Supporting Information

Synthesis of functionalized tetrahydrofuran derivatives from 2,5-dimethylfuran through cascade reactions

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1. Thermodynamic calculations

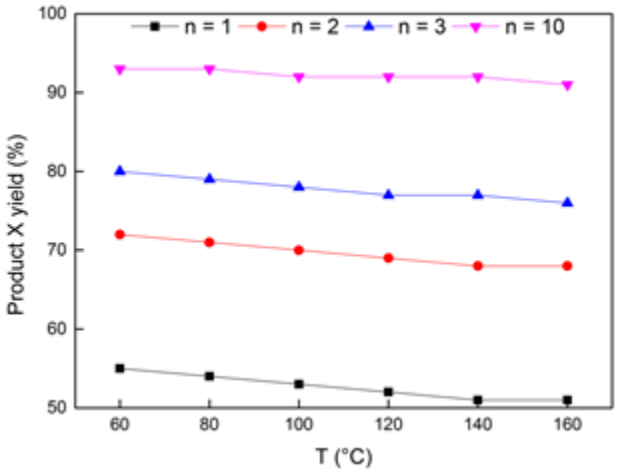


Fig S1. Equilibrium product yields as a function of temperature for different equivalents of benzaldehyde (calculations).

2. IR spectroscopy analysis of A26.

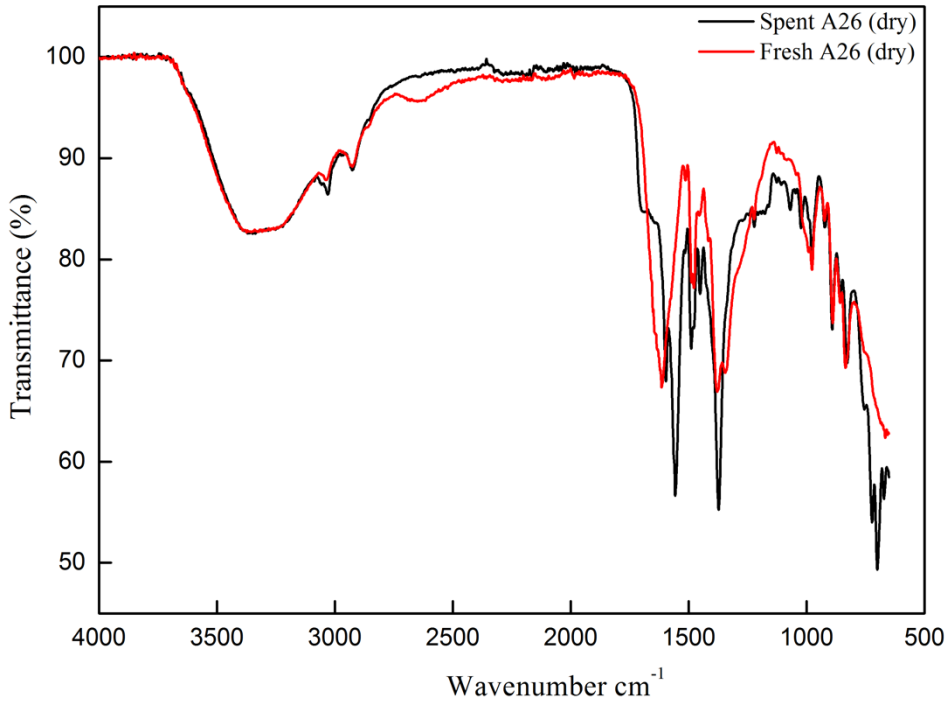


Fig S2. FT-IR spectroscopy of the fresh A26 (dry) and the spent A26 (dry).

3. TGA analysis

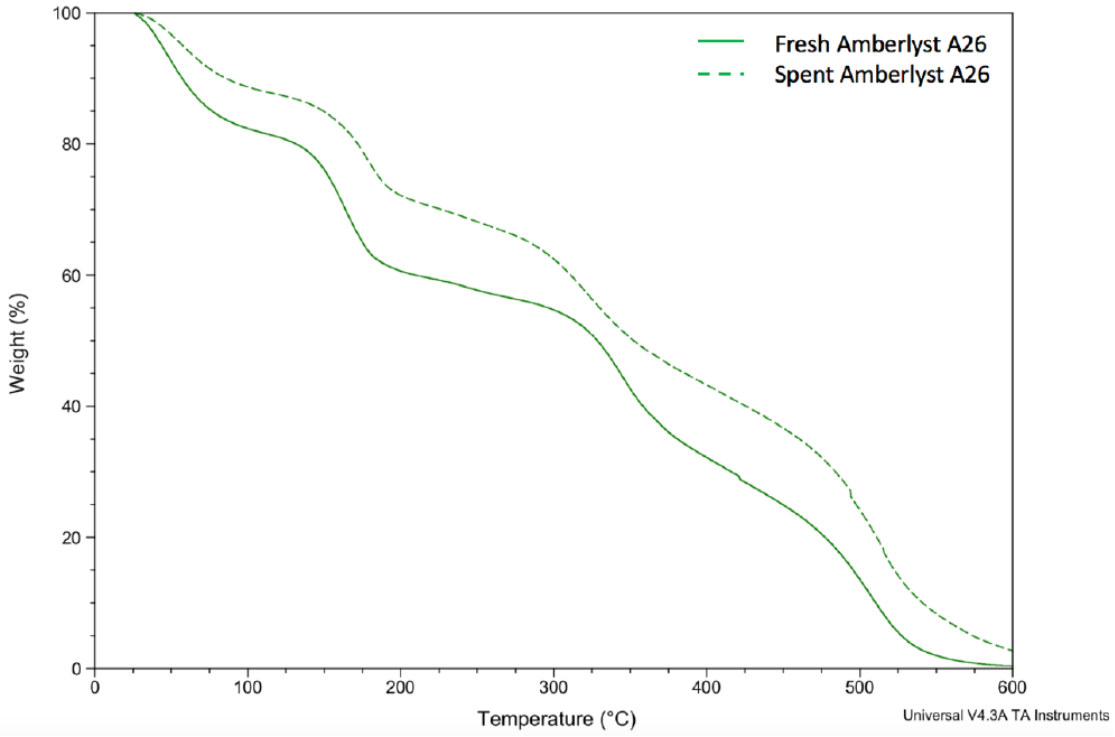


Fig S3. TGA analysis of fresh and spent A26 catalyst.

