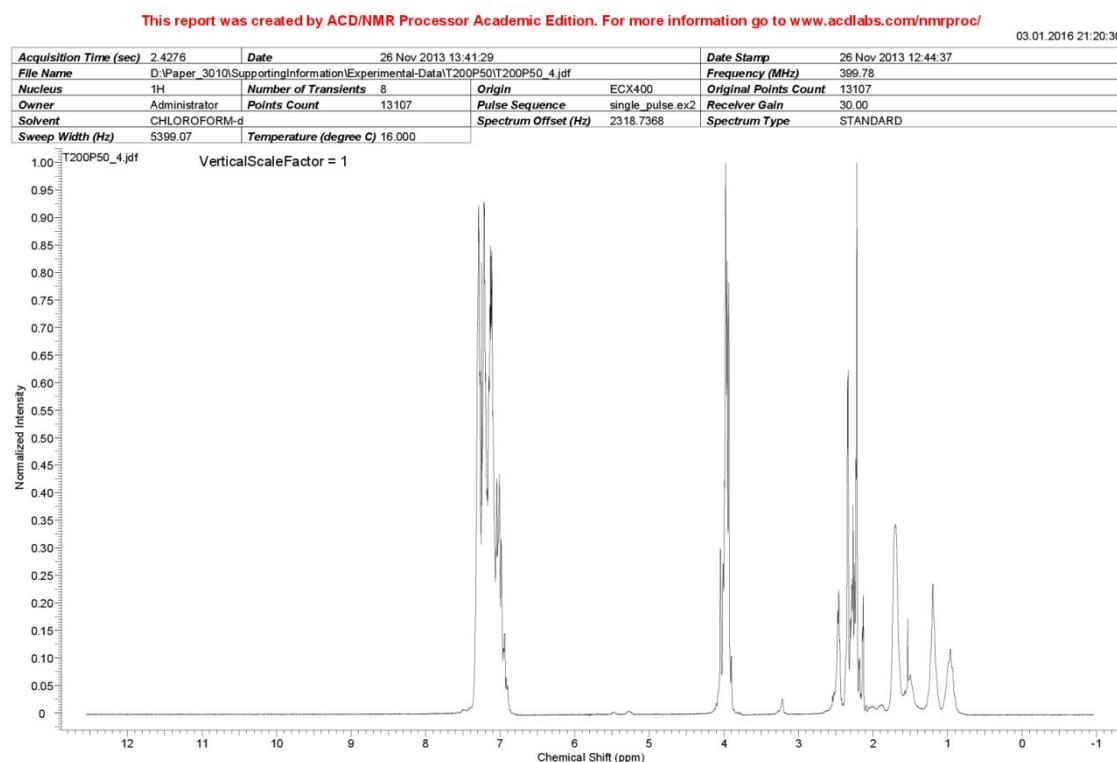


Figure S 72: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 4 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:20:19

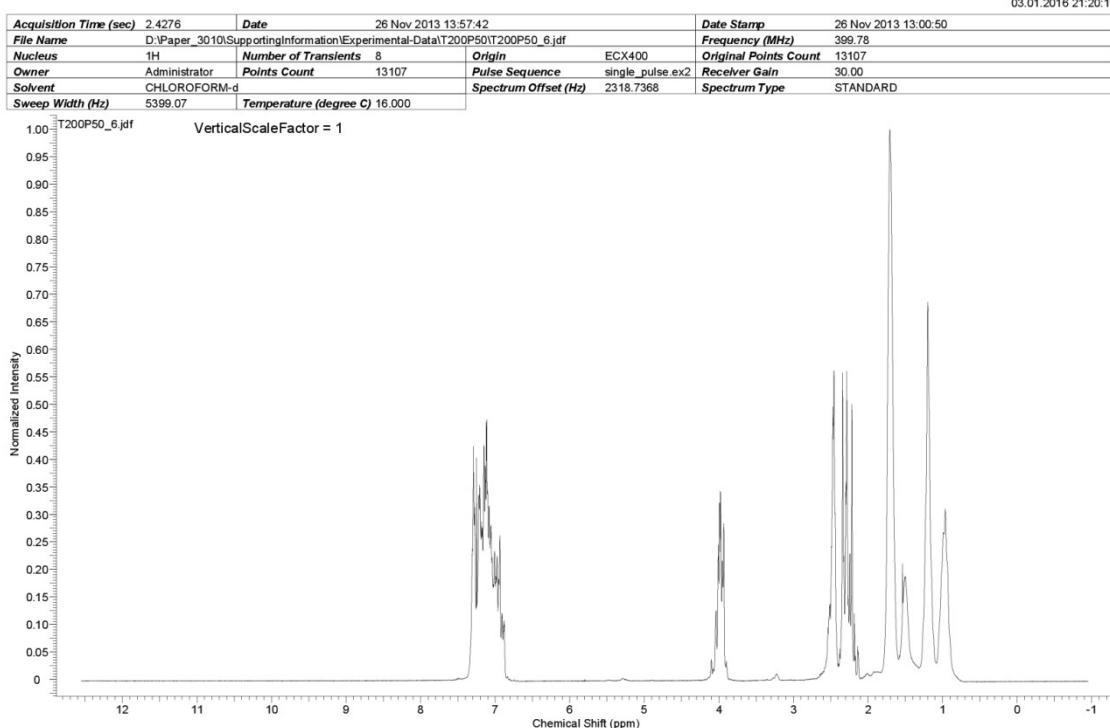


Figure S 73: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 6 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:20:10

