^{1}H NMR Analysis of the Metathesis Reaction between 1-Hexene and (*E*)-Anethole Using Grubbs 2nd Generation Catalyst: Effect of Reaction Conditions on (*E*)-1-(4-methoxyphenyl)-1-hexene formation and decomposition

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Supplementary Information

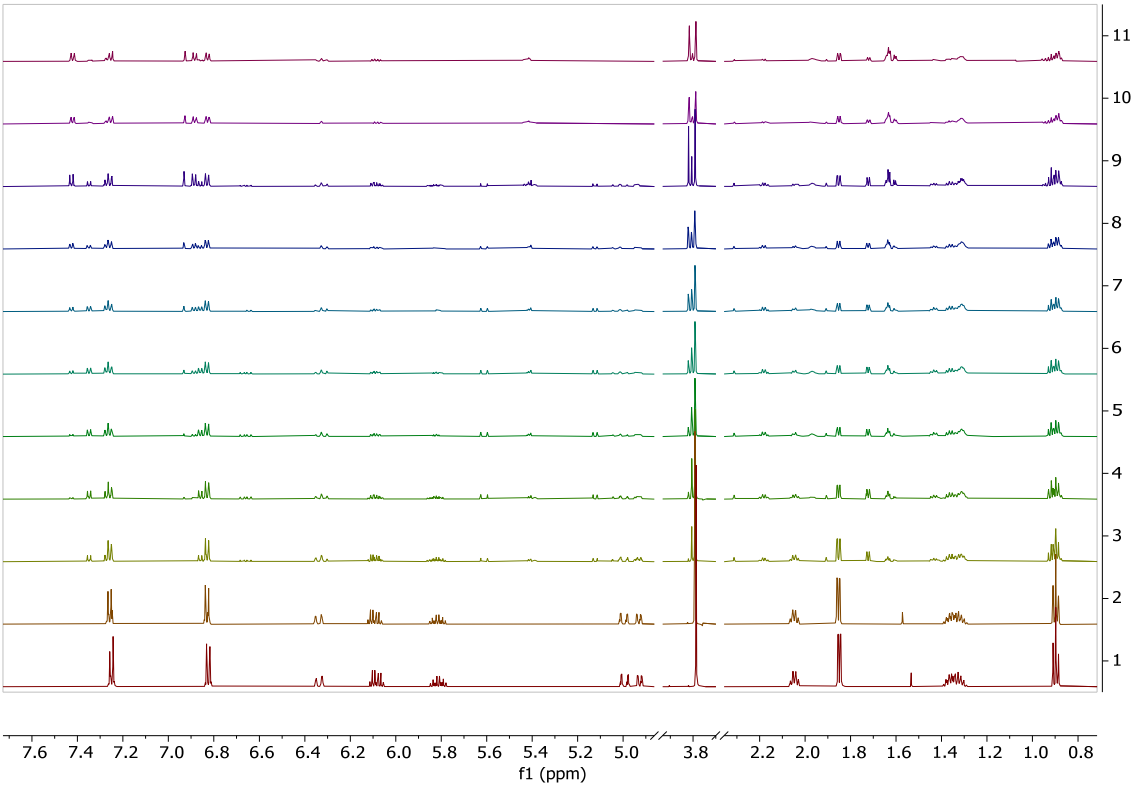

Figure S1. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.5) in the presence of Grubbs 2nd generation catalyst at 15 °C in $CDCl_3$ (experiment 1). The spectra at times t = 0 min. (1), t = 4 min. (2), t = 16 min. (3), t = 49 min. (4), t = 102 min. (5), t = 175 min. (6), t = 268 min. (7), t = 371 min. (8), t = 504 min. (9), t = 657 min. (10) and t = 724 min. (11).

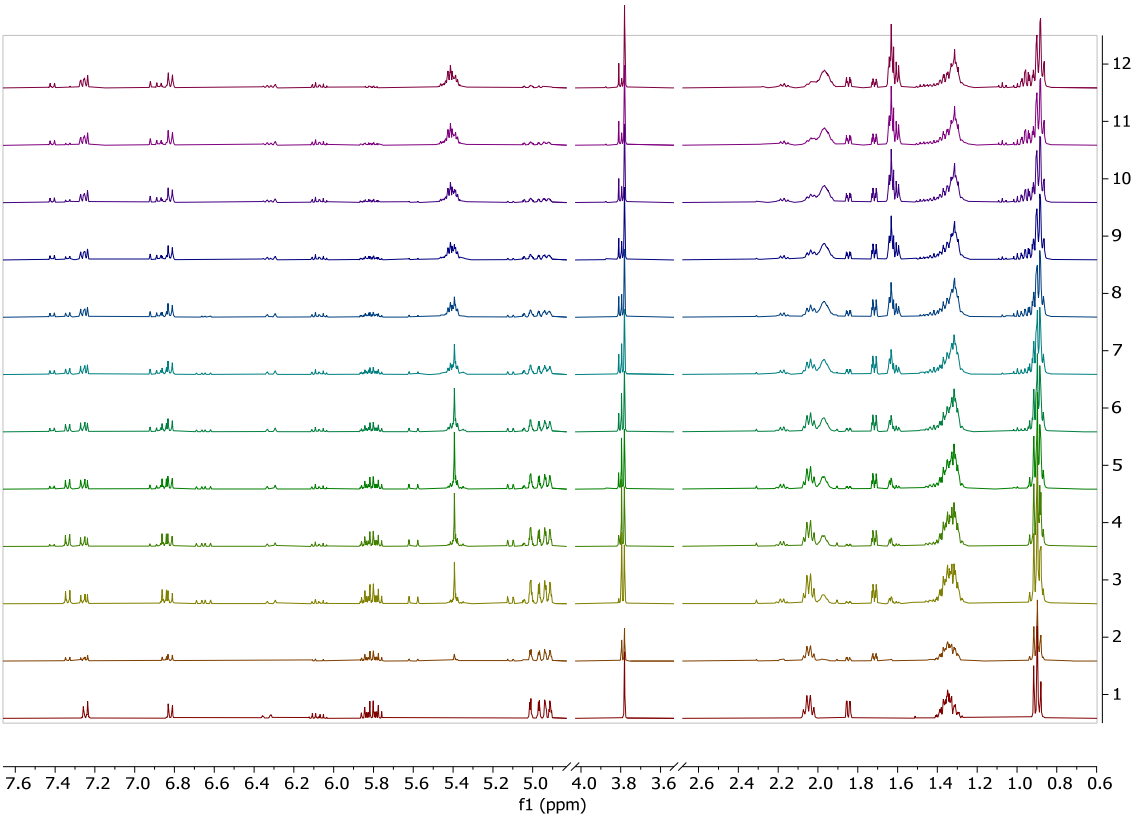

Figure S2. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.17) in the presence of Grubbs 2nd generation catalyst at 25 °C in $CDCl_3$ (experiment 2). The spectra at times t=0 min. (1), t=4 min. (2), t=16 min. (3), t=49 min. (4), t=102 min. (5), t=175 min. (6), t=268 min. (7), t=371 min. (8), t=504 min. (9), t=657 min. (10), t=830 min. (11) and t=1023 min. (12).

