Supporting Information for

Co-Catalysis of Rhodium–Phosphoramidite Catalyst and ZSM-35(10) for Tandem Hydroformylation–Acetalization of Olefins

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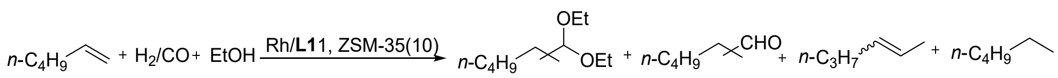
1. General methods

Unless otherwise noted, all manipulations involving air or moisture-sensitive compounds were performed in a nitrogen-filled glovebox or using standard Schlenk techniques. Solvents were dried according to standard procedures. ^{1}H NMR spectra were recorded on 400 MHz or 600 MHz and ^{13}C NMR spectra were recorded on 101 MHz by using a Bruker Avance 400 spectrometer. Chemical shifts (δ values) were reported in ppm with internal TMS (^{1}H NMR), $CDCl_3$ (^{13}C NMR), or external 85% H_3PO_4 (^{31}P NMR) as the standard, respectively. The IR spectra were measured on a Thermo (SCIENTIFC) NICOLET iS10 spectrometer. N_2 sorption isotherm was obtained on a Micromeritics ASAP 2460. HRMS (ESI) were determined on Agilent 1290-6545XT. GC analyses were measured on an Agilent 7820A system using an FID detector.

2. Screening the conditions for catalytic hydroformylation-acetalization of 1-hexene.

Table S1. Selected results of screening the conditions for catalytic hydroformylation-acetalization of 1-hexene[a]



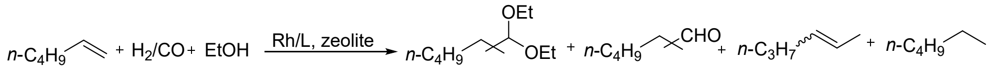
1 1a 1b 1c 1d

Entry	Rh/L	ZSM-35(10). (mg)	H_2/CO (bar)	Temp. (°C)	Solv. (mL)	Conv. (%)	*l/b*[b]	**1a**[c] (%)	**1b**[d] (%)	**1c**[e] (%)	**1d**[f] (%)
1	1:1	40	20/20	120	5.0	99.21	19.83	94.76	2.99	1.18	0.29
2	1:3	40	20/20	120	5.0	99.65	22.23	85.72	12.49	1.05	0.38
3	1:5	40	20/20	120	5.0	99.65	77.10	97.35	1.56	0.43	0.31
4	1:7	40	20/20	120	5.0	99.11	78.20.	91.11	6.33	1.51	0.15
5	1:5	20	20/20	120	5.0	98.48	12.85	77.89	17.12	2.09	1.38
6	1:5	60	20/20	120	5.0	99.55	43.63	96.36	2.10	0.42	0.67
7	1:5	40	20/20	110	5.0	99.51	32.12	95.77	2.90	0.39	0.44
8	1:5	40	20/20	100	5.0	99.63	29.51	93.43	4.43	0.87	0.91
9	1:5	40	20/20	90	5.0	99.20	35.14	86.68	5.56	3.76	0.74
10	1:5	40	10/10	120	5.0	98.74	26.43	77.30	13.49	1.39	6.55
11	1:5	40	25/25	120	5.0	99.64	63.10	90.64	7.25	1.08	0.68
12	1:5	40	20/20	120	2.5	99.60	50.45	70.80	27.16	0.91	0.73
13	1:5	40	20/20	120	7.5	99.45	75.50	95.10	2.54	0.95	0.86

[a]1-Hexene (3.8 mmol), $Rh(acac)(CO)_2$ (3.8×10^{-4} mmol), S/C_{Rh} (ratio of substrate to catalyst rhodium) = 10000, EtOH (5.0 mL), 24 h, decane as the internal standard. [b]Linear/branched acetal ratio, determined by GC analysis. [c]Yield of all acetals. [d]Yield of all aldehydes.

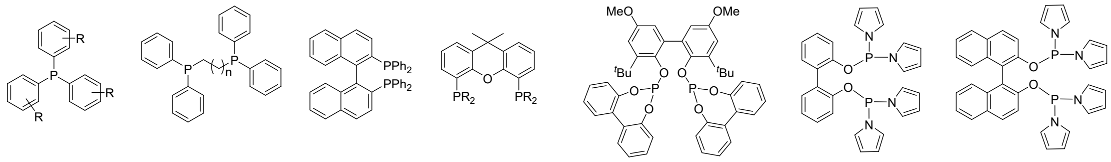
[e]Yield of hydrogenation product. [f]Yield of isomerization product.

Table S2. Selected results of screening the optimal conditions for catalytic hydroformylation-acetalization of 1-hexene[a]



1 1a 1b 1c 1d

Entry	Ligand	zeolites	conv. (%)	**1a**[b] (%)	*l/b*[c]	**1b**[d] (%)	**1c** (%)	**1d** (%)	TON[e]
1	**L1**	ZSM-35(10)	98.4	81.2	2.7	15.4	0.7	1.0	9660
2	**L2**	ZSM-35(10)	98.7	77.3	0.9	18.9	-	2.4	9620
3	**L3**	ZSM-35(10)	98.3	80.0	2.7	17.3	-	1.0	9730
4	**L4**	ZSM-35(10)	98.4	69.9	2.5	25.4	1.90	1.2	9530
5	**L5**	ZSM-35(10)	75.8	60.5	4.2	9.6	2.57	3.1	7010
6	**L6**	ZSM-35(10)	97.2	61.3	2.3	12.8	5.08	18.1	7410
7	**L7**	ZSM-35(10)	98.4	82.5	1.2	15.9	-	-	9840
8	**L8**	ZSM-35(10)	99.0	89.6	66.5	7.3	-	4.1	9690
9	**L9**	ZSM-35(10)	99.0	76.1	2.5	22.9	-	-	9900
10	**L10**	ZSM-35(10)	99.1	91.6	25.2	5.5	0	1.7	9710
11	**L11**	ZSM-35(10)	99.9	97.7	77.1	2.3	-	-	10000
12	**L11**	MCM-41	99.5	78.9	1.2	19.3	0.24	1.1	9820
13	**L11**	ZSM-5	99.3	85.9	8.0	12.3	0.29	0.8	9820
14	**L11**	β-Zeolite	98.9	85.4	23.8	9.1	1.0	3.4	9450
15	**L11**	ZSM-35(100)	99.4	82.1	20.2	16.2	0	1.1	9830



L1: R = H; **L2**: R = *o*-CH3; **L3**: R = *p*-OCH3; **L4**: n = 1; **L5**: n = 3; **L6**: BINAP; **L7**: R = *t*-Bu; **L8** (Xantphos): R = Ph; **L9**: Biphephos; **L10**: BPa; **L11**: BINAPa

[a]1-Hexene (3.8 mmol), $Rh(acac)(CO)_2$ (3.8×10^{-4} mmol), ligand (1.9×10^{-3} mmol), S/C_{Rh} (ratio of substrate to catalyst rhodium) = 10000, zeolites (40 mg), H_2/CO (20/20 bar), EtOH (5.0 mL), 120 °C, 24 h, decane as the internal standard, yields were determined by GC analysis. [b]Yield of all acetals. [c]Linear/branched acetal ratio. [d]Yield of all aldehydes. [e]Turnover Number of the Rh with respect to the yield of oxo products.

3. N_2 sorption isotherm and pore size distribution of zeolites.

Table S3. Textural parameters of zeolites[a]

Entry	zeolites	surface area (m^2/g)	pore volume (cm^3/g)	pore size (nm)
1	MCM-41	1,062.94	0.94	1.19-1.88; 2.98-4.05
2	β-Zeolite	454.85	0.34	0.53-0.84
3	ZSM-5	262.78	0.15	0.65-0.79; 1.09-2.51
4	ZSM-35(10)	277.98	0.16	0.65-0.73
5	ZSM-35(100)	329.59	0.19	0.65-0.85

[a]Analysed by BET (Brunauer-Emmett-Teller) method.