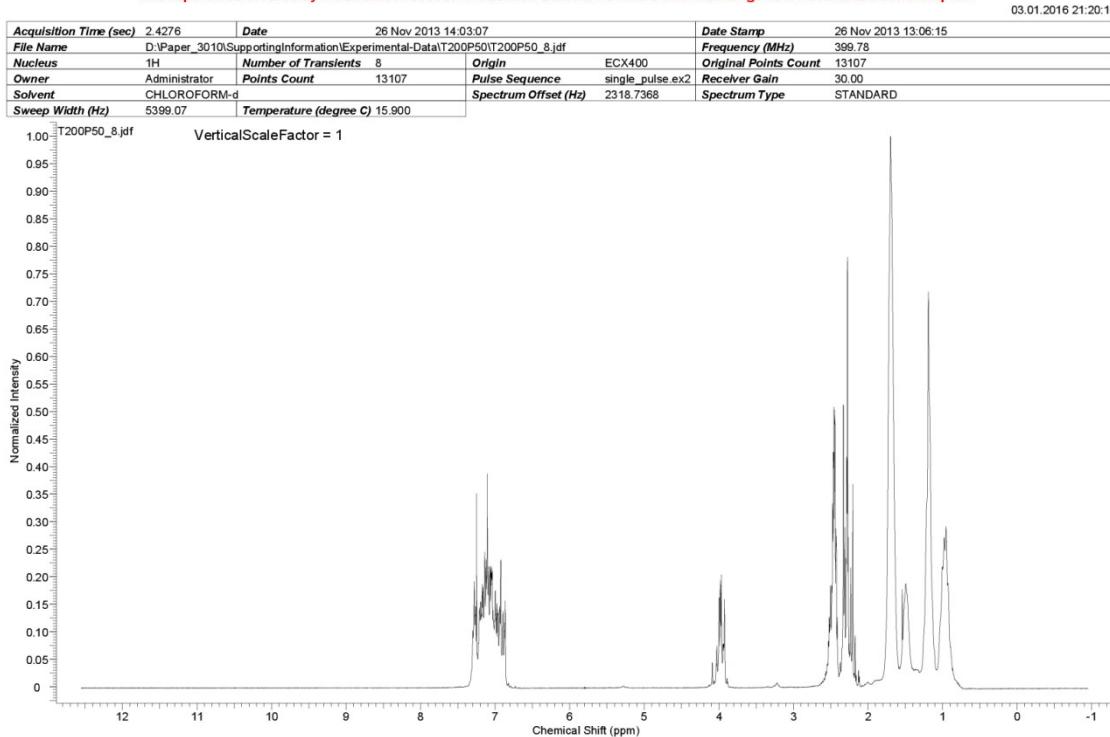


Figure S 74: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 8 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:20:02

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 12:16:15	Date Stamp	26 Nov 2013 11:19:23
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.200	Spectrum Type	STANDARD

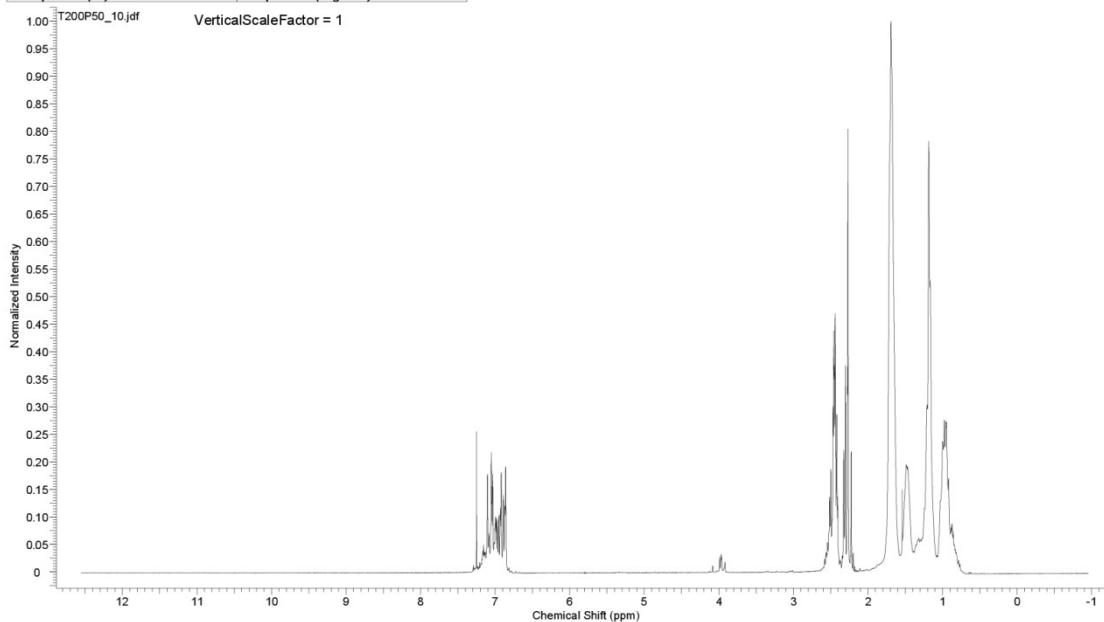


Figure S 75: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 10 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:19:52