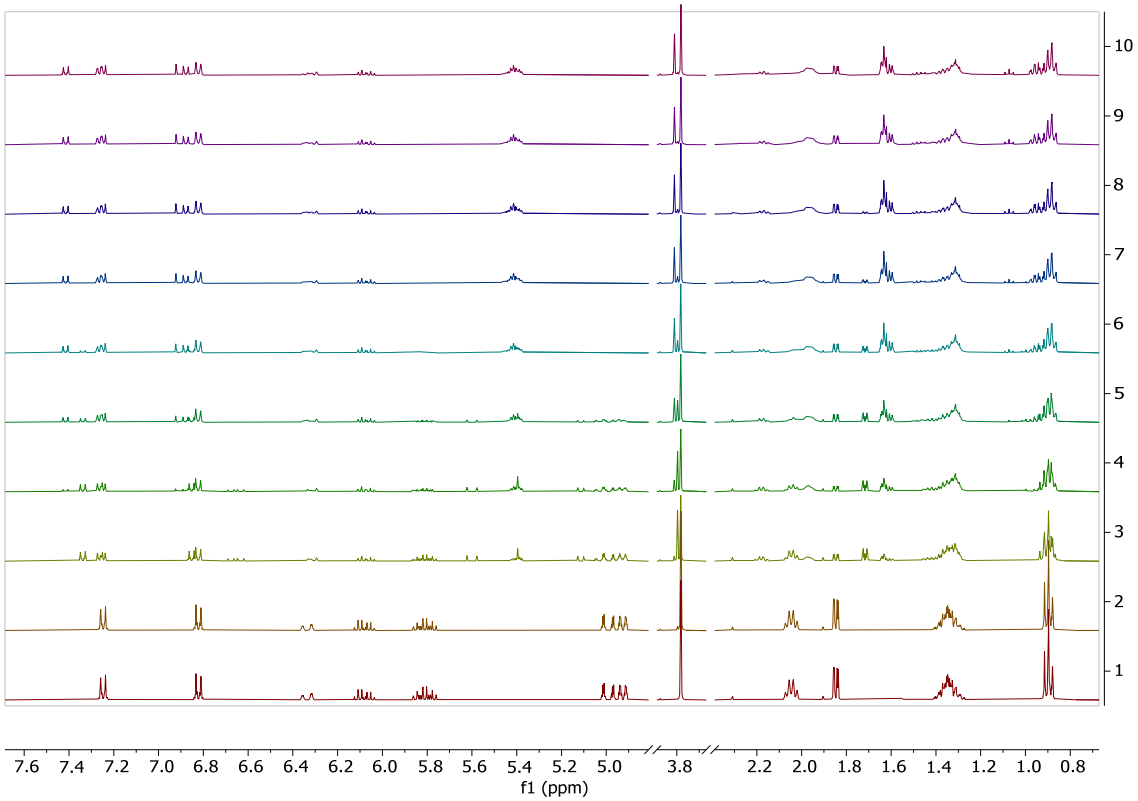

Figure S3. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.23) in the presence of Grubbs 2nd generation catalyst at 25 °C in $CDCl_3$ (experiment 3). The spectra at times t=0 min. (1), t=4 min. (2), t=16 min. (3), t=49 min. (4), t=102 min. (5), t=175 min. (6), t=268 min. (7), t=371 min. (8), t=504 min. (9) and t=657 min. (10).

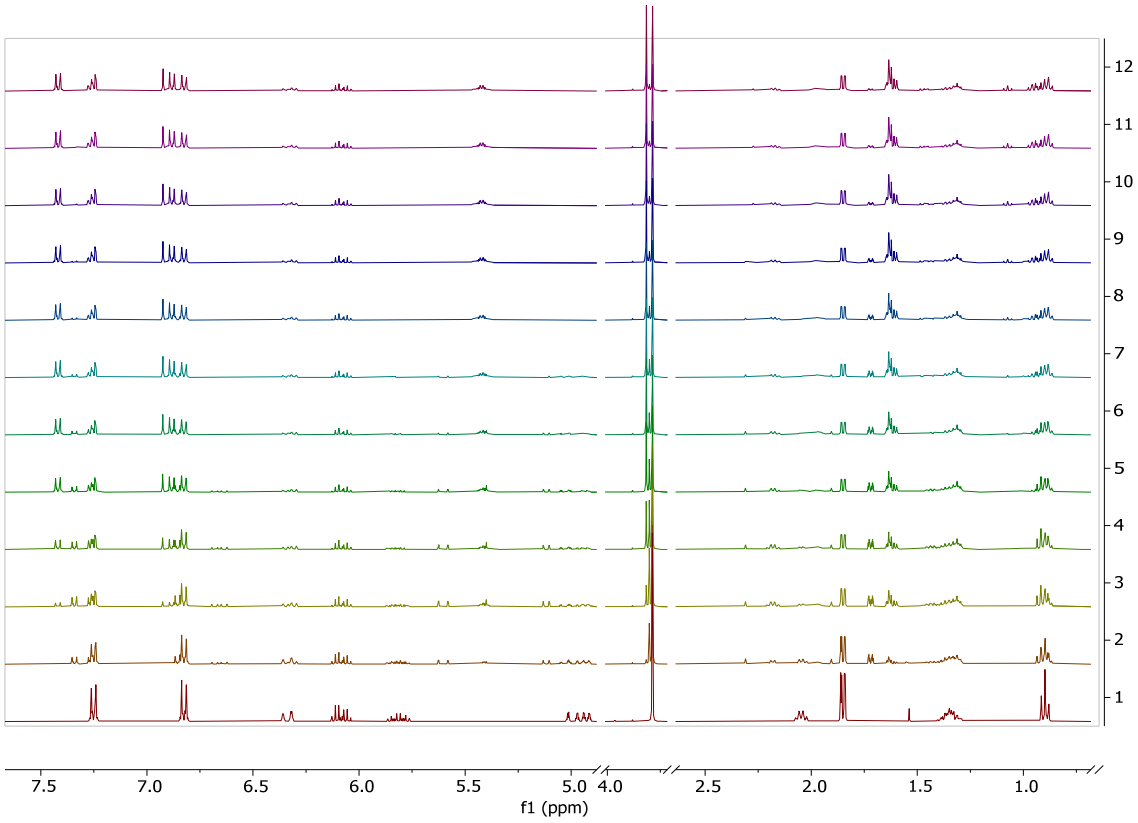

Figure S4. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.5) in the presence of Grubbs 2nd generation catalyst at 25 °C in $CDCl_3$ (experiment 4). The spectra at times t=0 min. (1), t=4 min. (2), t=16 min. (3), t=49 min. (4), t=102 min. (5), t=175 min. (6), t=268 min. (7), t=371 min. (8), t=504 min. (9), t=657 min. (10), t=830 min. (11) and t=1023 min. (12).