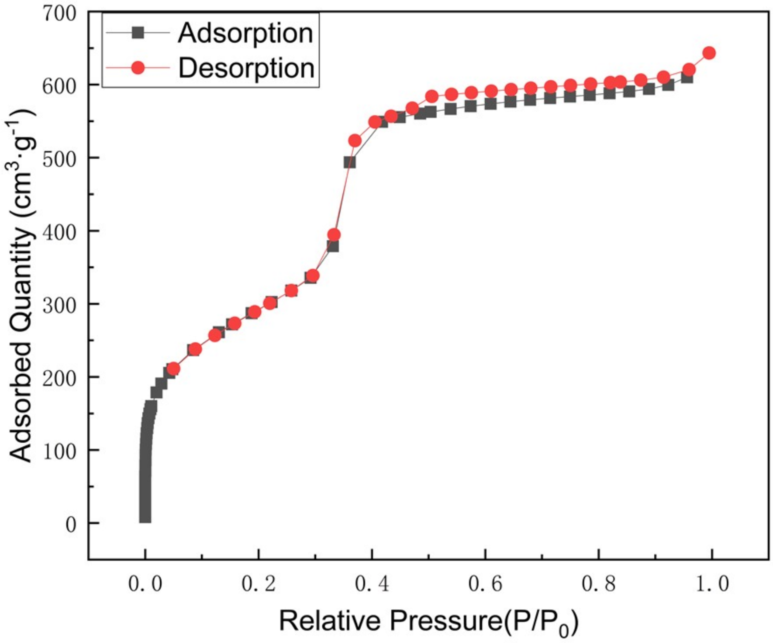


Figure S1. N_2 sorption isotherm of MCM-41

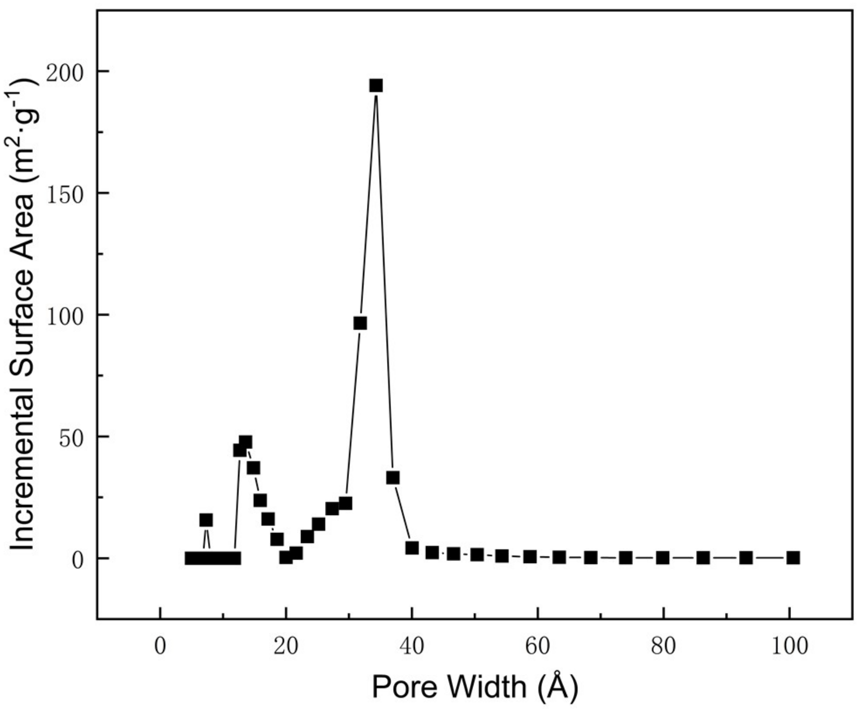


Figure S2. pore size distribution MCM-41

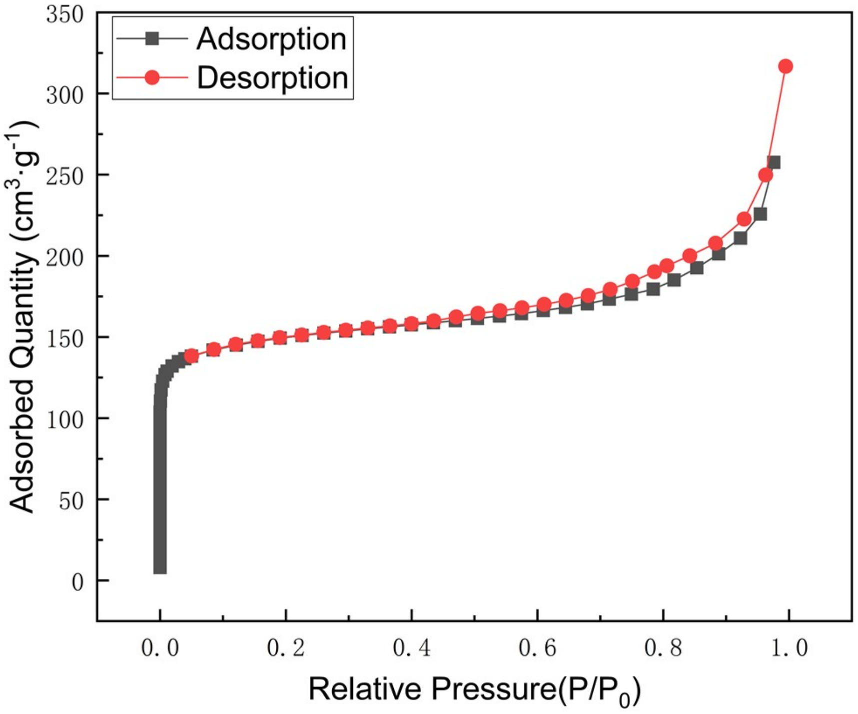


Figure S3. N_2 sorption isotherm of β-Zeolite

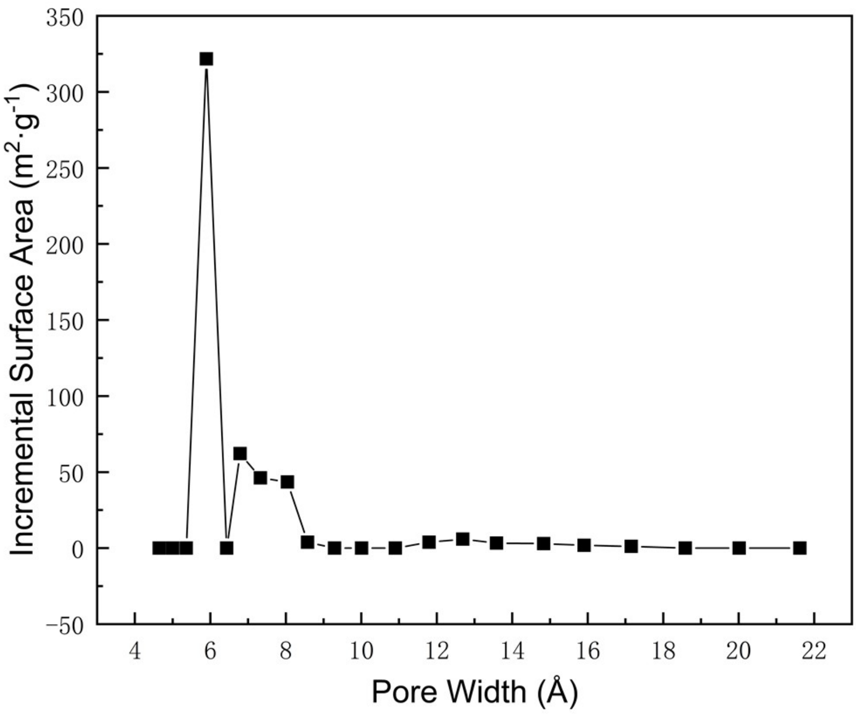


Figure S4. pore size distribution of β-Zeolite