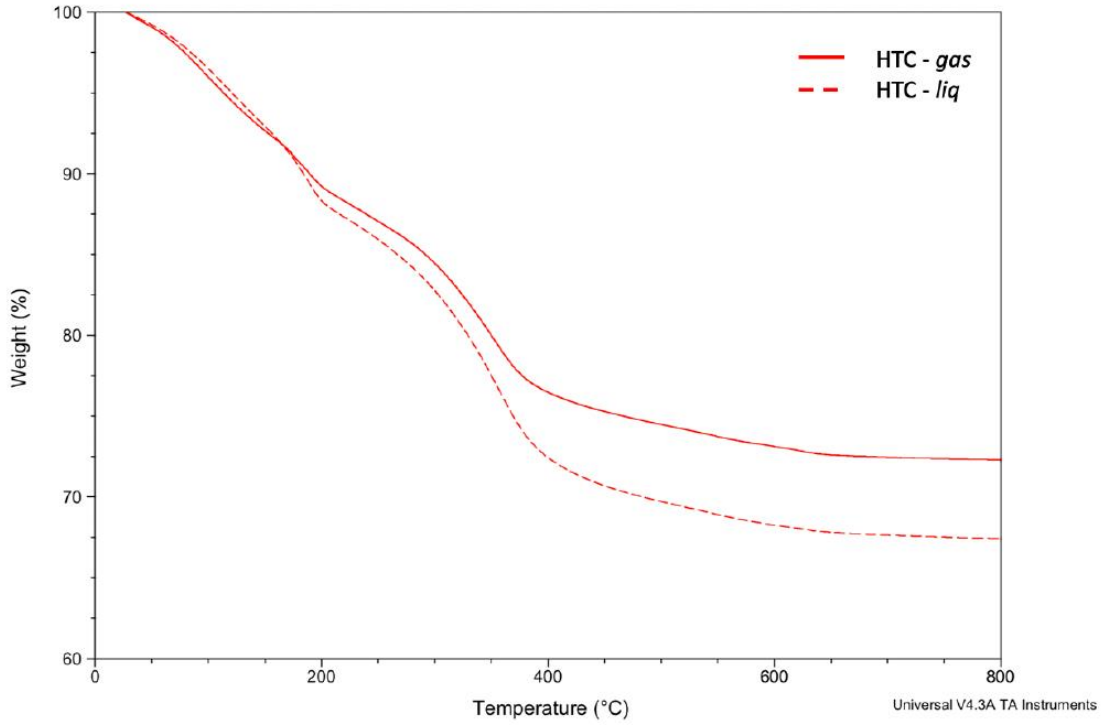


Fig S4. TGA analysis of fresh HTC-gas and HTC-liq catalysts.

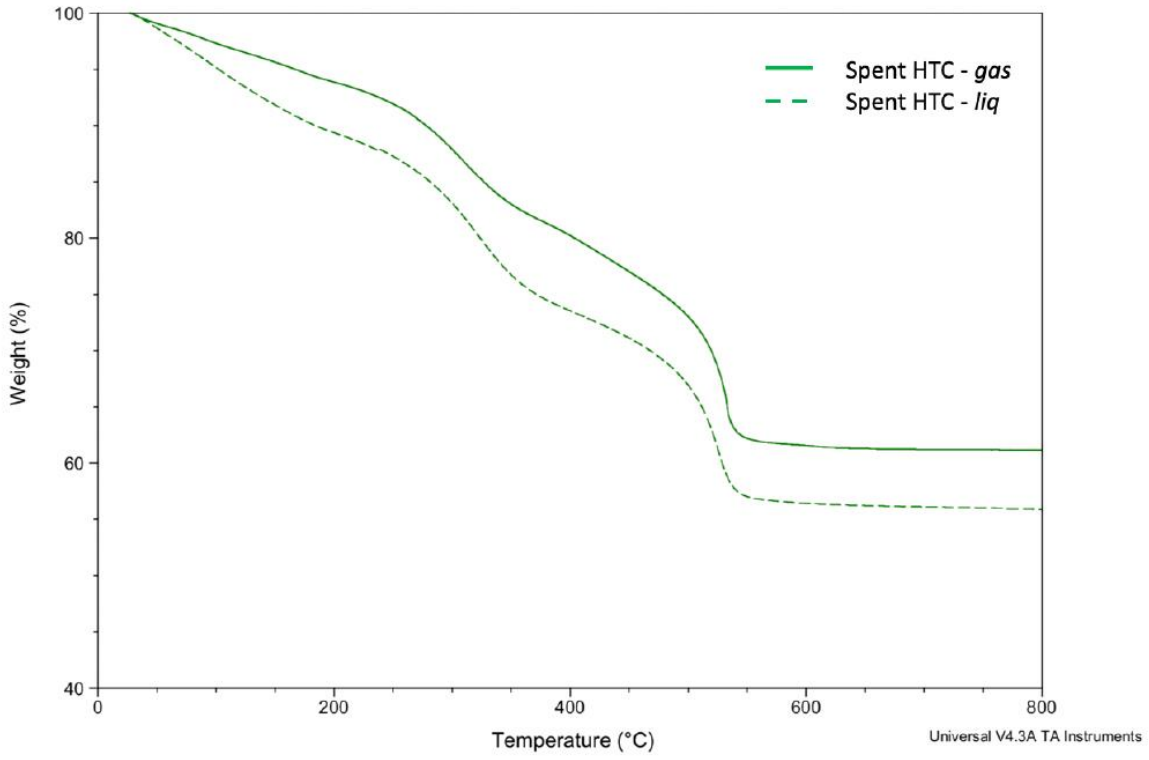


Fig S5. TGA analysis of HTC-gas and HTC-liq catalysts after reaction.