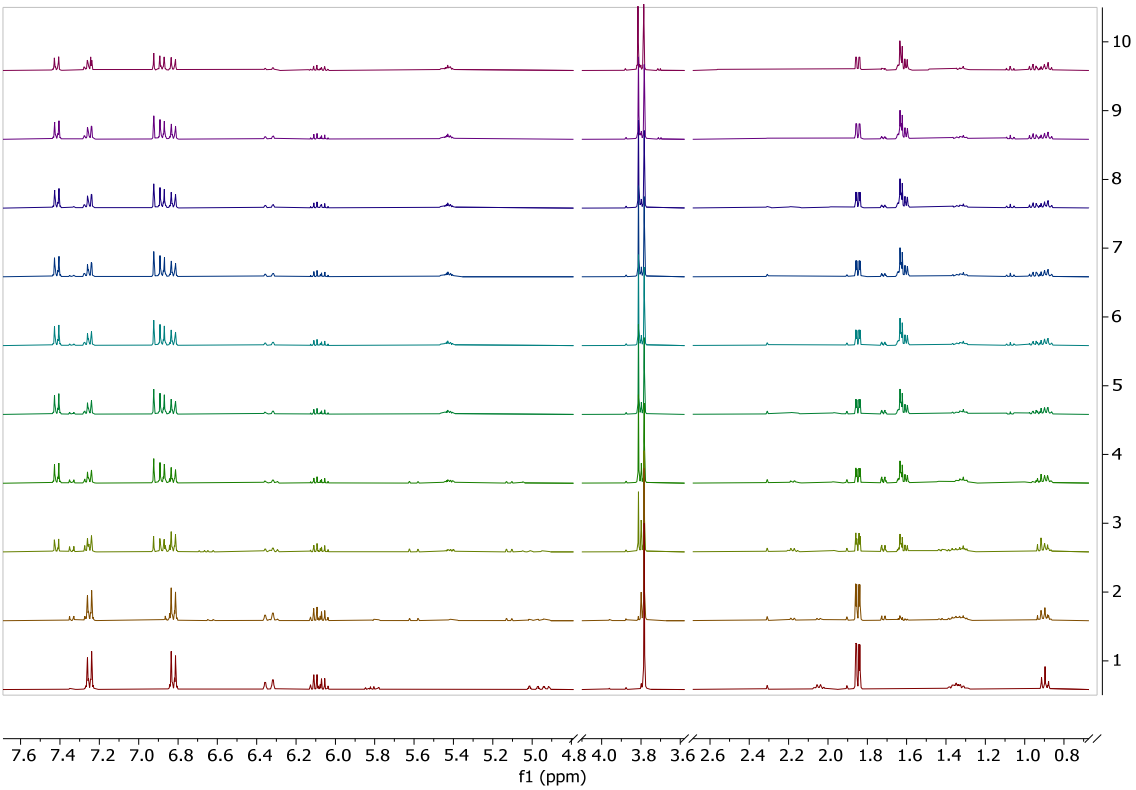

Figure S5. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.71) in the presence of Grubbs 2nd generation catalyst at 25 °C in $CDCl_3$ (experiment 5). The spectra at times t=0 min. (1), t=4 min. (2), t=16 min. (3), t=49 min. (4), t=102 min. (5), t=175 min. (6), t=268 min. (7), t=371 min. (8), t=504 min. (9) and t=657 min. (10).

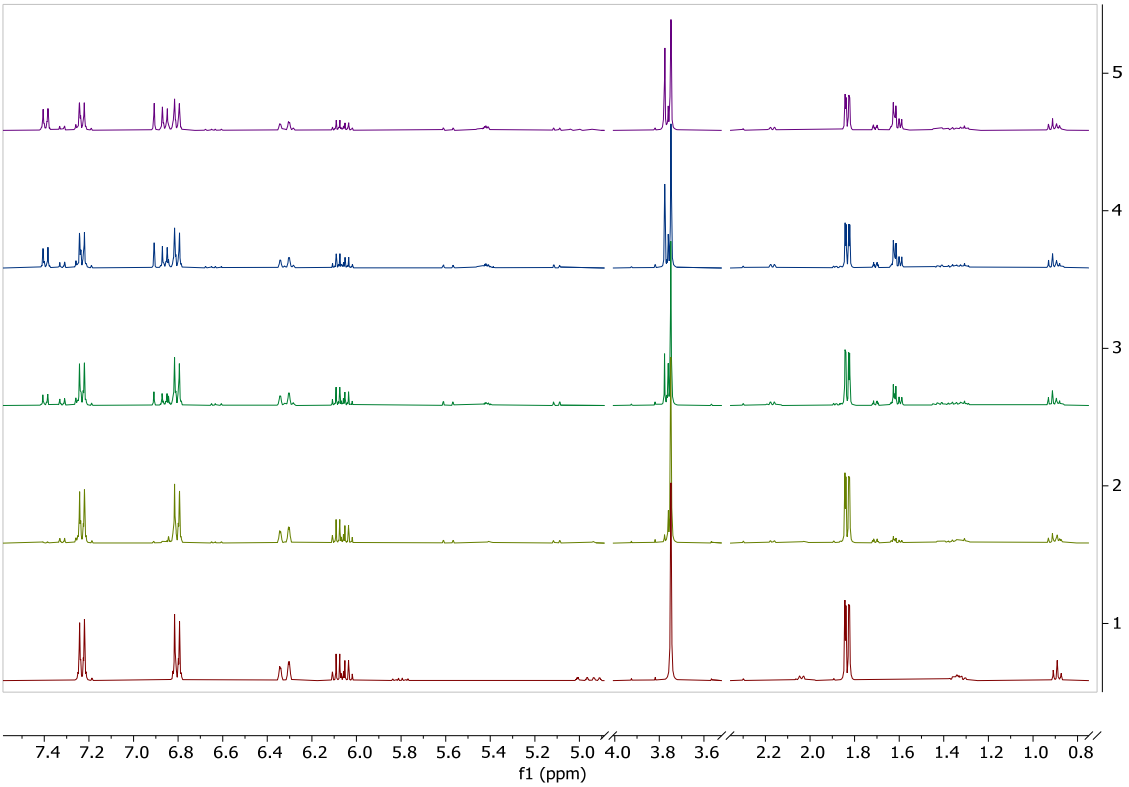

Figure S6. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.83) in the presence of Grubbs 2nd generation catalyst at 25 °C in $CDCl_3$ (experiment 6). The spectra at times t=0 min. (1), t=5 min. (2), t=8 min. (3), t=14 min. (4), t=21 min. (5).