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 12:21:40	Date Stamp	26 Nov 2013 11:24:48
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T200P50\T200P50_12.5.jdf	Frequency (MHz)	399.78		
Nucleus	¹ H	Number of Transients	8	Origin	ECX400
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	28.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.300	Spectrum Type	STANDARD

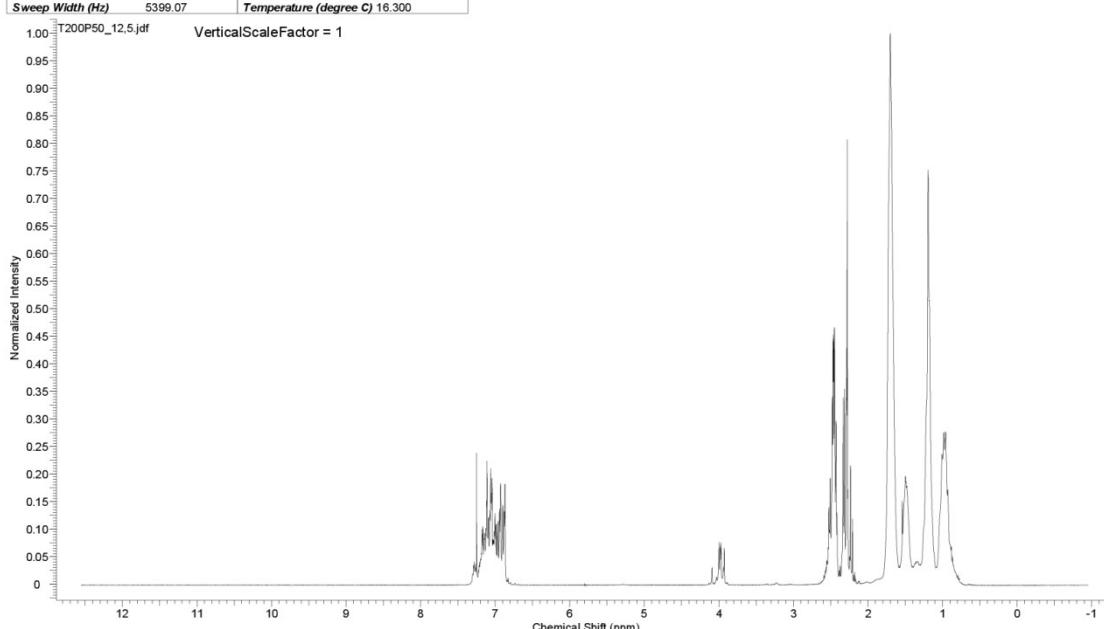


Figure S 76: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 12.5 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:19:40