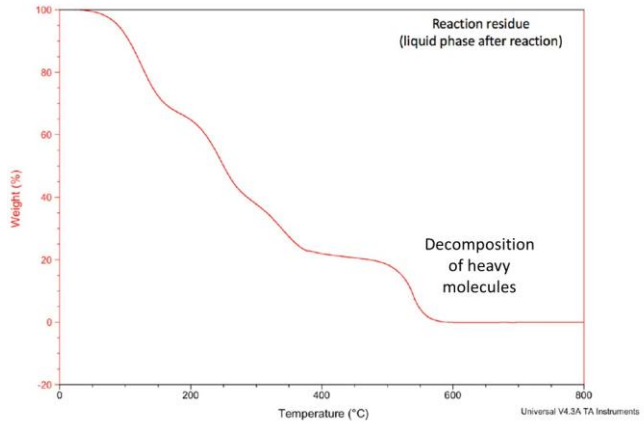


Fig S6. TGA analysis of the reaction media after catalytic run in the presence of HTC.

4. XPS analysis

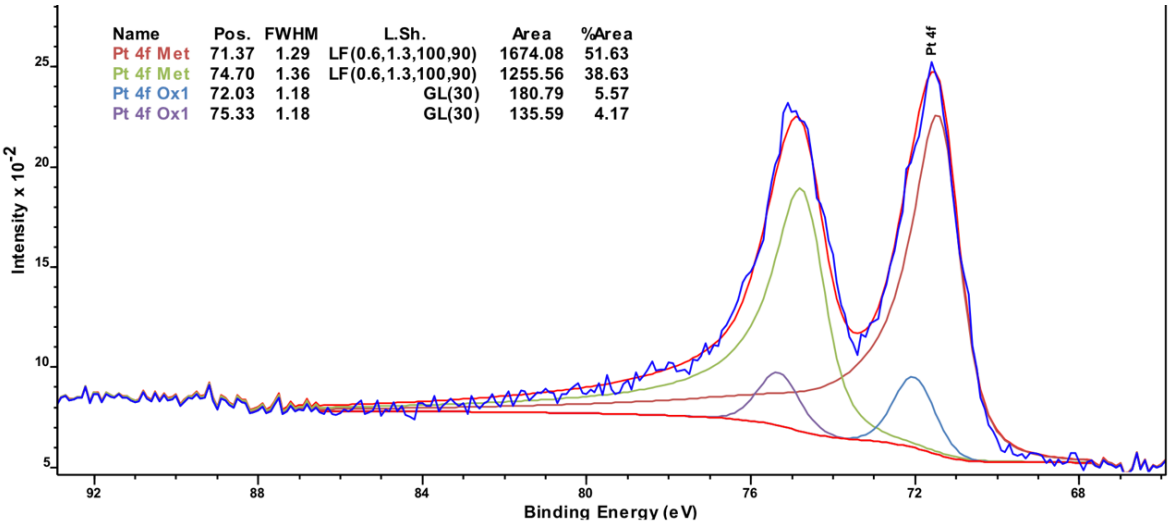


Figure S7. XPS analysis of the spent Pt/C after the 5th run.

Table S1: XPS analysis of spent and fresh catalyst

Element	Eb	RSF	Pt/C (Fresh)	Pt/C (After 5 runs)
C1s	284.4	0.28	91.6	87
O1s	532	0.78	7.8	10.5
Pt4f	71	5.58	0.6	0.4
S2p	168	0.668		1.5
N1s	400	0.477		0.6
Ca2p			traces	