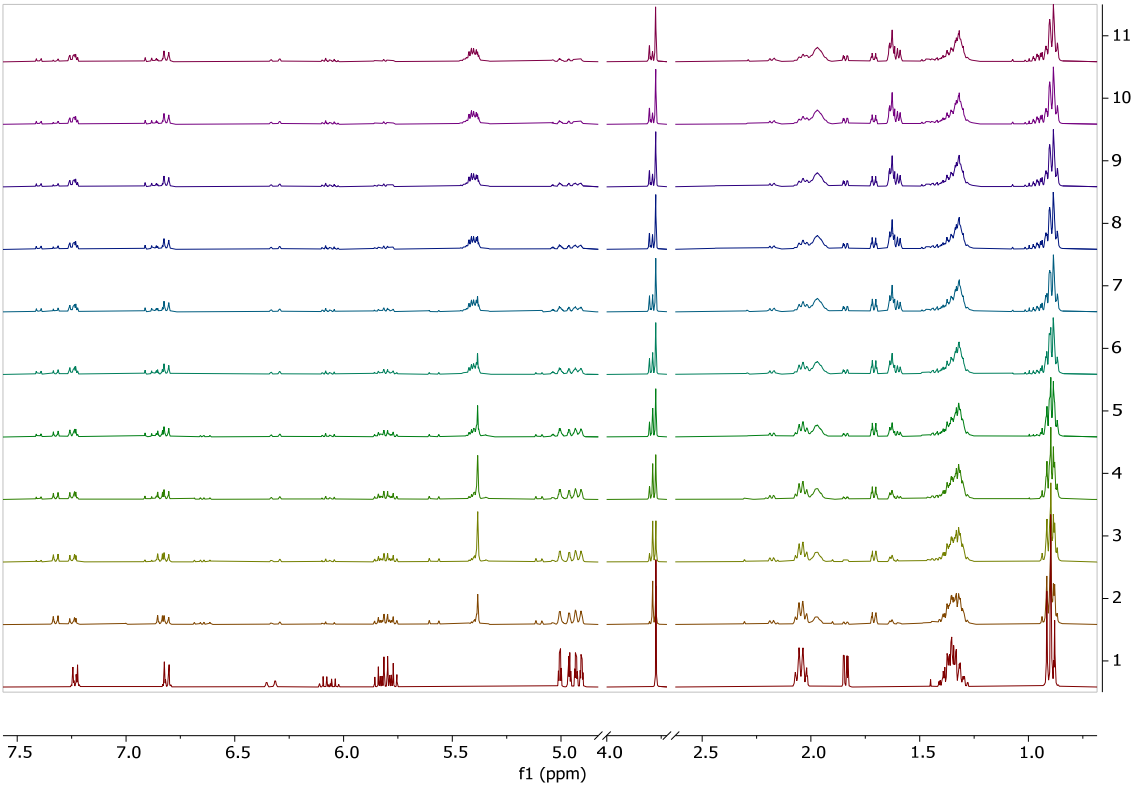

Figure S7. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.17) in the presence of Grubbs 2nd generation catalyst at 45 °C in $CDCl_3$ (experiment 7). The spectra at times t=0 min. (1), t=4 min. (2), t=7 min. (3), t=16 min. (4), t=30 min. (5), t=49 min. (6), t=73 min. (7), t=102 min. (8), t=136 min. (9), t=175 min. (10) and t=210 min. (11).

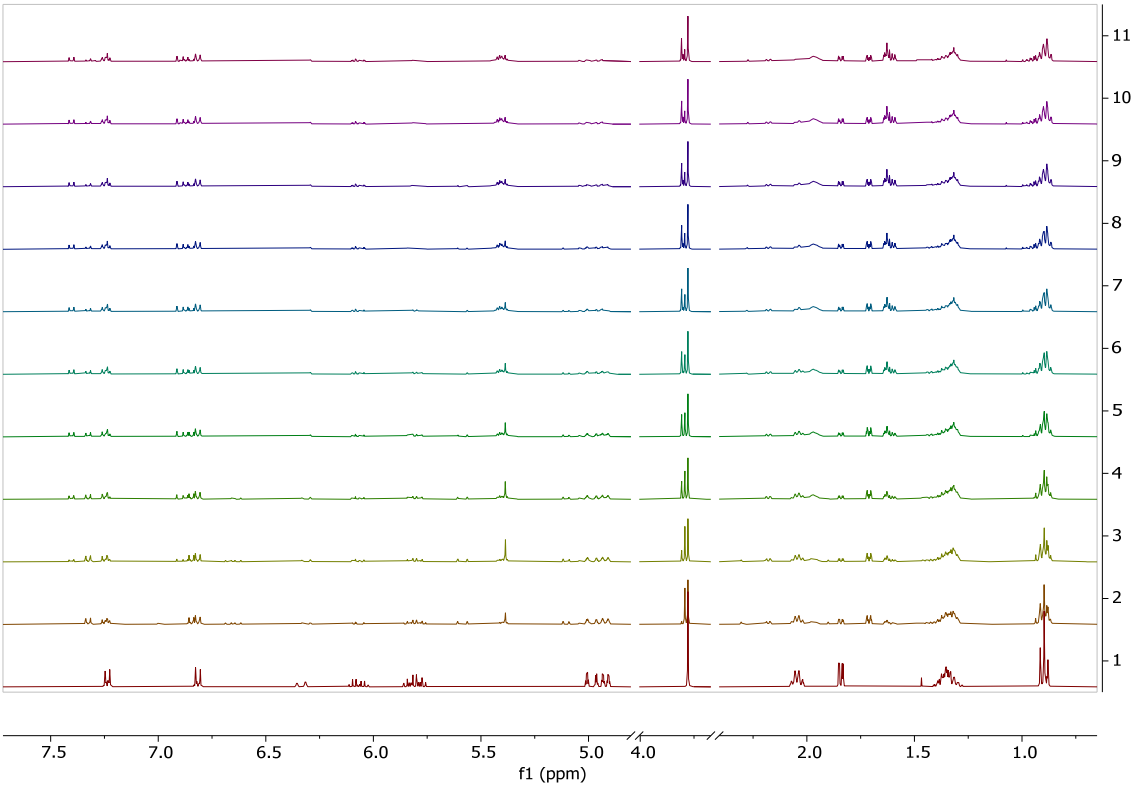

Figure S8. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.23) in the presence of Grubbs 2nd generation catalyst at 45 °C in $CDCl_3$ (experiment 8). The spectra at times t=0 min. (1), t=4 min. (2), t=7 min. (3), t=16 min. (4), t=30 min. (5), t=49 min. (6), t=73 min. (7), t=102 min. (8), t=136 min. (9), t=175 min. (10) and t=219 min. (11).