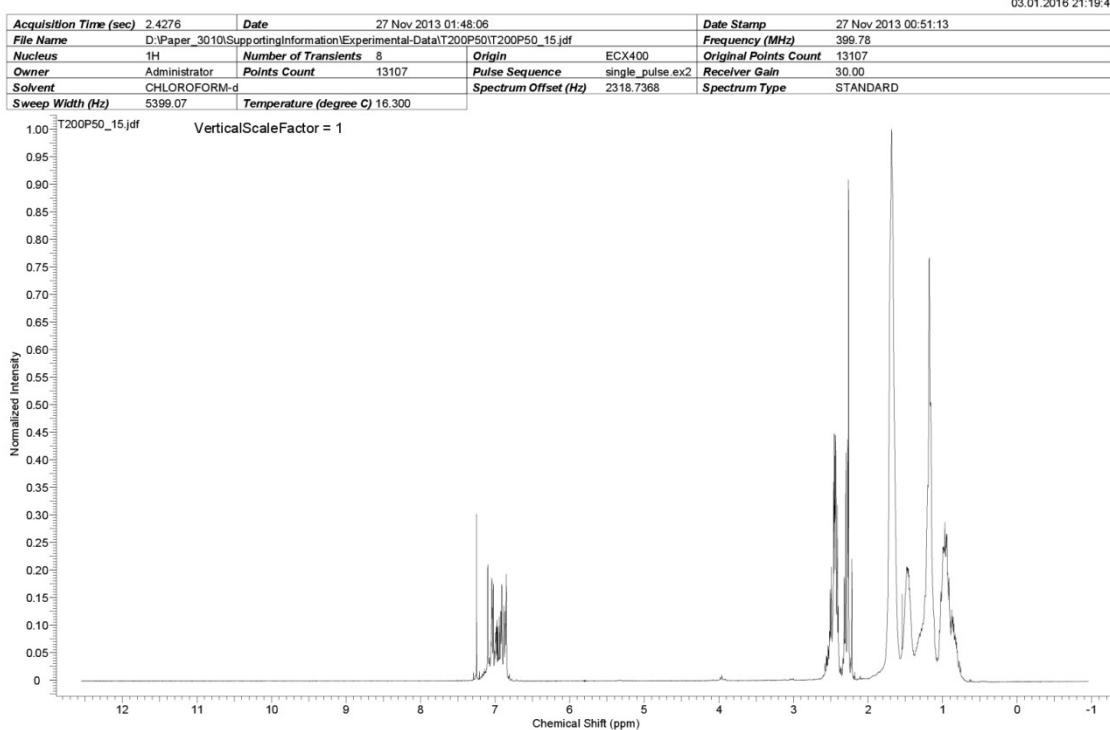


Figure S 77: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 15 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:19:32

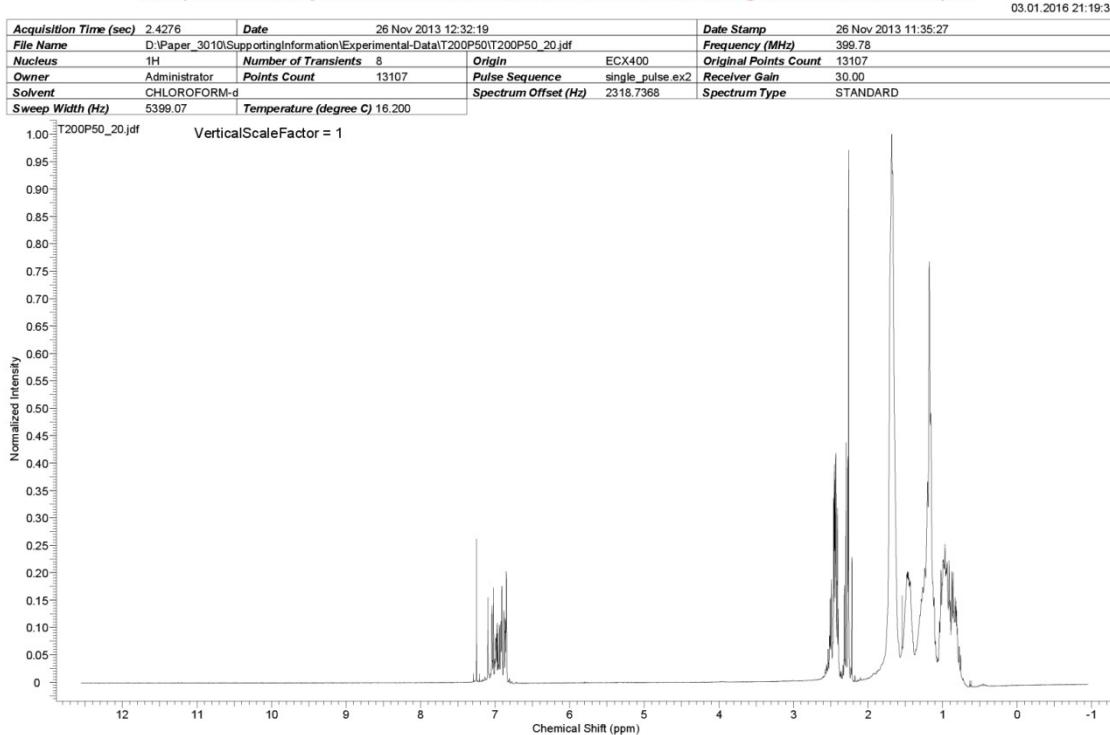


Figure S 78: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 20 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:19:21