Eb: Binding Energy
RSF: Relative Sensitivity Factor

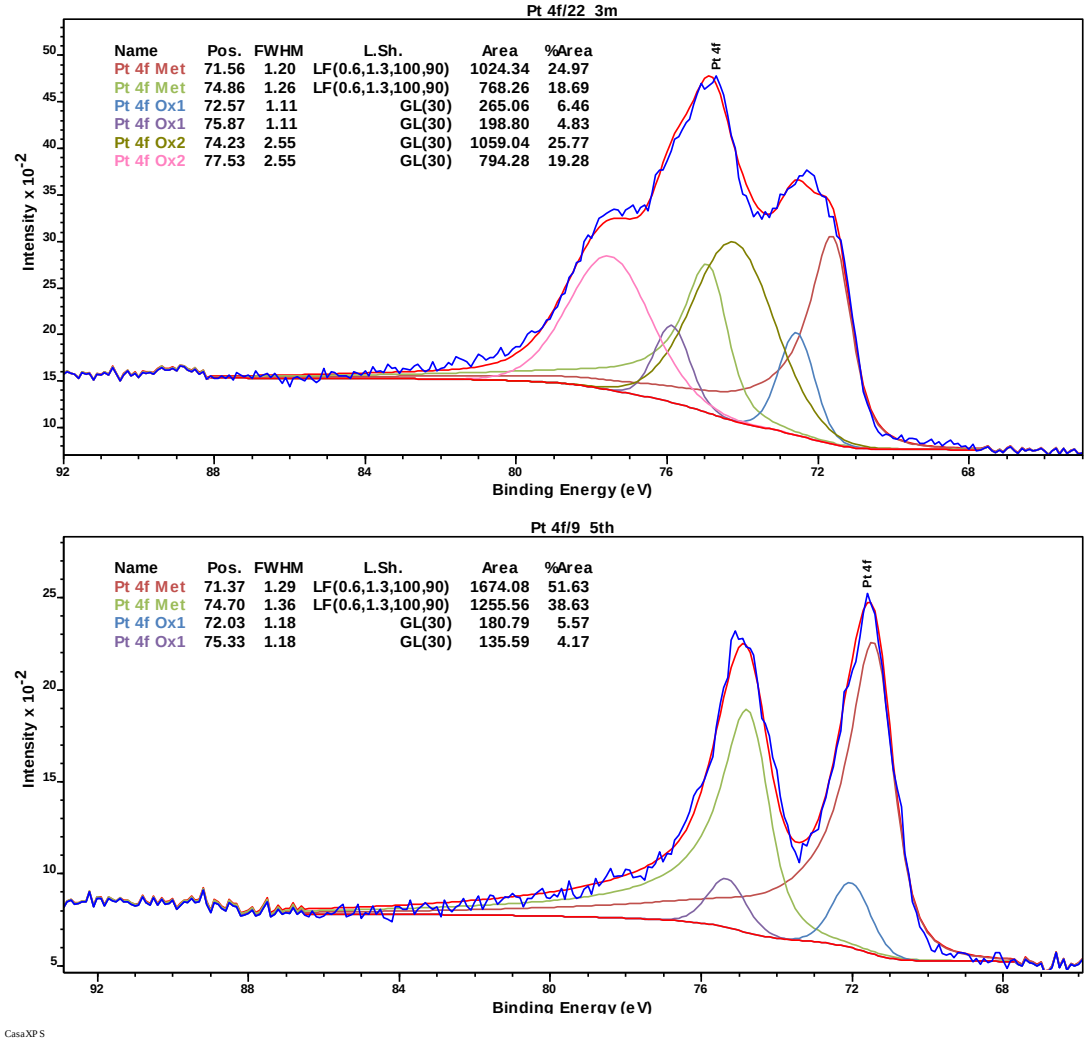
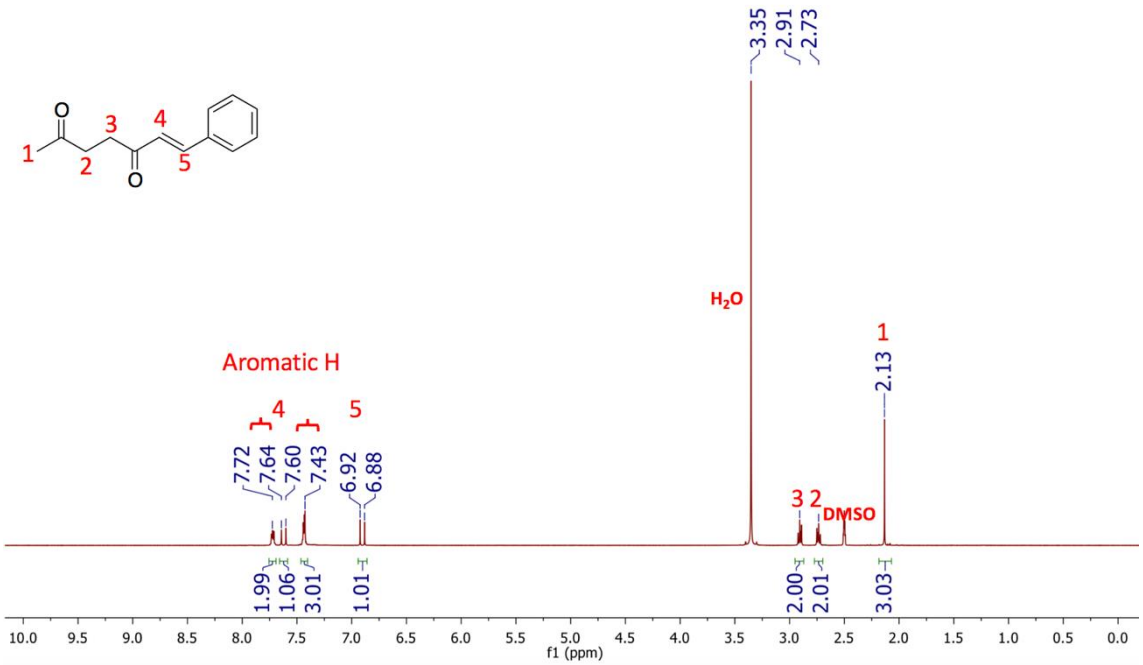
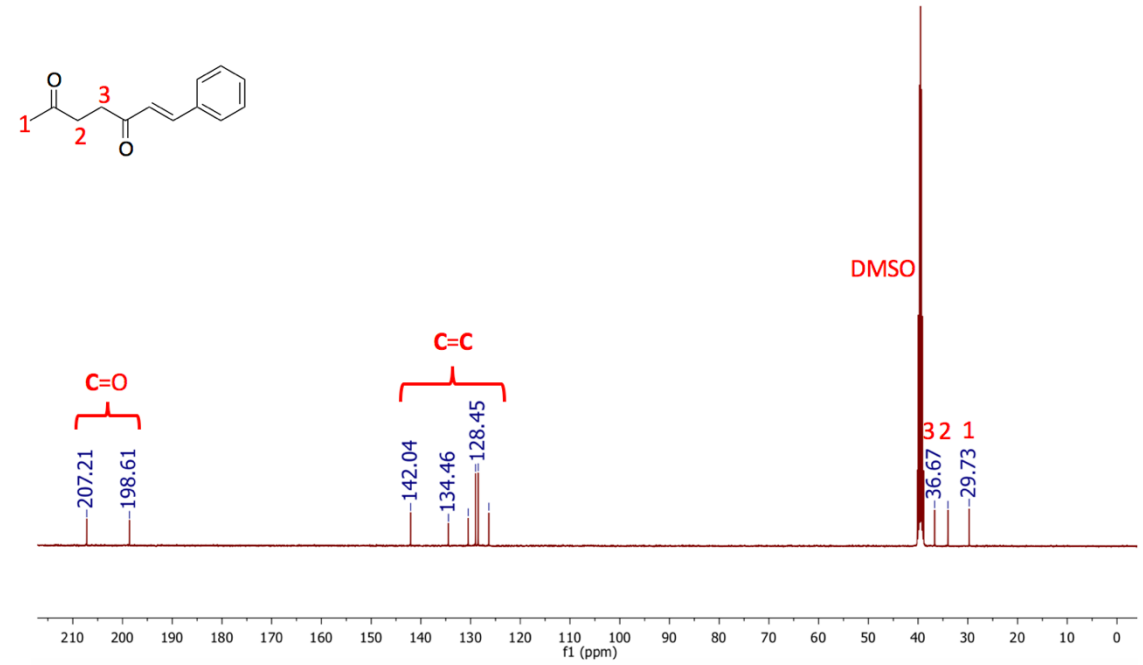