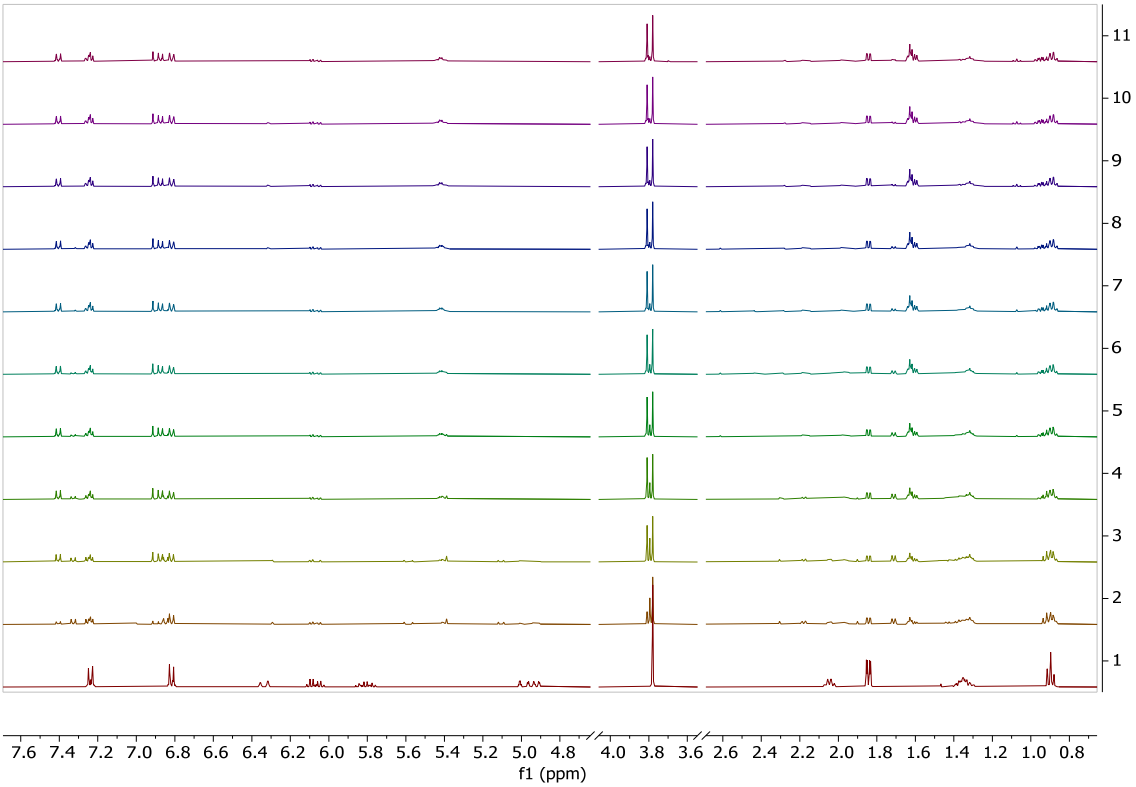

Figure S9. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.5) in the presence of Grubbs 2nd generation catalyst at 45 °C in $CDCl_3$ (experiment 9). The spectra at times t=0 min. (1), t=4 min. (2), t=7 min. (3), t=16 min. (4), t=30 min. (5), t=49 min. (6), t=73 min. (7), t=102 min. (8), t=136 min. (9), t=175 min. (10) and t=228 min. (11).