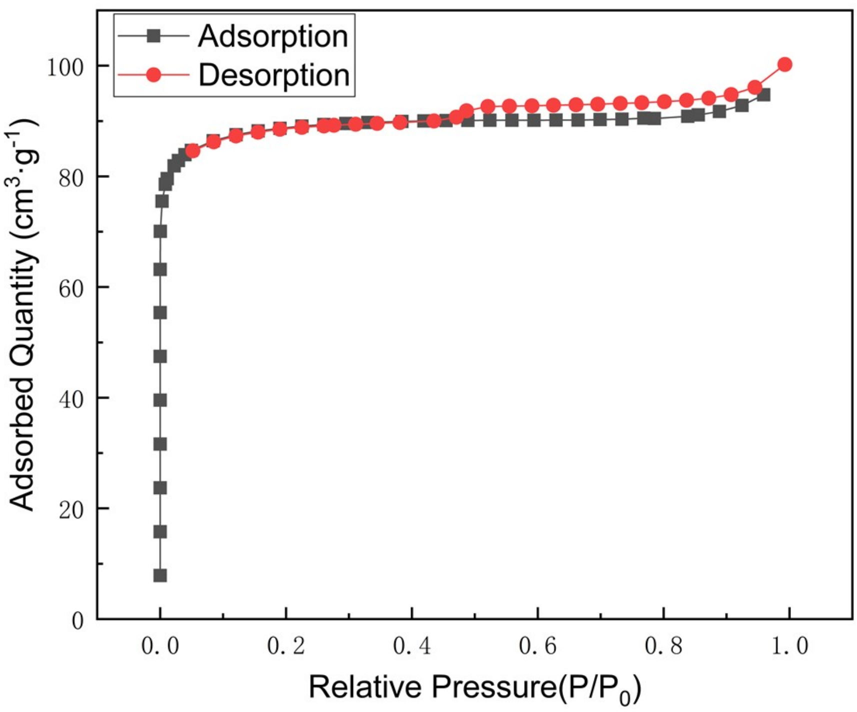


Figure S5. N_2 sorption isotherm of ZSM-5

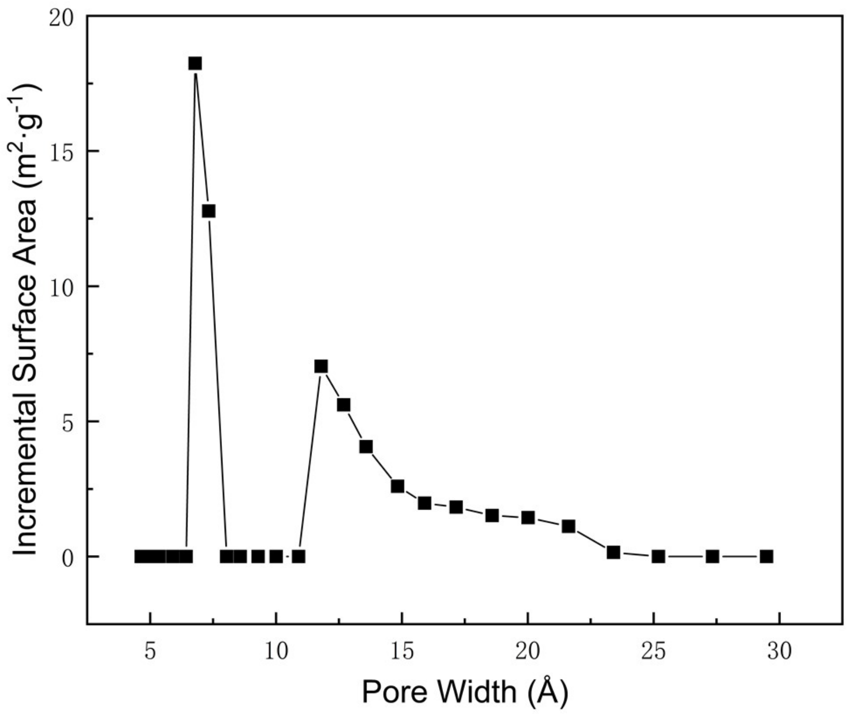


Figure S6. pore size distribution of ZSM-5

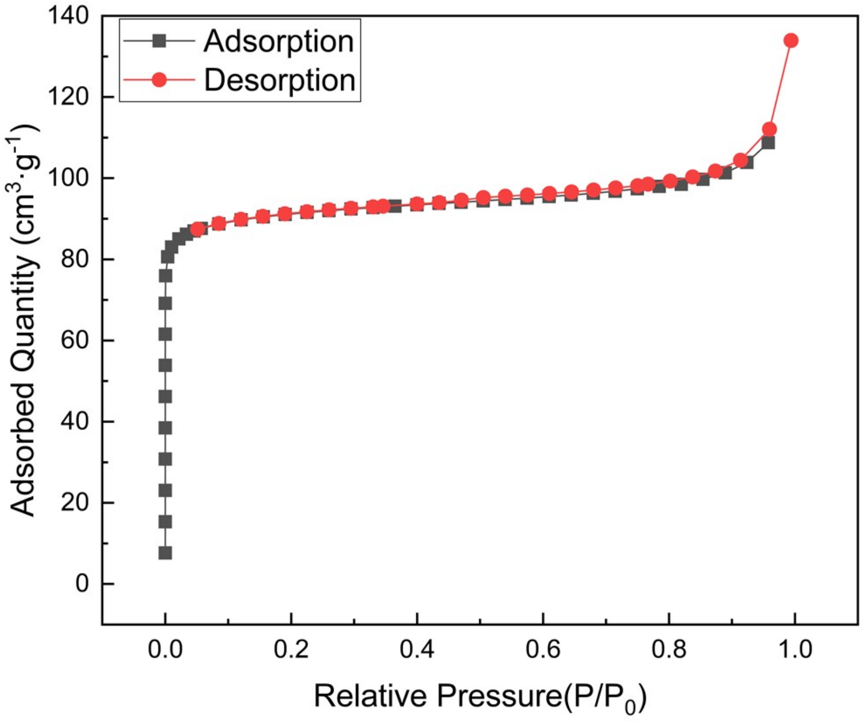


Figure S7. N_2 sorption isotherm of ZSM-35(10)

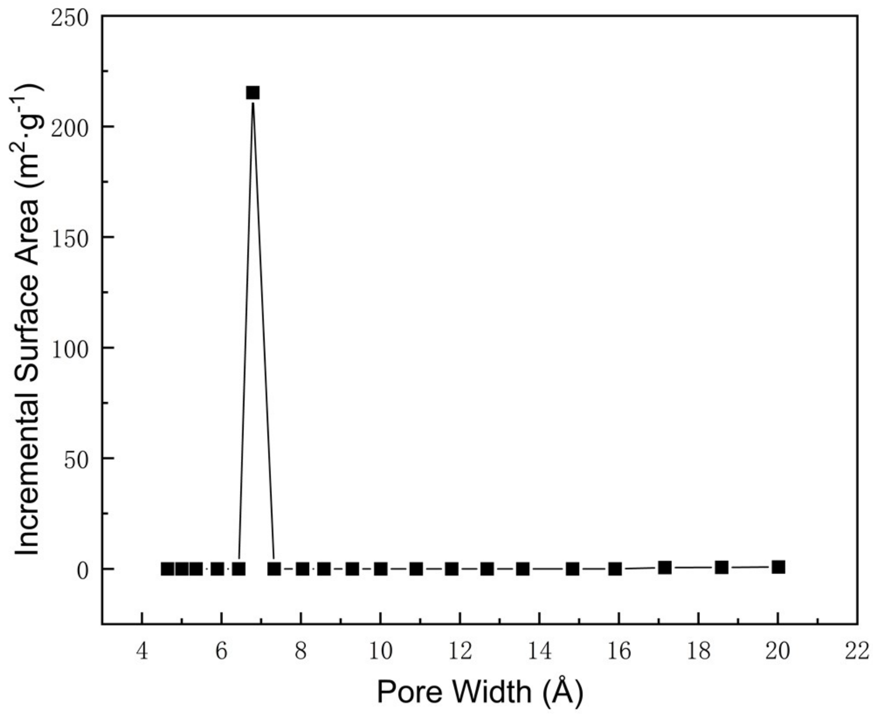


Figure S8. pore size distribution of ZSM-35(10)