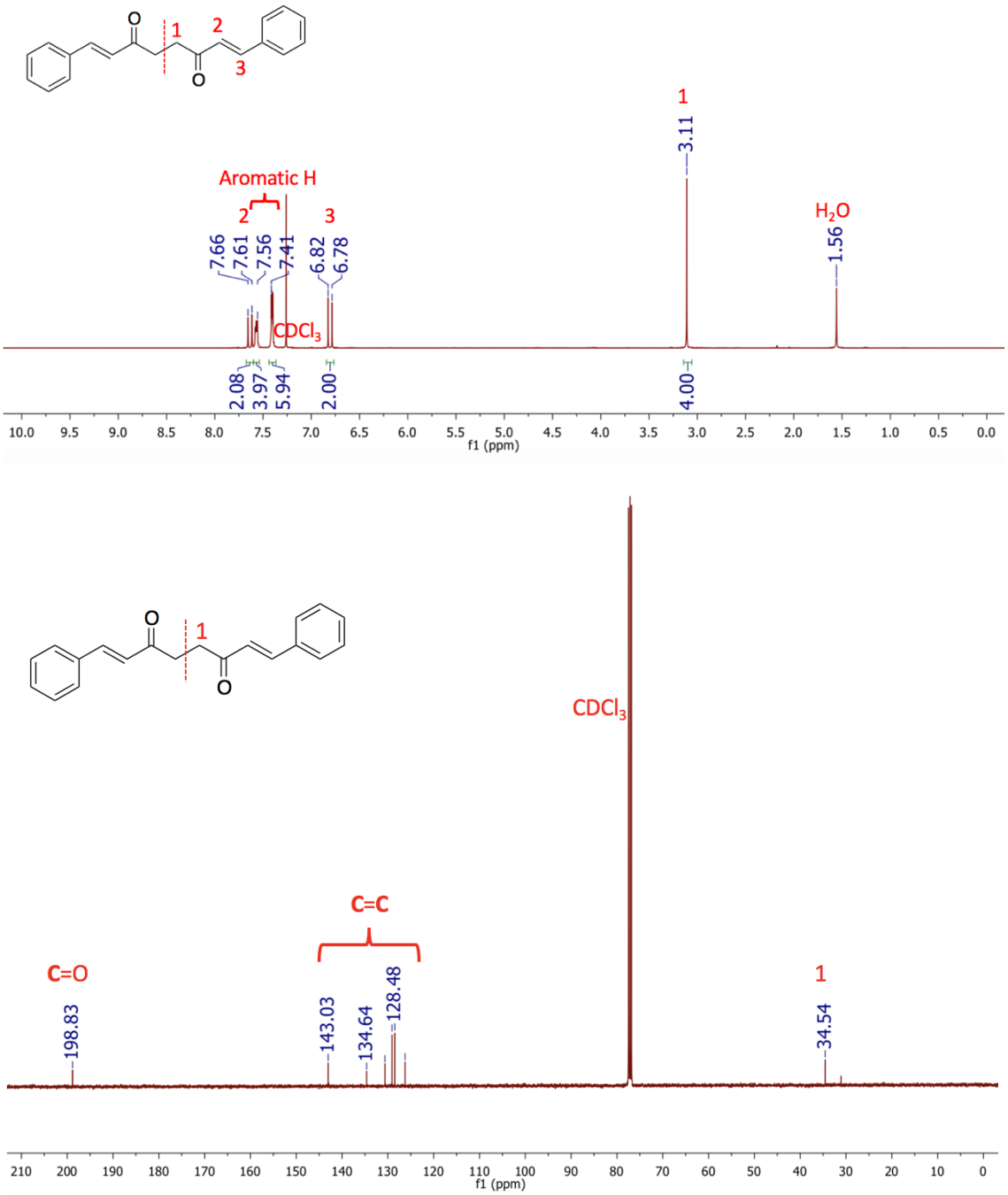
Fig S8. Deconvolution for Pt for fresh catalyst (up) and spent catalyst (down)

5. ^{1}H and ^{13}C NMR spectra of products of interest.