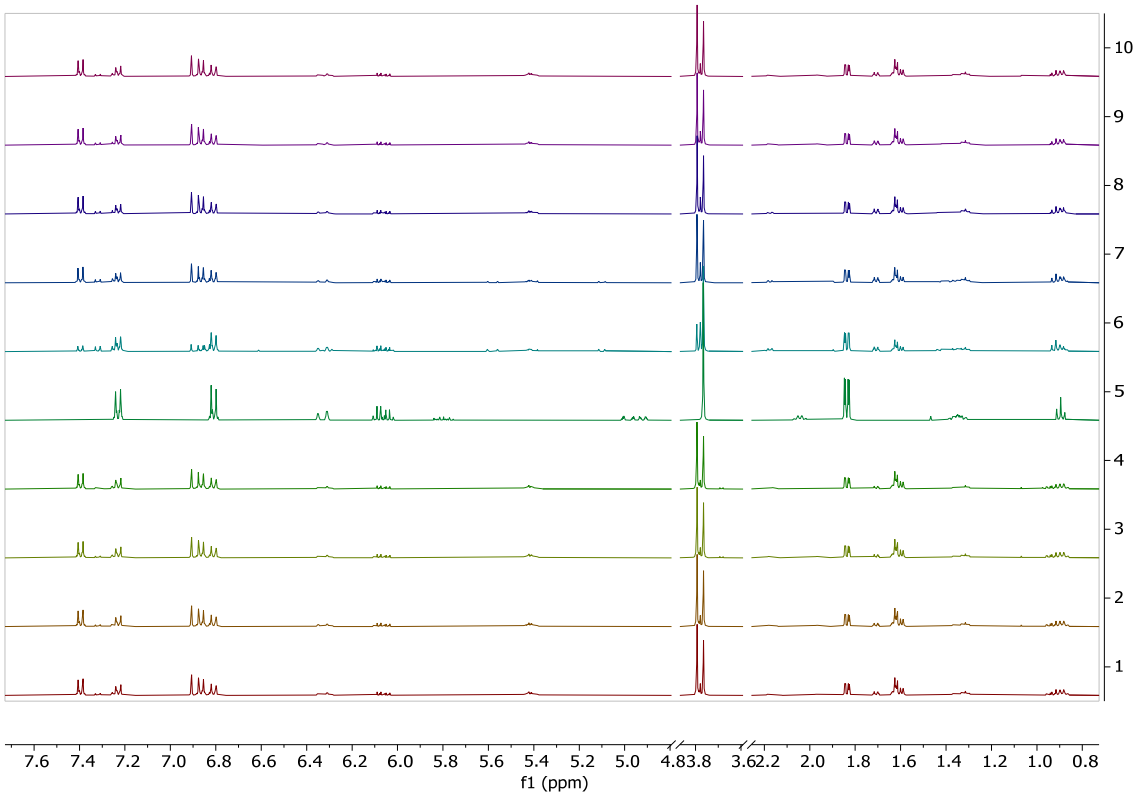

Figure S10. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.71) in the presence of Grubbs 2nd generation catalyst at 45 °C in $CDCl_3$ (experiment 10). The spectra at times t=0 min. (1), t=4 min. (2), t=7 min. (3), t=16 min. (4), t=30 min. (5), t=49 min. (6), t=73 min. (7), t=102 min. (8), t=136 min. (9) and t=192 min. (10).

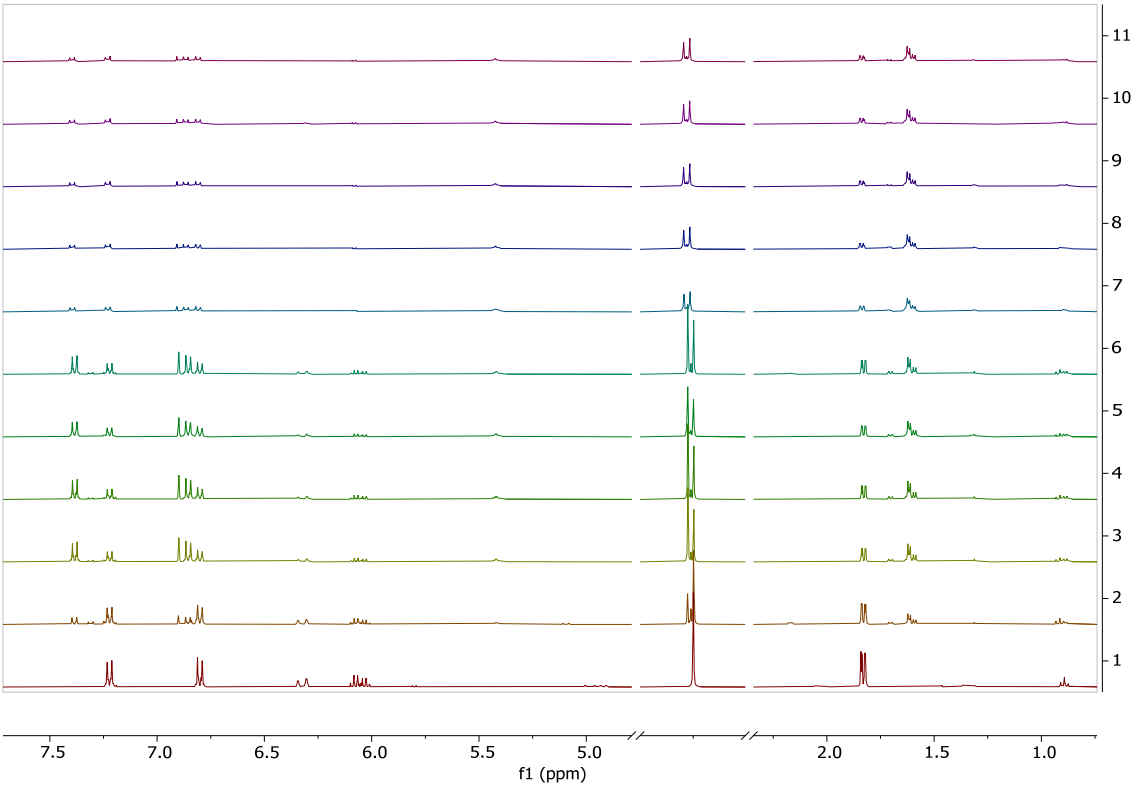

Figure S11. The time dependent ^{1}H NMR spectra of crude metathesis reaction mixture between (*E*)-anethole and 1-hexene ($X_{Anethole}$ = 0.83) in the presence of Grubbs 2nd generation catalyst at 45 °C in $CDCl_3$ (experiment 11). The spectra at times t=0 min. (1), t=4 min. (2), t=7 min. (3), t=16 min. (4), t=30 min. (5), t=49 min. (6), t=73 min. (7), t=102 min. (8), t=136 min. (9), t=175 min. (10) and t=201 min. (11).