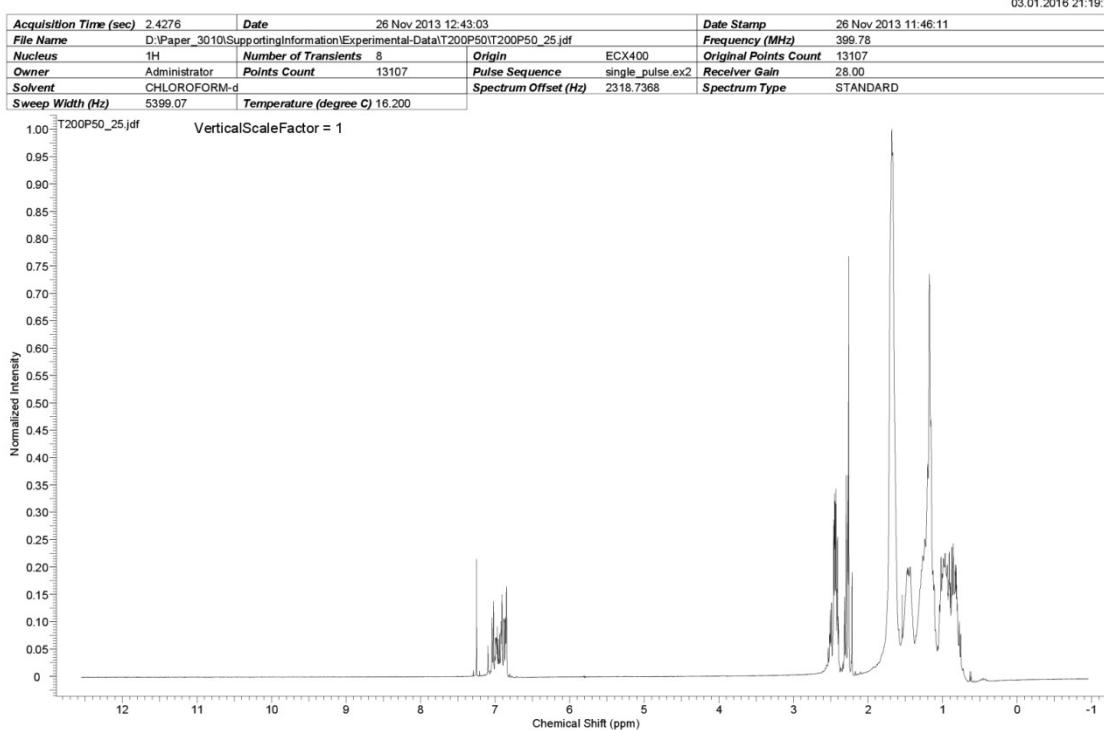


Figure S 79: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 25 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:19:13

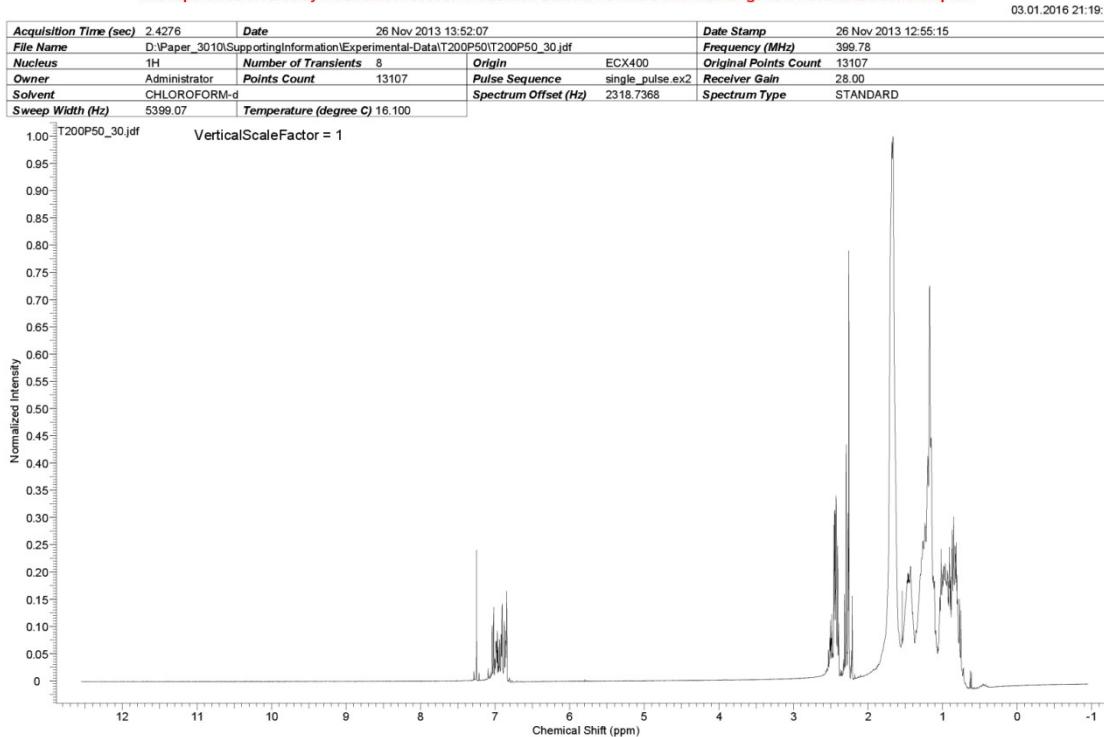


Figure S 80: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 30 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:19:05

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 12:53:44	Date Stamp	26 Nov 2013 11:56:52
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T200P50\T200P50_35.jdf	Frequency (MHz)	399.78		
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.000	Spectrum Type	STANDARD