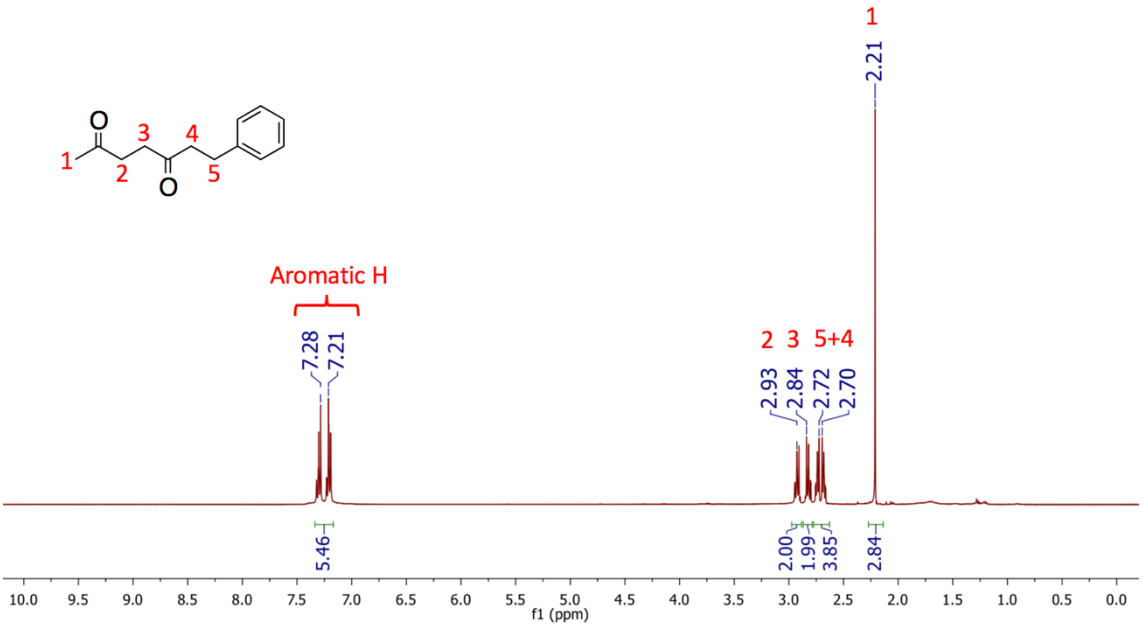


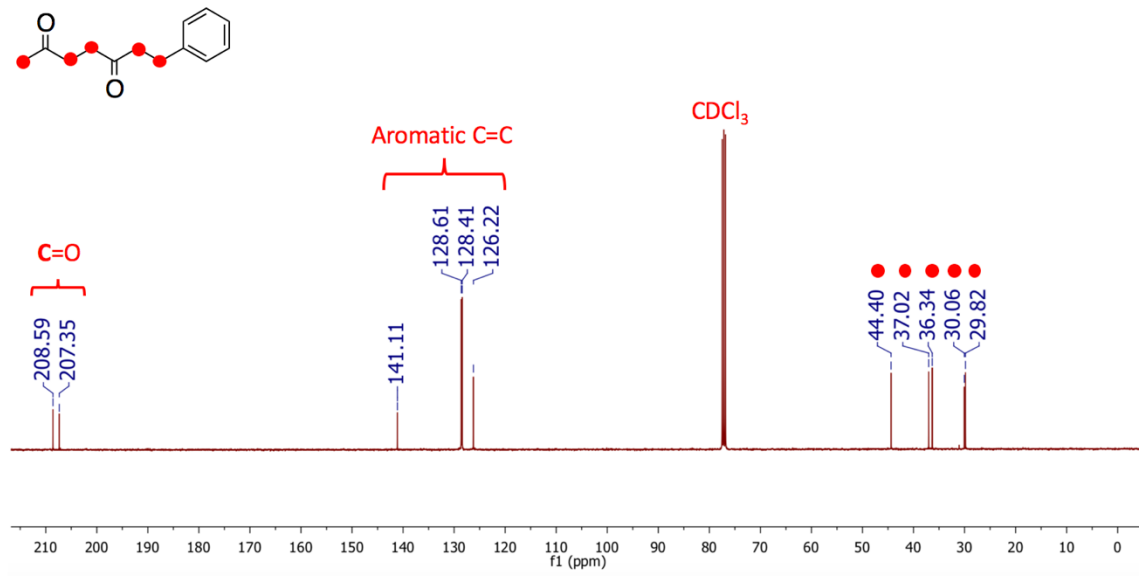


7-Phenylhept-6-ene-2,5-dione ^{1}H NMR (300 MHz, DMSO-d_6) δ = 7.72 (m, 2H, Ar), 7.64-7.60 (d, J = 16, 1H), 7.43 (m, 3H, Ar), 6.92-6.88 (d, J = 16, 1H), 2.91 (t, 2H), 2,73 (t, 2H), 2.13 (s, 3H). ^{13}C NMR (75MHz, DMSO-d_6) δ = 207.21, 198.61, 142.04, 134.46, 130.47, 128.99, 128.45, 126.32, 36.67, 34.02, 29.73.