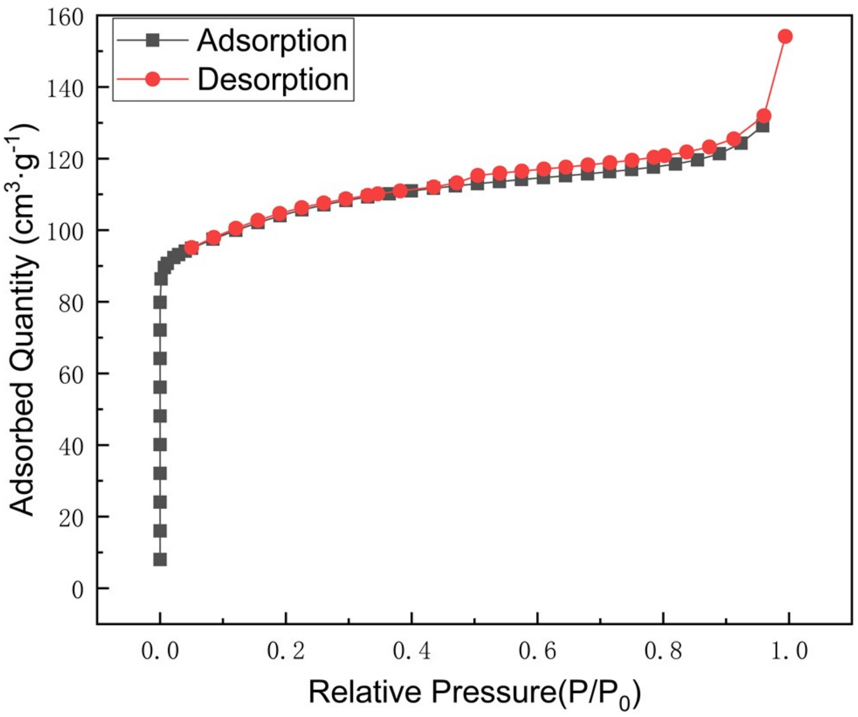


Figure S9. N_2 sorption isotherm of ZSM-35(100)

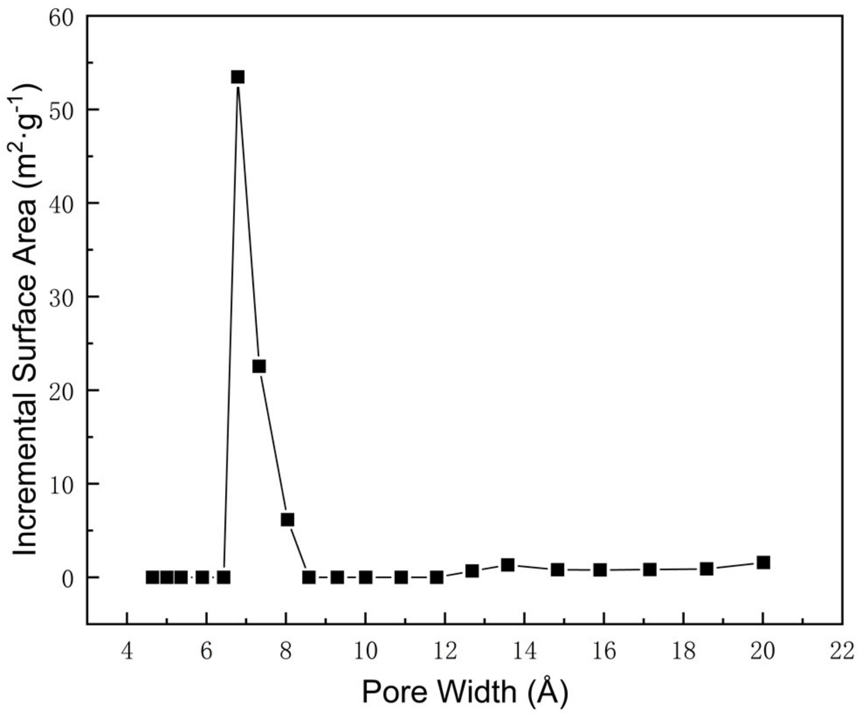


Figure S10. pore size distribution of ZSM-35(100)

4. General procedure for tandem hydroformylation–acetalization of olefins.

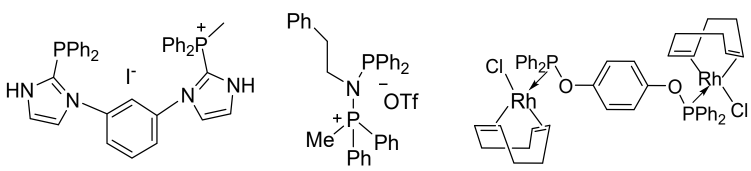
In a glove box, an autoclave with a magnetic stirring bar was charged with EtOH (5.0 mL), ZSM-35(10) (40 mg), $Rh(acac)(CO)_2$ (0.1 mg, 3.8×10^{-4} mmol), BINAPa (1.16 mg, 1.9×10^{-3} mmol), 1-hexene (0.47 mL, 3.8 mmol) and decane (16 μL) as the internal standard. The mixture was purged with hydrogen for three times and subsequently charged with CO (20 bar) and H_2 (20 bar). The autoclave was then heated to 120 °C (oil bath) and was kept at this temperature for 24 h. The autoclave was cooled in ice water, and the gas was carefully released in a well-ventilated hood. The mixture subsequently was analyzed by gas chromatography (GC).

GC analysis condition: SE-54, 30 m×0.32 mm×0.33 mm, flow rate 2.0 mL min^{-1}, method: 50°C was maintained for 5 min, and then ramped from 50 °C to 120 °C at a rate of 10 °C min^{-1}, 120 °C was maintained for 2 min; then ramped from 120 °C to 250 °C at a rate of 20 °C min^{-1}, 250 °C was maintained for 10 min.

5. Comparison of catalytic performance of catalysts reported in literature and in this study

Table S4. Comparison of catalytic performance of catalysts reported in literature and in this study

catalyst	yield	*l*/*b*	TON_{oxo}[a]
Rh/BINAPa, ZSM-35(10)	50.6-98.4	≥30.5	43000
$Rh(acac)(CO)_2$/**L12**[12b]	84.3-92.1	1.1-1.9	1900
$Rh(acac)(CO)_2$/**L13**[12a]	39.2-94.1	0.4-2.1	980
Rh/P complex[7c]	81.0-99.0	0.9-1.6	2475
$RhCl_3\cdot3H_2O/PPh_3$[11a]	96.9	3.0	980
$[Rh(cod)_2]BF_4$/Xantphos[11b]	5.8-86.2	9.1-89.2	184



L12 **L13** Rh/P complex

[a]The highest TON_{oxo} value in the literature and in this work. The references see the main text.

6. Preparation and characterization of Rh-H complexes

In a glovebox, the mixture of $Rh(acac)(CO)_2$ (4.1 mg, 0.016 mmol), BINAPa (9.8 mg, 0.016 mmol), ZSM-35(10) (10 mg), in toluene-d_8 (2.0 mL) was stirred for 0.5 hour at room temperature in a 10 mL glass vial, which was then transferred into a stainless-steel autoclave and sealed. The autoclave was purged with H_2 three times and subsequently charged with CO (10 bar) and H_2 (10 bar). The autoclave was then heated to 40 °C (oil bath) and stirred at the temperature for 10 h. After cooling the autoclave to 0 °C, the syngas was carefully released, and the solution was submitted to NMR analysis.