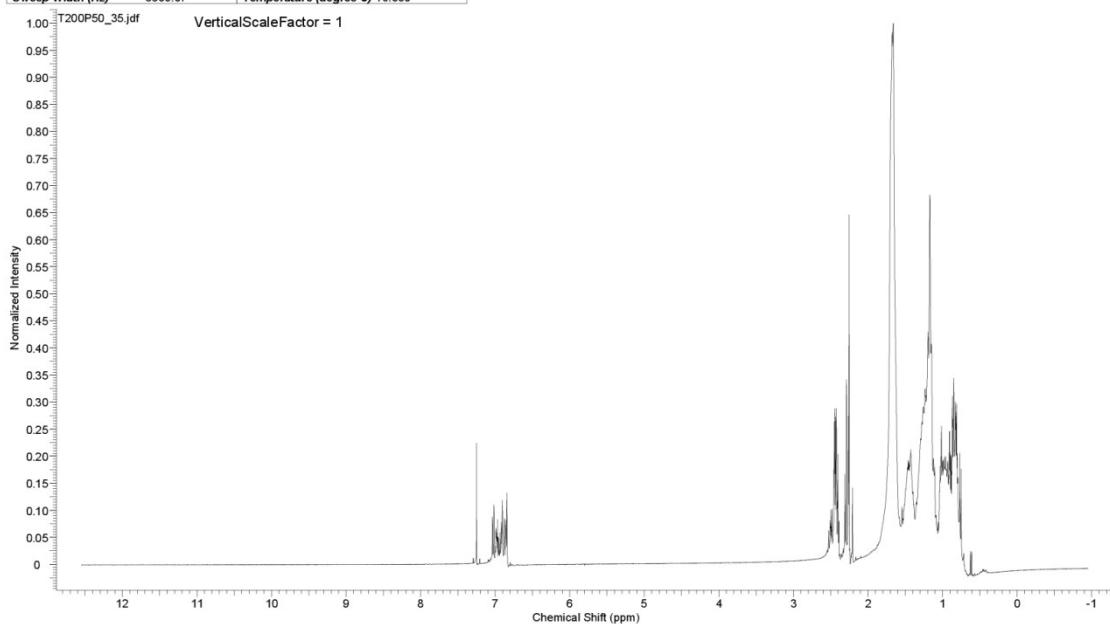


Figure S 81: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 35 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:18:57

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 13:36:25	Date Stamp	26 Nov 2013 12:39:33
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T200P50\T200P50_40.jdf	Frequency (MHz)	399.78		
Nucleus	¹ H	Number of Transients	8	Original Points Count	13107
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	26.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.100	Spectrum Type	STANDARD

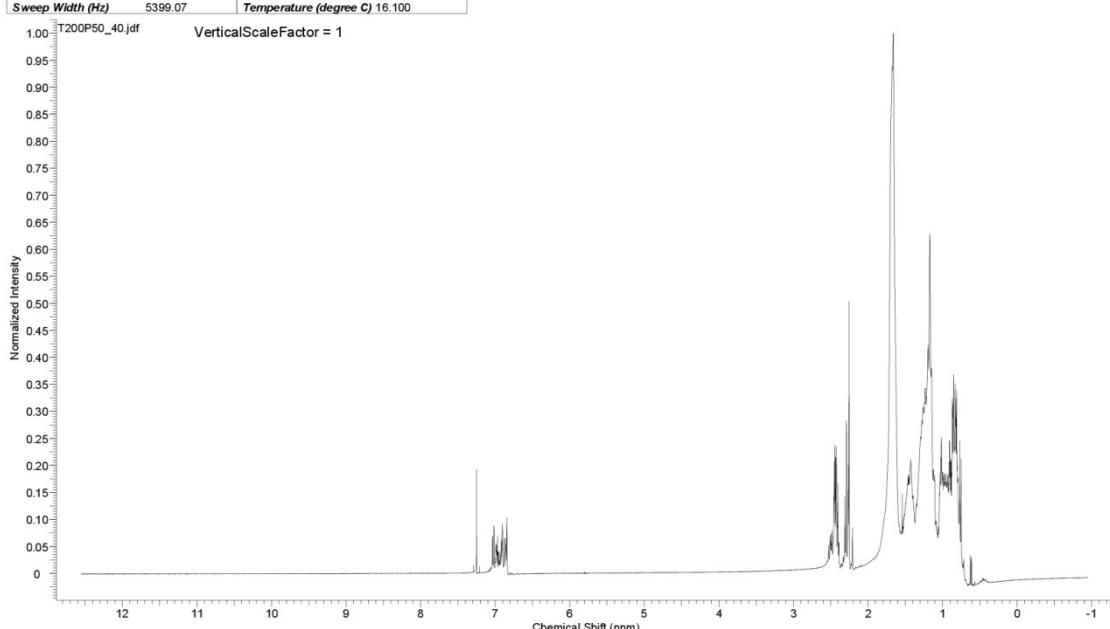


Figure S 82: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 40 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:18:44

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 12:37:34	Date Stamp	26 Nov 2013 11:40:42
File Name	D:\Paper_3010\SupportingInformation\Experimental-Data\T200P50\T200P50_50.jdf	Frequency (MHz)	399.78		
Nucleus	¹ H	Number of Transients	8	Original Points Count	13107
Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	30.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.300	Spectrum Type	STANDARD