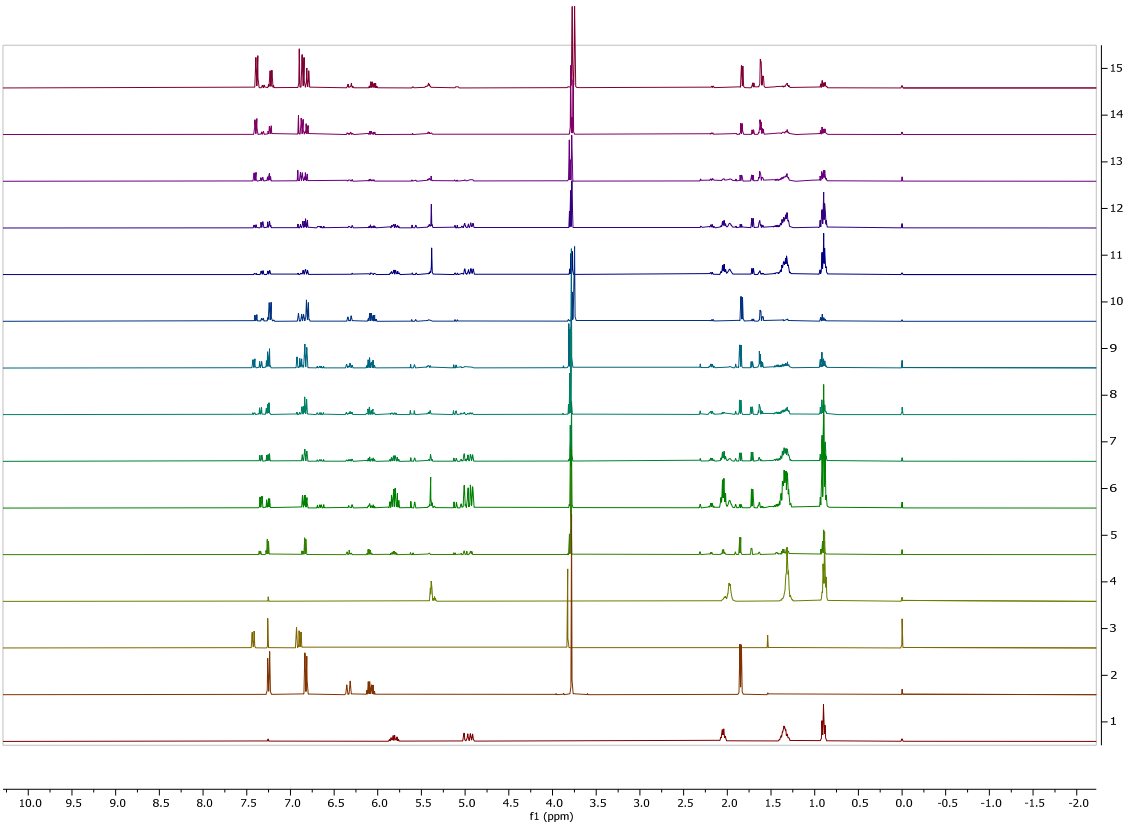

Figure S12. Expanded ^{1}H NMR spectra of reagents (1) 1-hexene (**1**); (2) (*E*)-anethole (**2**); (3) SM product of (**2**), (*E*)-4,4'-dimethoxystilbene (**7**); (4) SM product of (**1**), (*E*)-5-decene (**5**); and the crude metathesis reaction mixture between (*E*)-anethole and 1-hexene in the presence of Grubbs 2nd generation at t=10 min. in $CDCl_3$ for (5) $X_{Anethole}$ = 0.5 at 15 °C; (6) $X_{Anethole}$ = 0.17 at 25 °C; (7) $X_{Anethole}$ = 0.29 at 25 °C; (8) $X_{Anethole}$ = 0.5 at 25 °C; (9) $X_{Anethole}$ = 0.71 at 25 °C; (10) $X_{Anethole}$ = 0.83 at 25 °C; (11) $X_{Anethole}$ = 0.17 at 45 °C; (12) $X_{Anethole}$ = 0.29 at 45 °C; (13) $X_{Anethole}$ = 0.5 at 45 °C; (14) $X_{Anethole}$ = 0.71 at 45 °C and; (15) $X_{Anethole}$ = 0.83 at 45 °C.

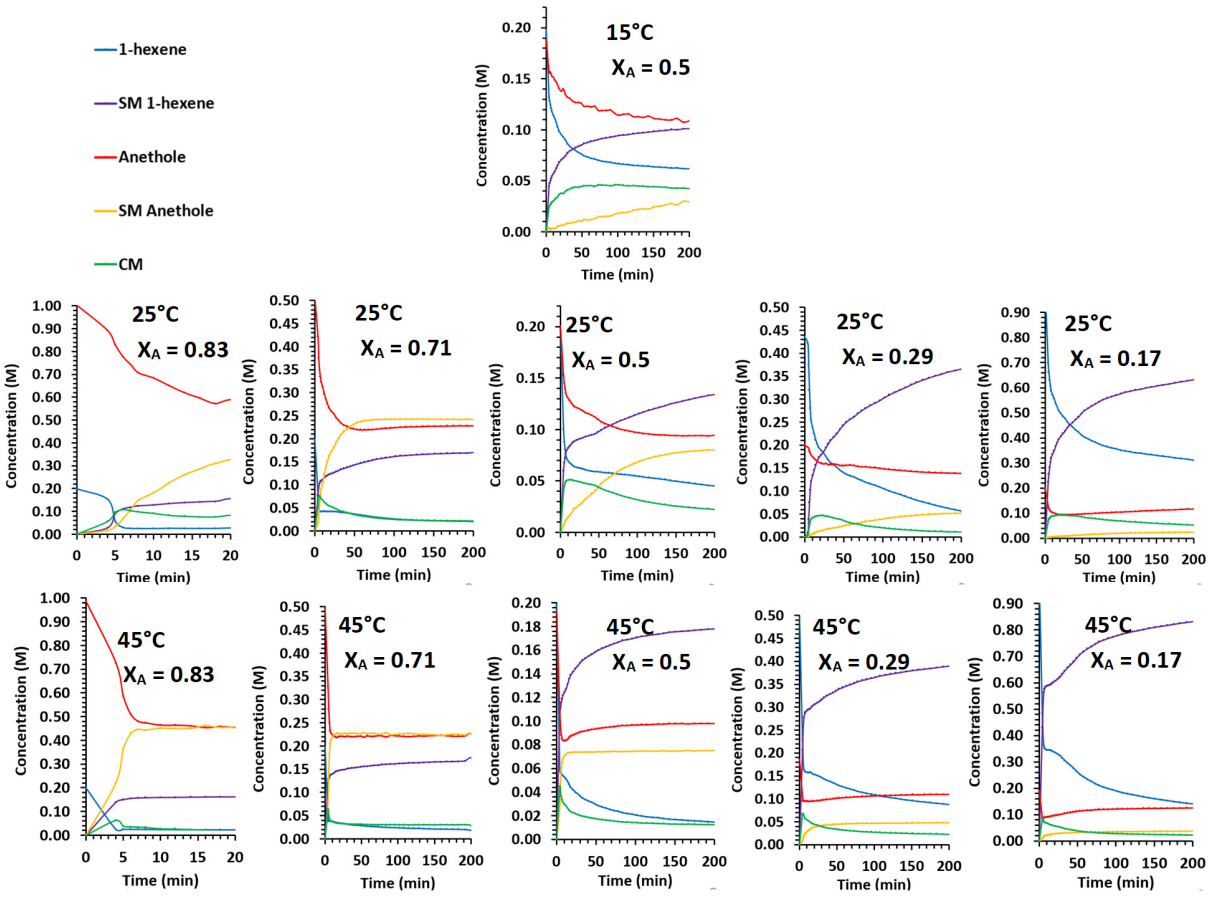

Figure S13. The time trace of the Grubbs' 2nd generation catalysed metathesis reaction between 1-hexene (**1**) and (*E*)-anethole (**2**) at 15 ºC (top row), 25 ºC (middle row), and 45 ºC (bottom row), the mole fraction of anethole is indicated on each graph. (*E*)-anethole (red -) and 1-hexene (blue -), and the formation of the different products, CM (3, green -), SM 1-hexene (5, purple -) and SM (*E*)-anethole (7, orange -).