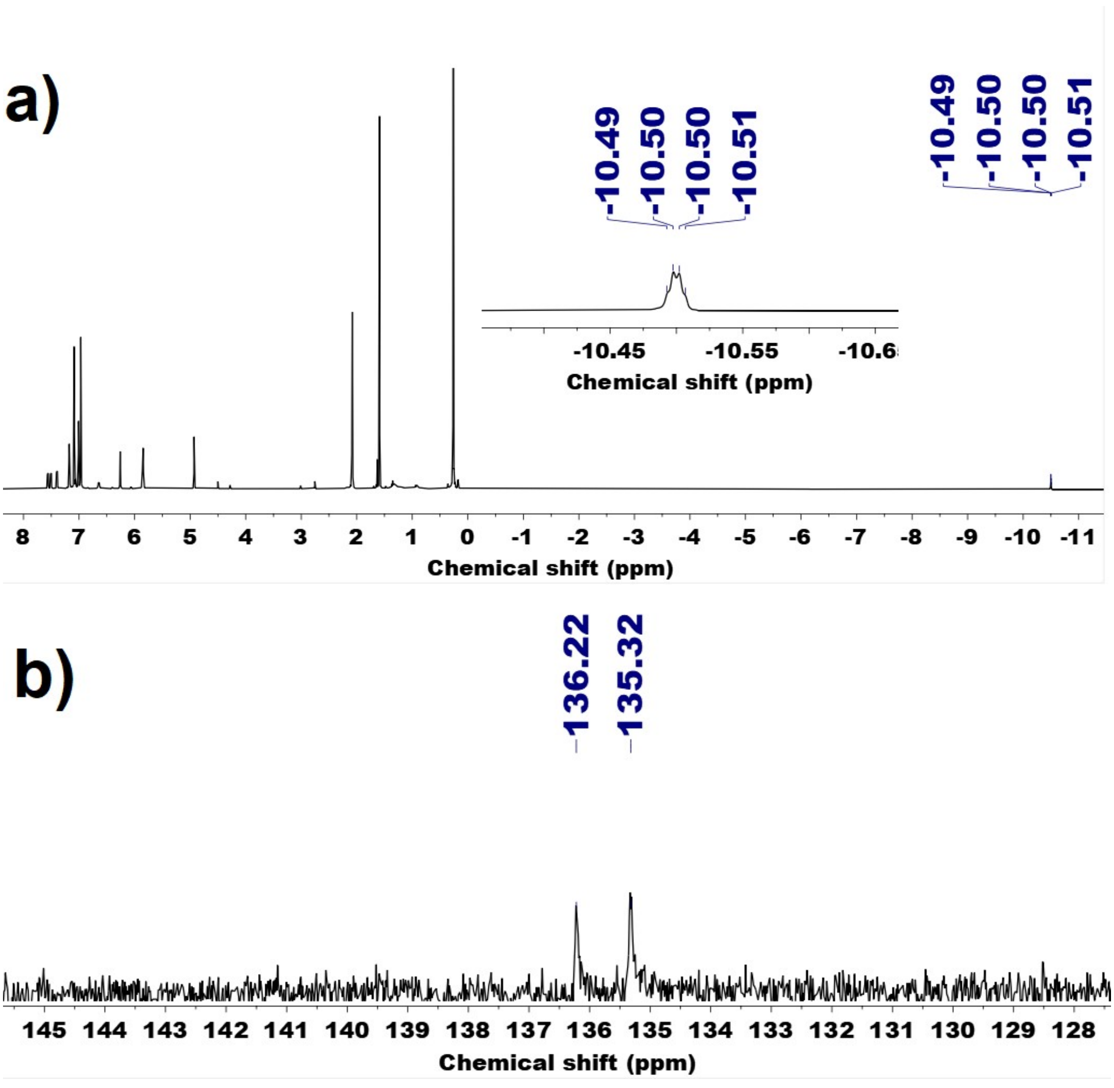
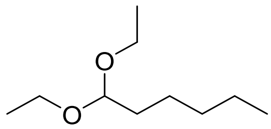
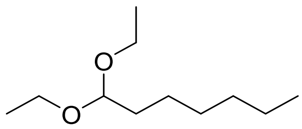


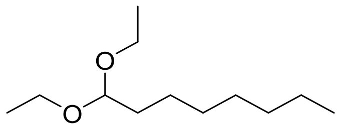
Figure S11. (a) ^1H NMR spectra, (b) ^{31}P NMR spectra of [HRh(CO)(BINAPa)] in the presence of

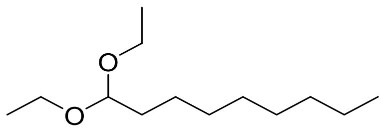
ZSM-35(10).

7. Characterization data for the products

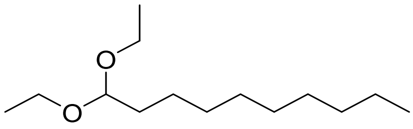
 **1,1-Diethoxyhexane (2a)[1]:** colorless oil, 608.20 mg, 91.9% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.42 (t, *J* = 5.6 Hz, 1H), 3.62-3.54 (m, 2H), 3.47-3.40 (m, 2H), 1.56-1.52 (m, 2H), 1.25 (m, 6H), 1.30-1.15 (t, *J* = 7.2 Hz, 6H), 0.83-0.82 (m, 3H) ppm.

 **1,1-Diethoxyheptane (1a)[2]:** colorless oil, 652.87 mg, 91.3% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.41 (t, *J* = 6.0 Hz, 1H), 3.61-3.53 (m, 2H), 3.46-3.39 (m, 2H), 1.55-1.51 (m, 2H), 1.25-1.22 (m, 8H), 1.13 (t, *J* = 7.2 Hz, 6H), 0.82-0.80 (m, 3H) ppm.

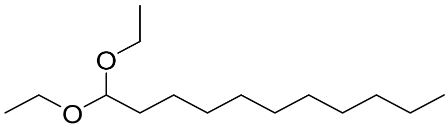
 **1,1-Diethoxyoctane (3a)[1]:** pale yellow oil, 674.59 mg, 87.8% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.43 (t, *J* = 6.0 Hz, 1H), 3.64-3.55 (m, 2H), 3.48-3.40 (m, 2H), 1.58-1.53 (m, 2H), 1.30-1.23 (m, 10H), 1.15 (t, *J* = 7.2 Hz, 6H), 0.83 (t, *J* = 6.8 Hz, 3H) ppm.

 **1,1-Diethoxynonane (4a):** pale yellow oil, 715.61 mg, 87.1% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.45 (t, *J* = 5.6 Hz, 1H), 3.65-3.58 (m, 2H), 3.50-3.43 (m, 2H), 1.59-1.56 (m, 2H), 1.32-1.25 (m, 12H), 1.18 (t, *J* = 7.2 Hz, 6H), 0.86 (t, *J* = 6.8 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$): δ 103.0, 60.8, 33.6, 31.9, 29.5, 29.5, 29.2, 24.8, 22.6, 15.3, 14.1 ppm; **FT-IR** υ max/cm^{-1} 2926.06, 2856.61,

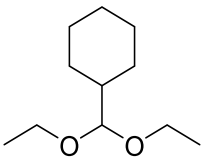
1461.89, 1376.18, 1119.20, 1059.82, 905.84, 731.13, 648.80; HRMS (ESI) m/z: Calcd. For $C_{13}H_{28}NaO_2^+$: 239.1982, Found: 239.1986 (M+Na^+).



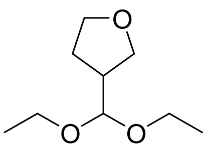
1,1-Diethoxydecane (5a) [3]: pale yellow oil, 755.86 mg, 86.4% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.41 (t, *J* = 5.6 Hz, 1H), 3.61-3.53 (m, 2H), 3.46-3.38 (m, 2H), 1.54-1.51 (m, 2H), 1.30-1.20 (m, 14H), 1.13 (t, *J* = 7.2 Hz, 6H), 0.81 (t, *J* = 6.8 Hz, 3H) ppm.



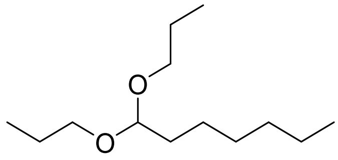
1,1-Diethoxydecane (6a) [2]: pale yellow oil, 748.99 mg, 80.7% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.31 (t, *J* = 5.6 Hz, 1H), 3.50-3.43 (m, 2H), 3.35-3.28 (m, 2H), 1.47-1.42 (m, 2H), 1.19-1.12 (m, 16H), 1.03 (t, *J* = 7.2 Hz, 6H), 0.73 (t, *J* = 7.2 Hz, 3H) ppm.

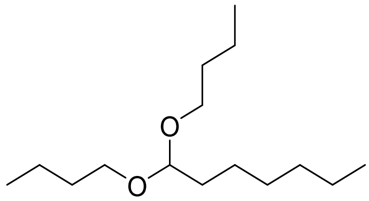


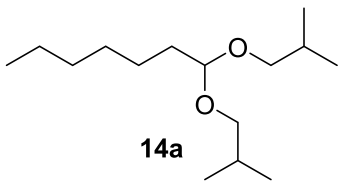
(Diethoxymethyl)cyclohexane (7a)[3]: pale yellow oil, 543.29 mg, 76.8% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.08 (d, *J* = 7.2 Hz, 1H), 3.65-3.57 (m, 2H), 3.49-3.41 (m, 2H), 1.78-1.68 (m, 4H), 1.63-1.51 (m, 2H), 1.23-1.11 (m, 9H), 0.99-0.91 (m, 2H) ppm.



3-(Diethoxymethyl)tetrahydrofuran(9a)[4]: pale yellow oil, 210.42 mg, 31.8% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.33 (d, *J* = 8.0 Hz, 1H), 3.85-3.80 (m, 2H), 3.73-3.67 (m, 2H), 3.65-3.60 (m, 2H), 3.55-3.45 (m, 2H), 2.60-2.51 (m, 1H), 2.01-1.92 (m, 1H), 1.80-1.71 (m, 1H), 1.22-1.16 (m, 6H) ppm.