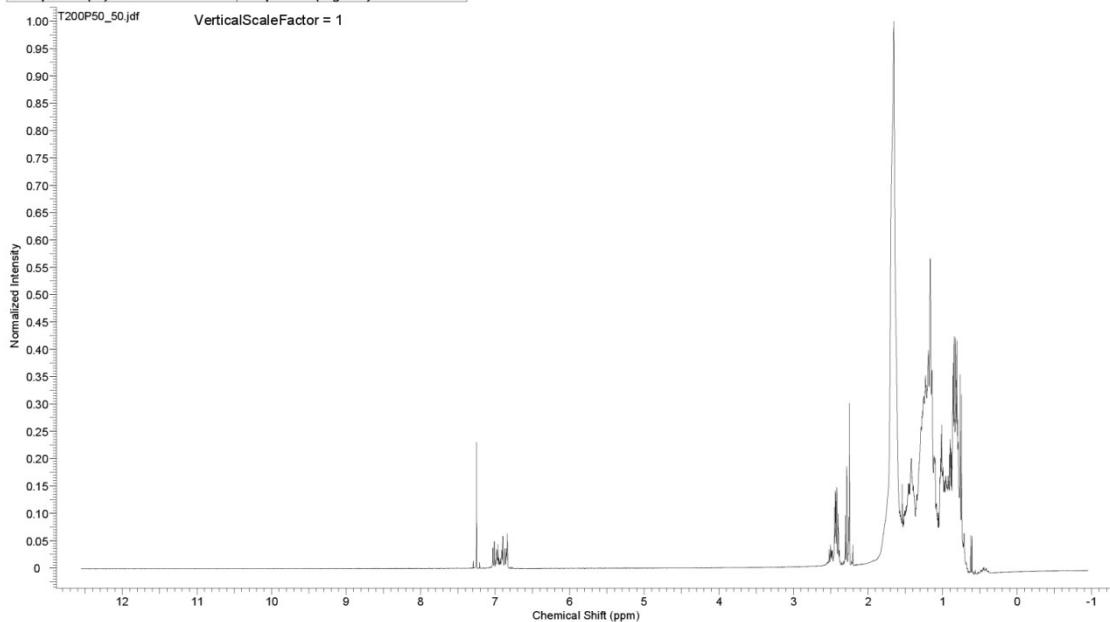


Figure S 83: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 50 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

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03.01.2016 21:18:34

Acquisition Time (sec)	2.4276	Date	26 Nov 2013 12:48:42	Date Stamp	26 Nov 2013 11:51:51
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Owner	Administrator	Points Count	13107	Pulse Sequence	single_pulse.ex2
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2318.7368	Receiver Gain	28.00
Sweep Width (Hz)	5399.07	Temperature (degree C)	16.100	Spectrum Type	STANDARD

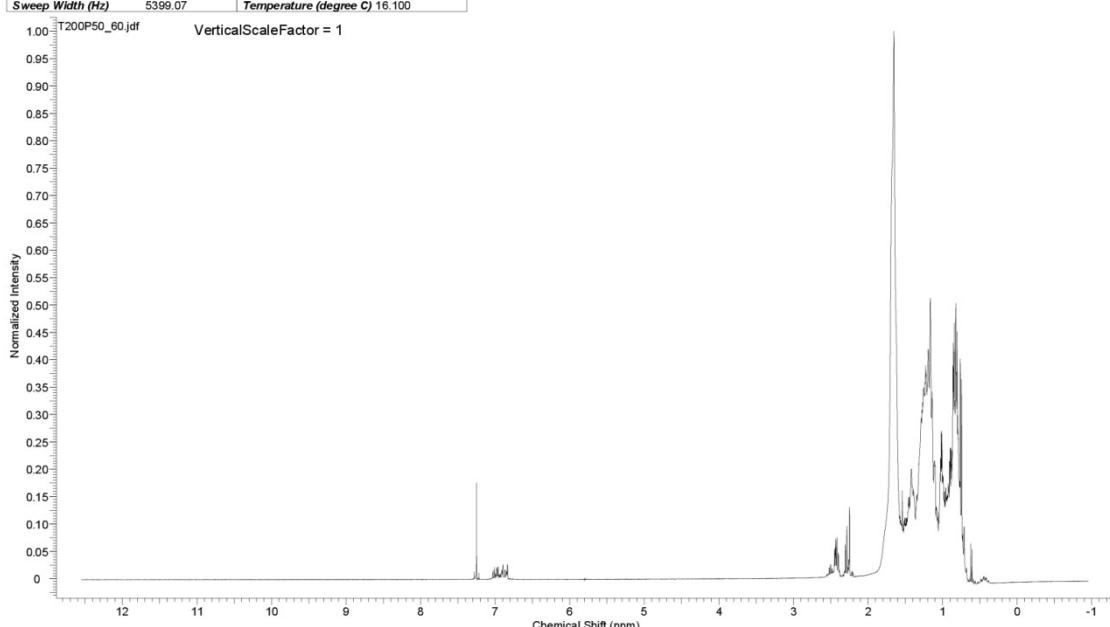


Figure S 84: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 60 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{HO-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:18:24