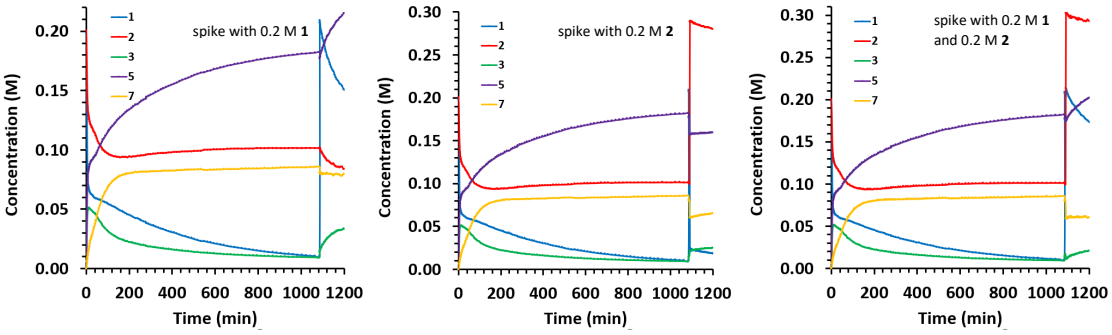

Figure S14. The time trace of the Grubbs 2nd generation catalysed (*E*)-anethole and 1-hexene ($X_{Anethole} \approx 0.5$) reaction at 25 °C in $CDCl_3$ spiked with (A) 0.2 M **1** (experiment 12), (B) 0.2 M **2** (experiment 13) and (C) 0.2 M **1** and 0.2 M **2** at 1086 min (experiment 14).

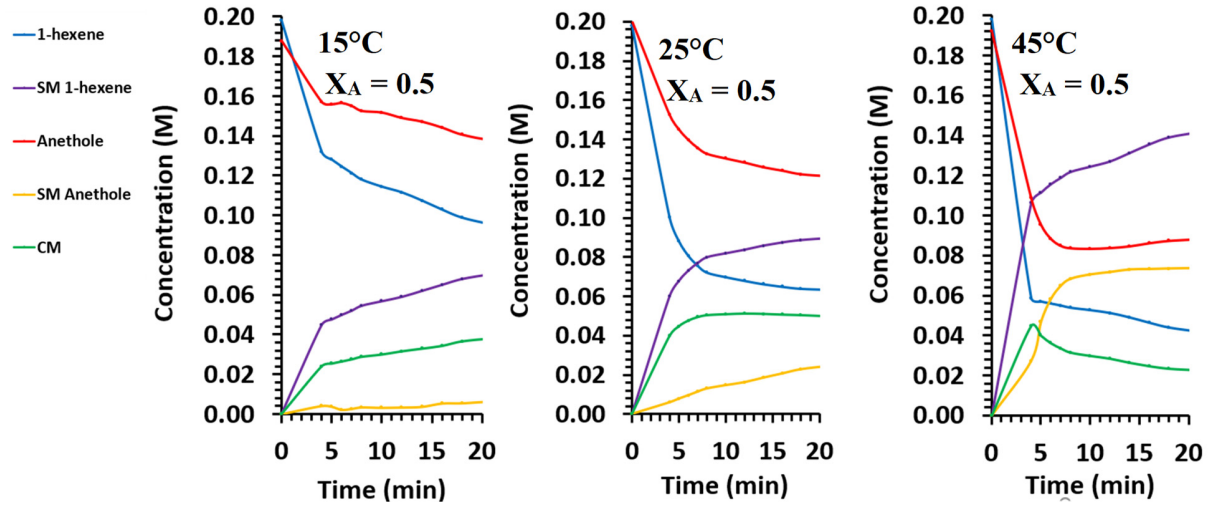

Figure S15. The time traces of the of the initial 20 min of the Grubbs' 2nd generation catalysed metathesis reaction between 1-hexene (**1**) and (*E*)-anethole (**2**) at 15 ºC (left), 25 ºC (middle), and 15 ºC (right), the mole fraction of anethole is indicated on each graph.

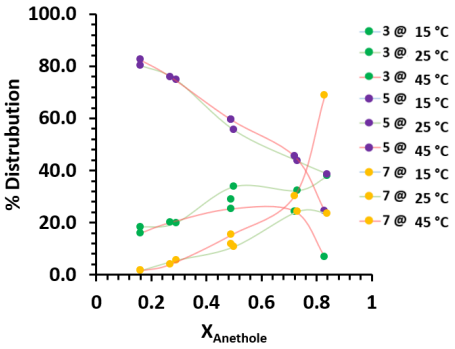

Figure S16. Graph of % distribution of metathesis products **3**, **5**, and **7** *vs* $X_{Anethole}$ at the different temperatures (as indicated) at the time where $[\mathbf{3}]_{max}$ was reached.

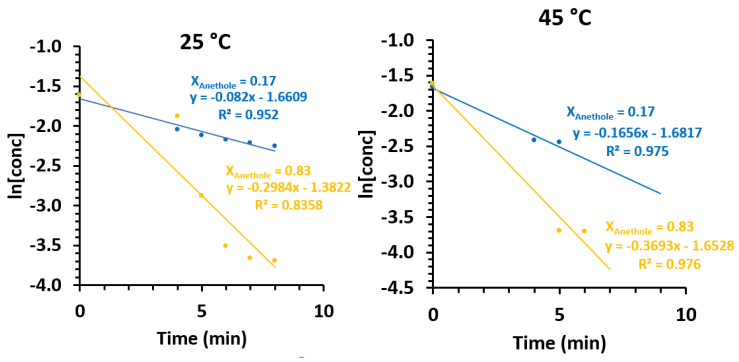

Figure S17. The kinetic plots of the disappearance of **1** (blue) and **2** (yellow) at (left) 25 °C and (right) 45 °C for the metathesis reactions (at the indicated $X_{Anethole}$) that leads to the apparent observed first order rate constant k'_{obs}.

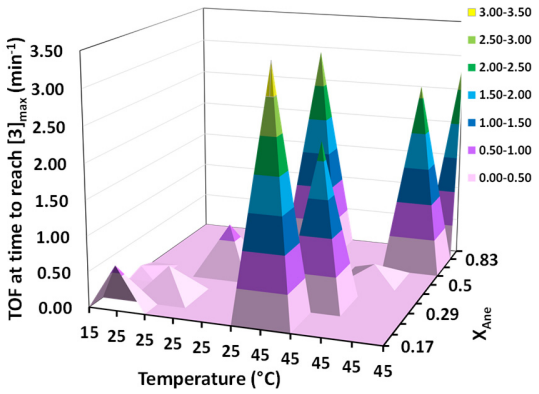

Figure S18. Graph comparing the TOF at the time when $[\mathbf{3}]_{max}$ is reached against the reaction conditions.