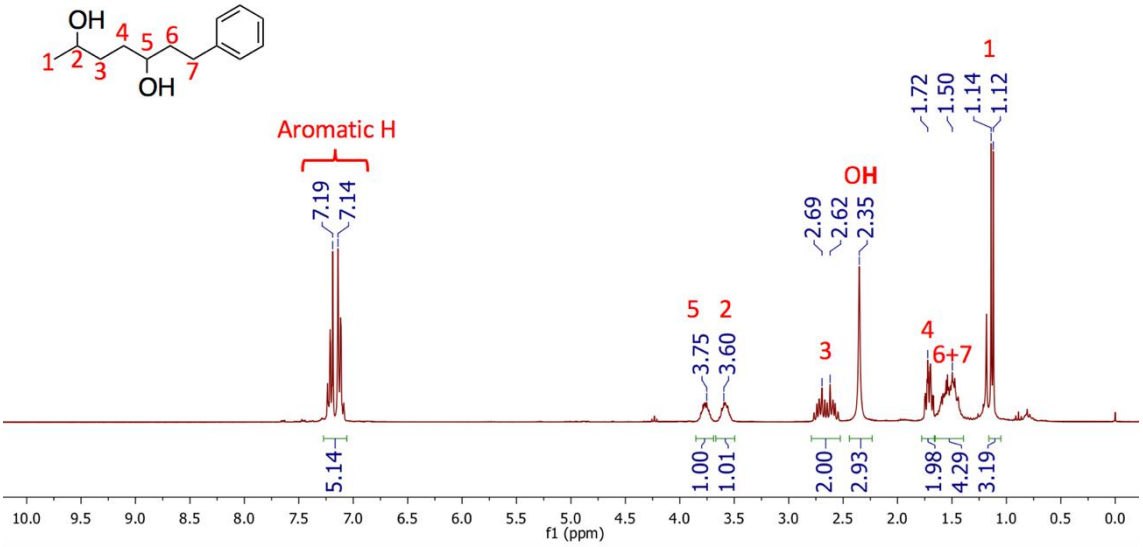


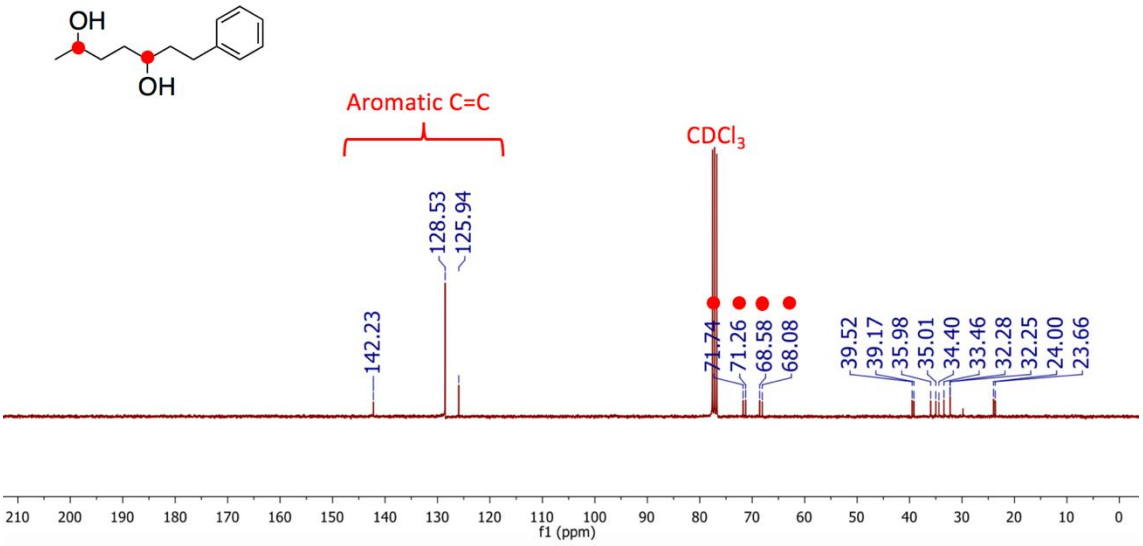
1,8-Diphenylocta-1,7-diene-3,6-dione ^{1}H NMR (300MHz, $CDCl_3$) δ = 7.66-7.61 (d, J = 20, 2H), 7.56 (m, 4H, Ar), 7.41 (m, 6H, Ar), 6.82-6.78 (d, J = 16, 2H), 3,11 (s, 4H). ^{13}C NMR (75MHz, $CDCl_3$) δ = 198.83, 143.03, 134.64, 130.65, 129.10, 128.48, 126.25, 34.54.



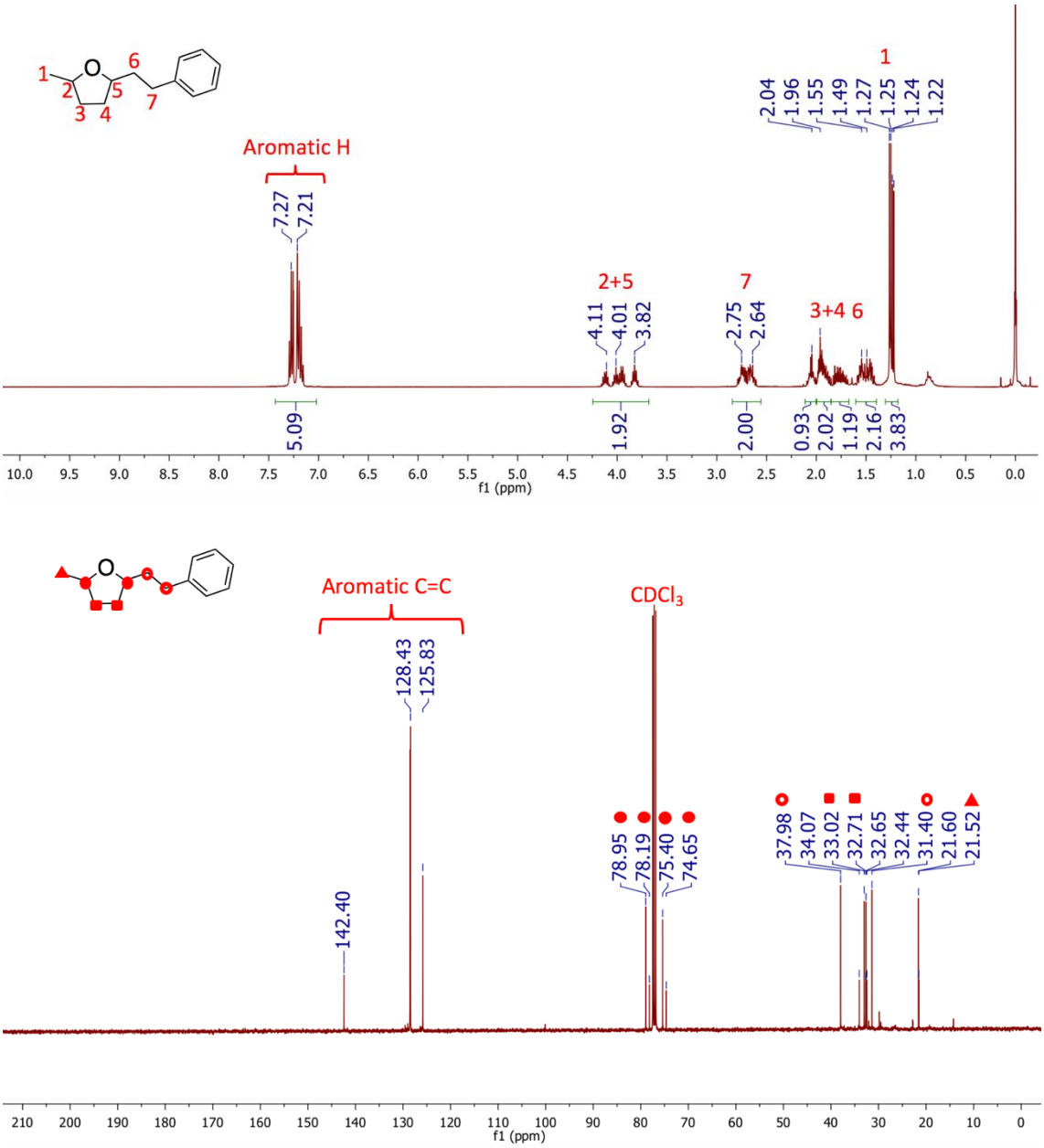


7-Phenylheptane-2,5-dione ^{1}H NMR (300MHz, $CDCl_3$) δ = 7.28-7.21 (m, 5H, Ar), 2.93 (t, 2H), 2.82 (t, 2H), 2.72-2.70 (m, 4H), 2.21 (s, 3H). ^{13}C NMR (75MHz, $CDCl_3$) δ = 208.59, 207.35, 141.11, 128.61, 128.41, 126.22, 44.40, 37.02, 36.34, 30.06, 29.82.