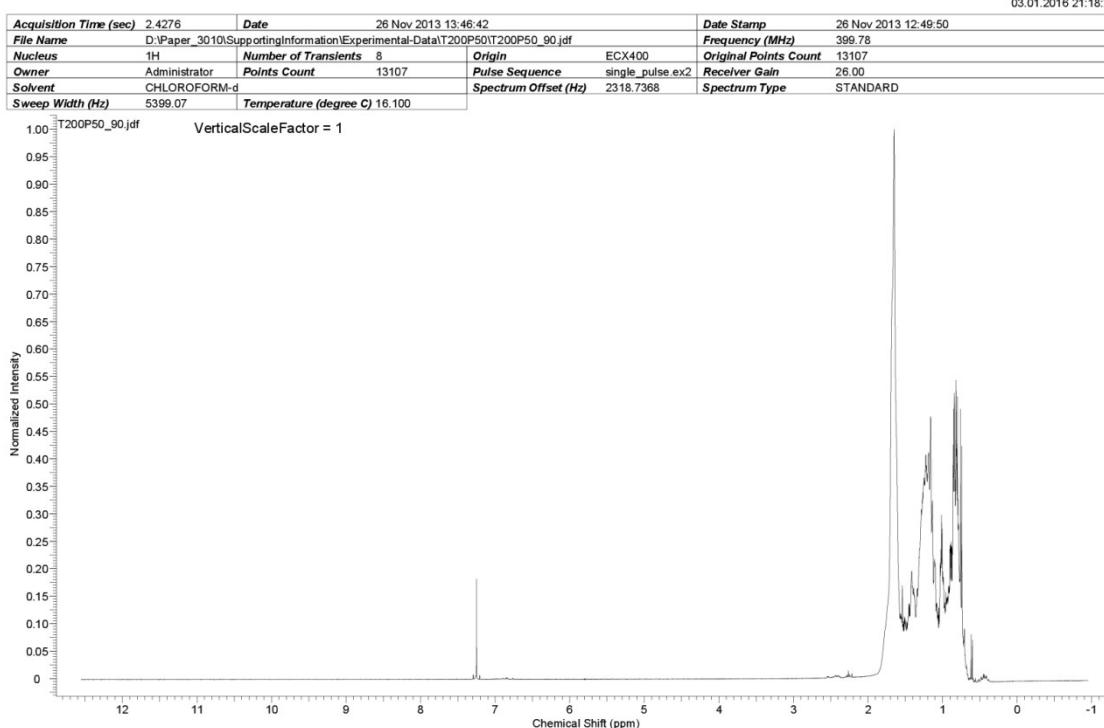


Figure S 85: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 90 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)

This report was created by ACD/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrproc/

03.01.2016 21:18:13

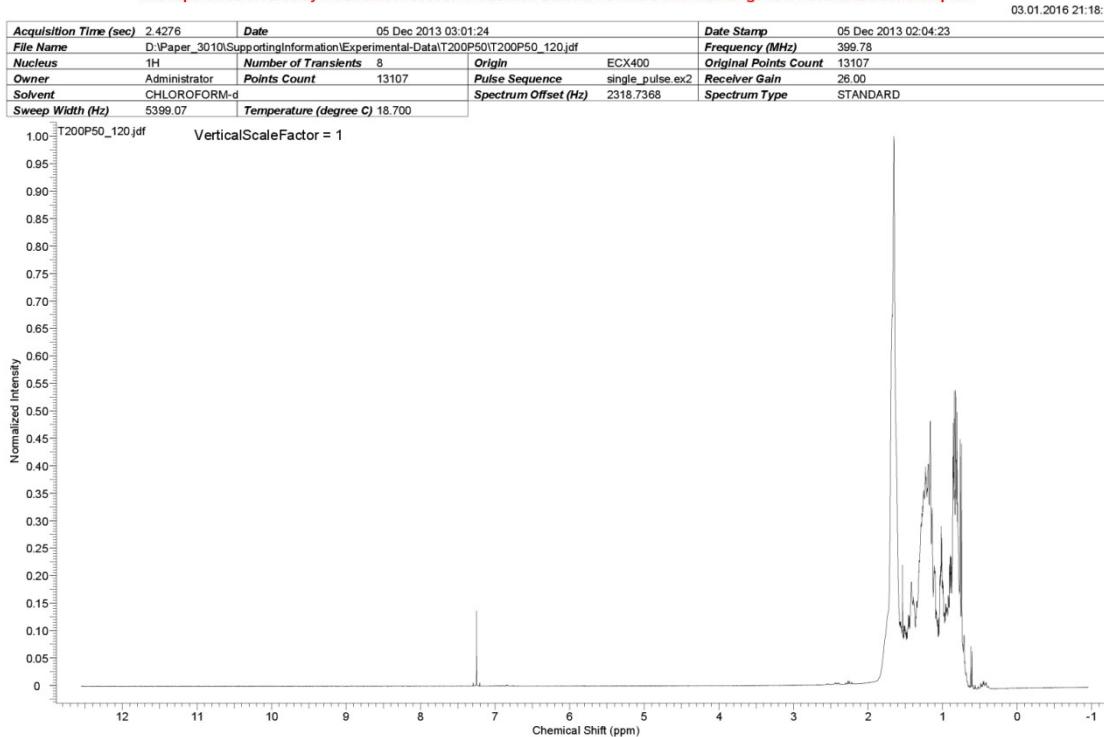


Figure S 86: Hydrogenation of Dibenzyltoluene $t_{\text{sample}} = 120 \text{ min}$ ($T=200^\circ\text{C}$; $P=50 \text{ bar}$; Cat.: 0.5 wt% Ru/ Al_2O_3 ; $m[\text{H}_2\text{-DBT}]=150 \text{ g}$; $n_{\text{Ru}}/n_{\text{Al}_2\text{O}_3}=0.25 \text{ mol\%}$)