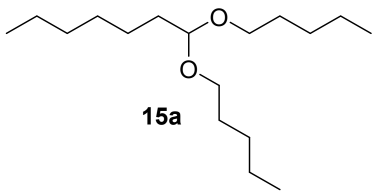
 **1,1-Dipropoxyheptane: (11a):** pale yellow oil, 713.15 mg, 86.8% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.36 (t, *J* = 6.0 Hz, 1H), 3.46-3.40 (m, 2H), 3.29-3.24 (m, 2H), 1.53-1.44 (m, 6H), 1.21-1.16 (m, 8H), 0.83 (t, *J* = 7.6 Hz, 6H), 0.78 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 103.1, 67.0, 33.4, 31.7, 29.1, 24.7, 23.0, 22.5, 13.9, 10.6 ppm; **FT-IR** υ max/cm^{-1} 2927.80, 2857.39, 1463.68, 1378.68, 1115.17, 1024.34, 907.23, 730.44, 647.34. HRMS (ESI) m/z: Calcd. For $C_{13}H_{28}NaO_2^+$: 239.1982, Found: 239.1986 ($M+Na^+$).

 **1,1-Dibutoxyheptane (12a):** pale yellow oil, 799.10 mg, 86.1% yield. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.35 (t, *J* = 6.0 Hz, 1H), 3.49-3.44 (m, 2H), 3.33-3.27 (m, 2H), 1.52-1.41 (m, 6H), 1.34-1.18 (m, 12H), 0.82 (t, *J* = 7.2 Hz, 6H), 0.78 (t, *J* = 6.8 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 103.1, 65.0, 33.4, 32.0, 31.7, 29.1, 24.7, 22.5, 19.4, 13.9, 13.8; **FT-IR** υ max/cm^{-1}: 2931.16, 2860.39, 1464.97, 1379.58, 1112.75, 1036.15, 906.34, 729.09, 647.63. HRMS (ESI) m/z: Calcd. For $C_{15}H_{32}NaO_2^+$: 267.2295, Found: 267.2302 ($M+Na^+$).



14a

1,1-Diisobutoxyheptane (14a): pale yellow oil, 797.25 mg，85.9% yield. **^{1}H NMR (**400 MHz, $CDCl_3$): δ 4.39 (t, *J* = 6.0 Hz, 1H), 3.30-3.27 (m, 2H), 3.12-3.09 (m, 2H), 1.78-1.76 (m, 2H), 1.56-1.55 (m, 2H), 1.23 (m, 8H), 0.86-0.83 (m, 15H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 103.4, 72.2, 33.5, 31.9, 29.3, 28.8, 24.9, 22.7, 19.6, 14.1 ppm; **FT-IR** υ max/cm^{-1}: 2930.5, 2872.5, 1461.7, 1376.3, 1111.9, 1033.9, 902.1, 726.1, 646.7. HRMS (ESI) m/z: Calcd. For $C_{15}H_{32}NaO_2^+$: 267.2295, Found: 267.2303 ($M+Na^+$).



15a

1,1-Bis(pentyloxy)heptane (15a): pale yellow oil, 847.36 mg, 81.9%. **^{1}H NMR (**400 MHz, $CDCl_3$): δ 4.45 (t, *J* = 4.0 Hz, 1H), 3.57-3.53 (m, 2H), 3.42-3.37 (m, 2H), 1.61-1.55 (m, 6H), 1.33-1.25 (m, 16H), 0.90-0.86 (m, 9H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 103.2, 65.4, 33.5, 31.8, 29.6, 29.1, 28.5, 24.8, 22.6, 22.5, 14.1, 14.04, 14.01 ppm; **FT-IR** υ max/cm^{-1}: 2928.5, 2873.6, 1458.7, 1372.3, 1114.9, 1030.8, 901.1, 724.2, 649.2. HRMS (ESI) m/z: Calcd. For $C_{17}H_{36}NaO_2^+$: 295.2608, Found: 295.2612 (M+Na$^+$).

8. Recycling tests of the ZSM-35(10) in tandem hydroformylation-acetalization of 1-hexene with EtOH

The recycling tests are followed the general procedure for tandem hydroformylation–acetalization of olefins. The ZSM-35(10) was separated from the mixture by using centrifuge, washed by EtOH, and heated at 120 °C for 8 h under vacuum condition. The reactivated ZSM-35(10) was used to test next recycling reaction with the same condition and procedure.

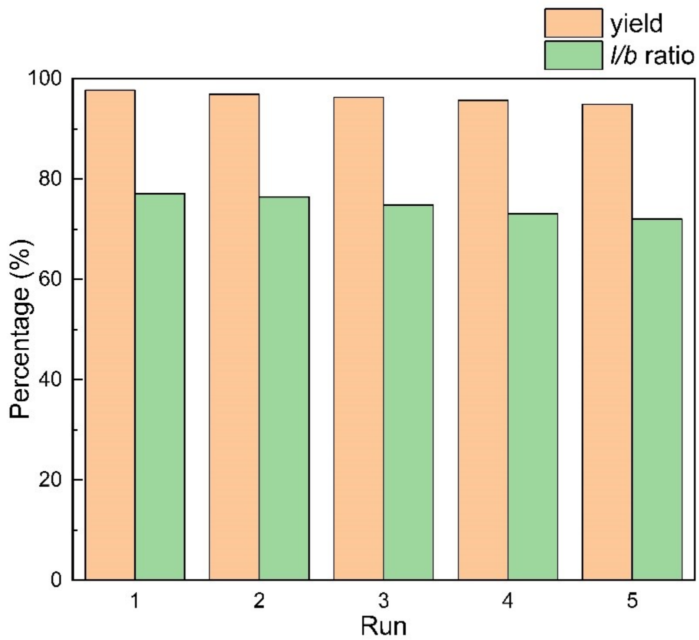


Figure S12. Recycling tests of ZSM-35(10)

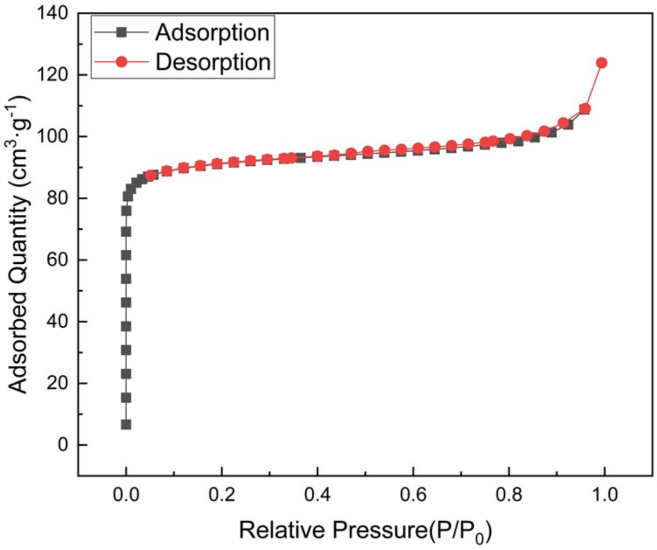


Figure S13. N_2 sorption isotherm of recovered ZSM-35(10)

The Brunauer−Emmett−Teller (BET) surface area and pore volume of recovered ZSM-35(10) are 264.2 m^2/g and 0.15 cm^3/g, respectively.