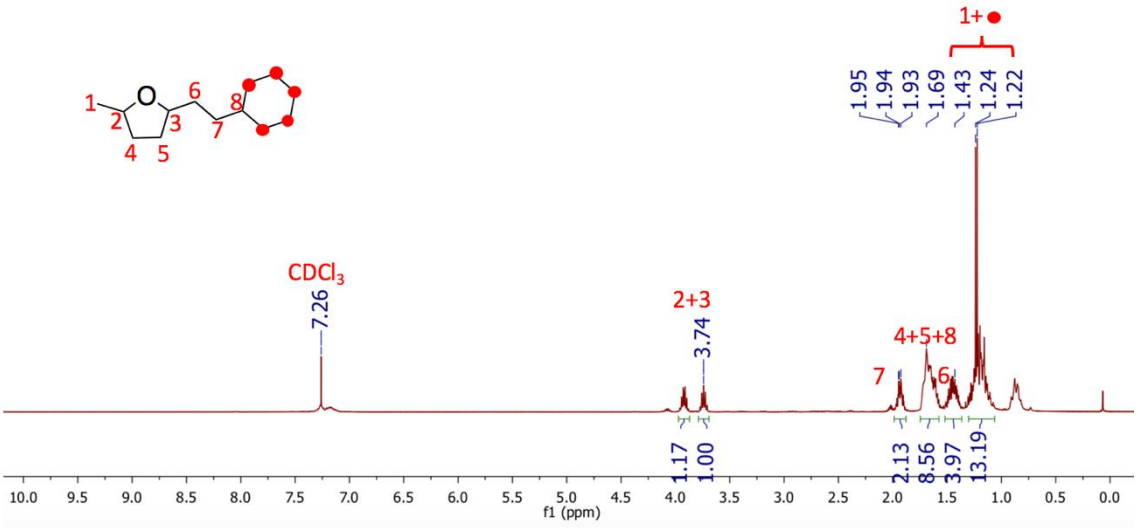


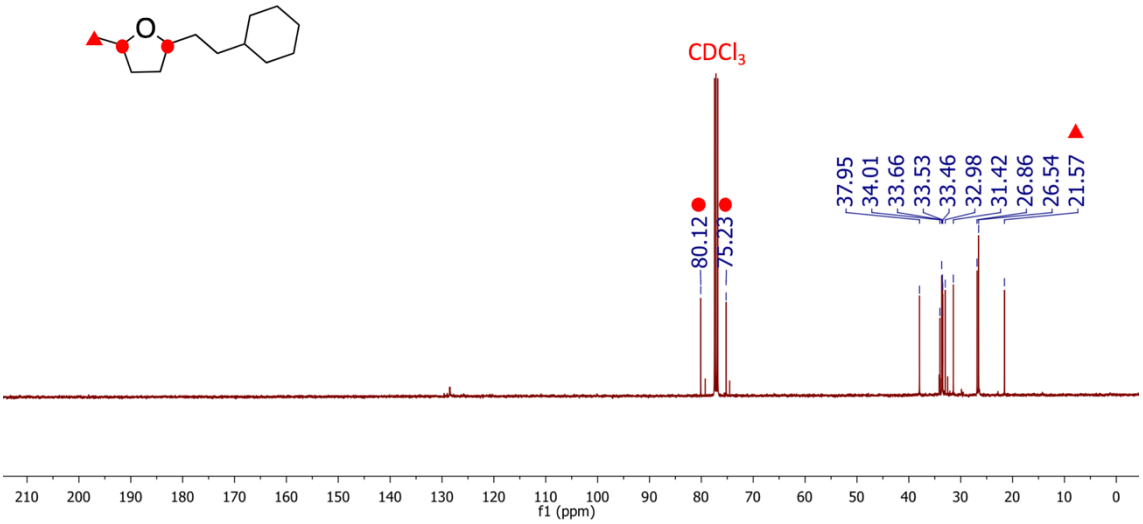


7-Phenylheptane-2,5-diol ^{1}H NMR (300MHz, $CDCl_3$): δ = 7.19-7.14 (m, 5H, Ar), 3,75 (m, 1H), 3.60 (m, 1H), 2.69-2.62 (m, 2H), 1.72 (m, 2H), 1.50 (m, 4H), 1.14-1.12 (d, 3H). ^{13}C NMR (75MHz, $CDCl_3$) δ = 142.23, 128.53, 125.94, 71.74, 71.26, 68.58, 68.08, 39.52, 39.17, 35.98, 35.01, 34.40, 33.46, 32.28, 32.25, 24.00, 23.66.



2-Methyl-5-phenethyltetrahydrofuran ^{1}H NMR (300MHz, $CDCl_3$) δ = 7.27-7.21 (m, 5H, Ar), 4.11-3.82 (m, 2H), 2.75-2.64 (m, 2H), 2.04-1.78 (m, 4H), 1.55-1.49 (m, 2H), 1.27-1.22 (d, d, 3H). ^{13}C NMR (75MHz, $CDCl_3$) δ = 142.40, 128.43, 125.83, 78.95, 78.19, 75.40, 74.65, 37.98, 34.07, 33.02, 32.71, 32.65, 32.44, 31.40, 21.60, 21.52.





2-(2-Cyclohexylethyl)-5-methyltetrahydrofuran ^{1}H NMR (300MHz, $CDCl_3$): δ = 3.93 (m, 1H), 3.74 (m, 1H), 1.94 (m, 2H), 1.69 (m, 5H), 1.43 (m, 4H), 1.24-1.22 (d, 3H), 1.20 (m, 10H). ^{13}C NMR (75MHz, $CDCl_3$): δ = 80.12, 75.23, 37.95, 34.01, 33.66, 33.53, 33.46, 32.98, 31.42, 26.86, 26.54, 21.57.