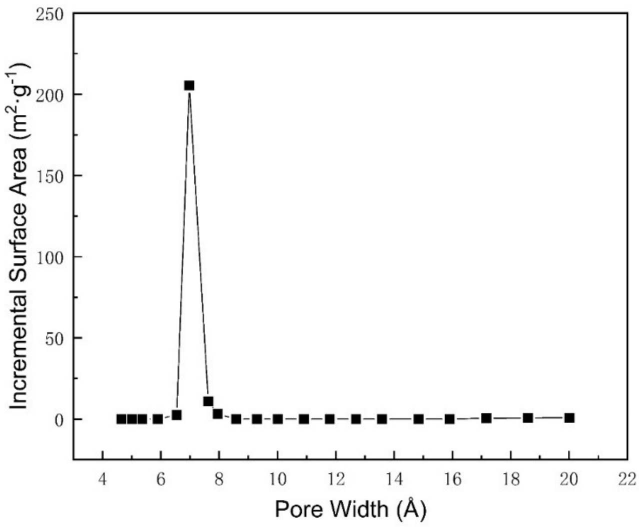
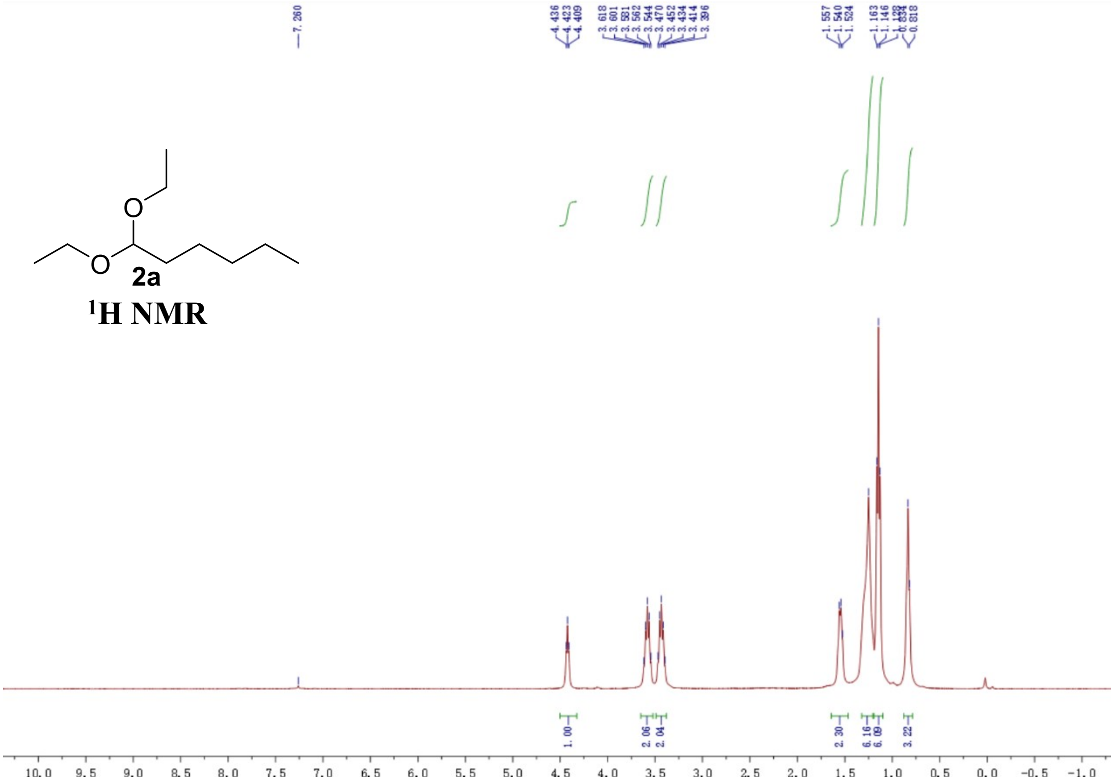
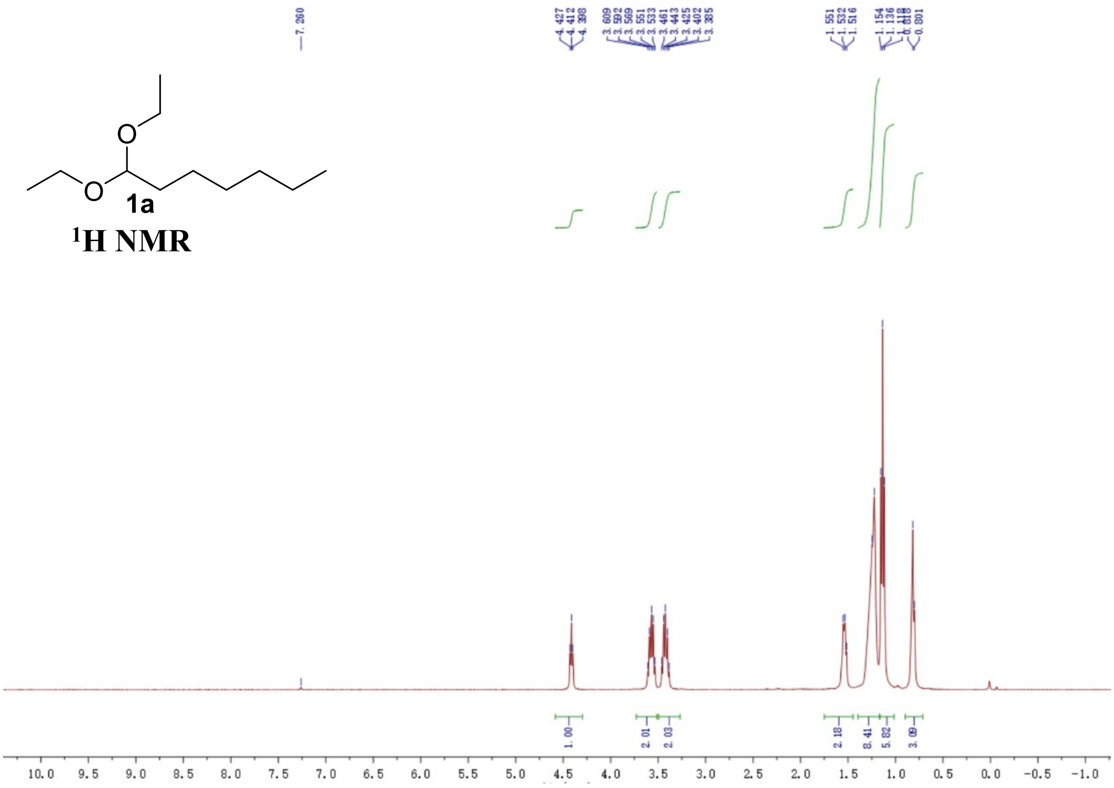
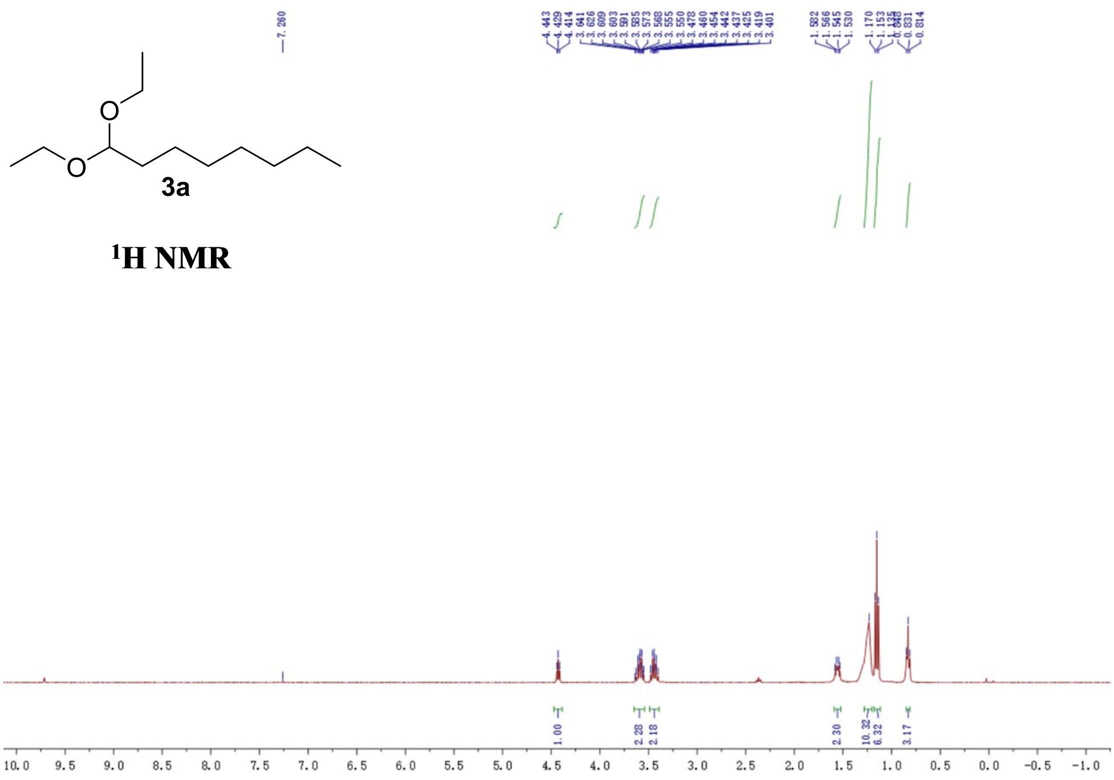


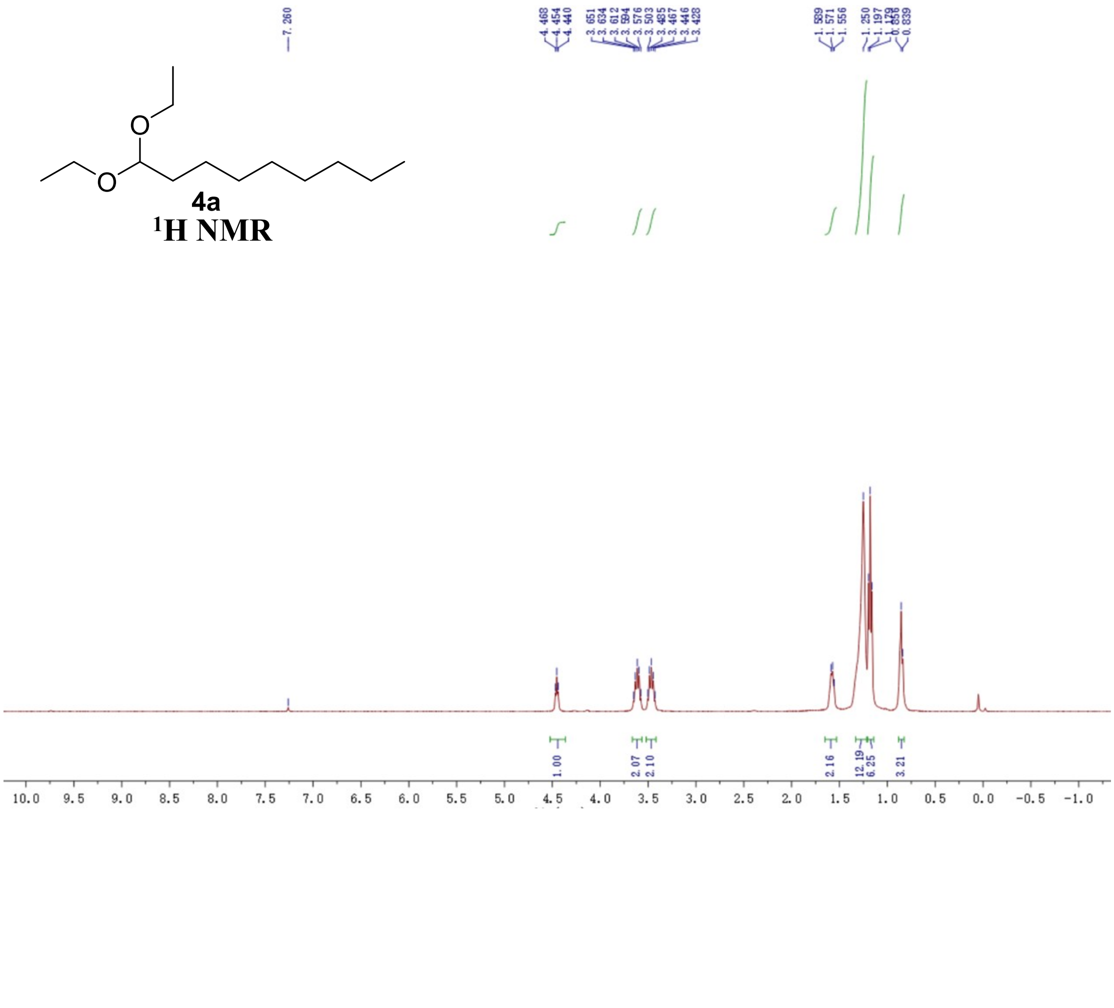
Figure S14. pore size distribution of recovered ZSM-35(10)

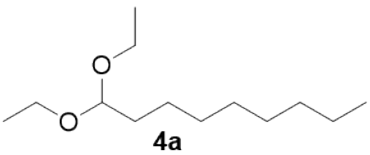
9. NMR spectra of major products





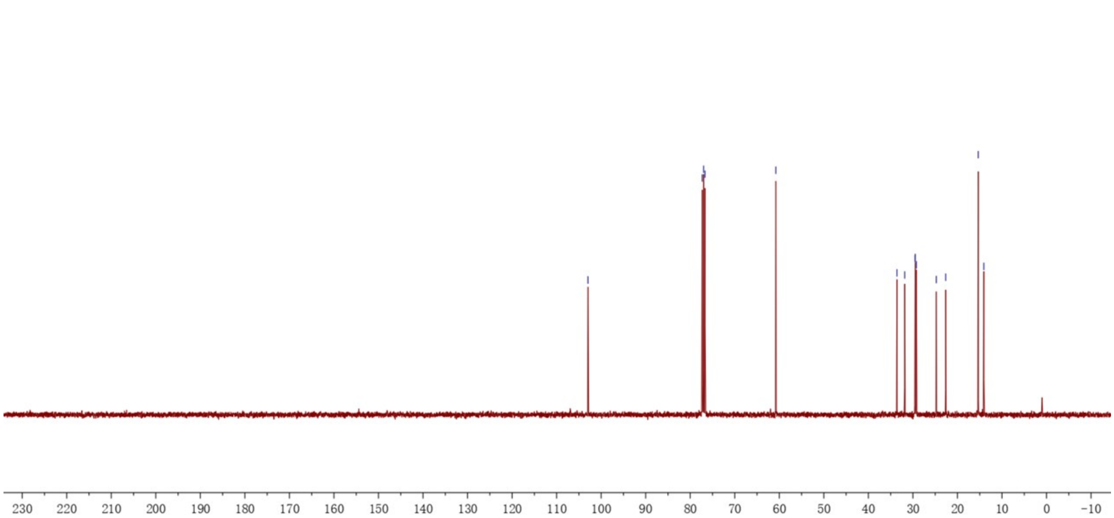

3a
^{1}H NMR

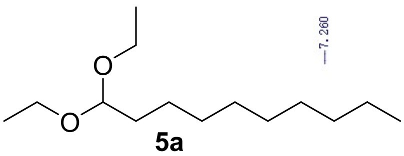

4a
^{1}H NMR



4a

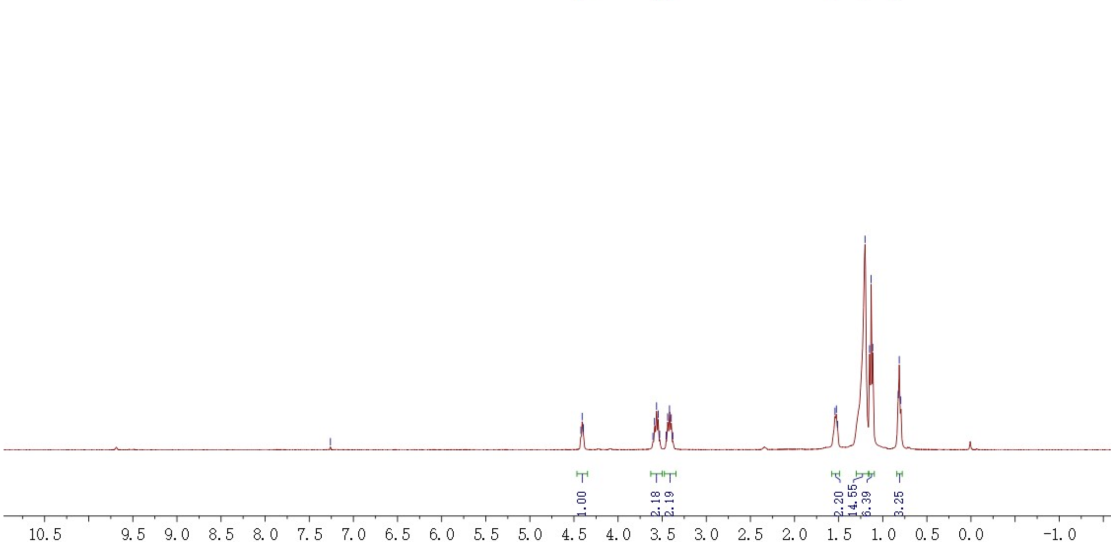
^{13}C NMR

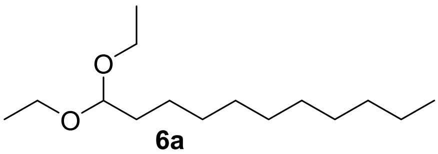




5a

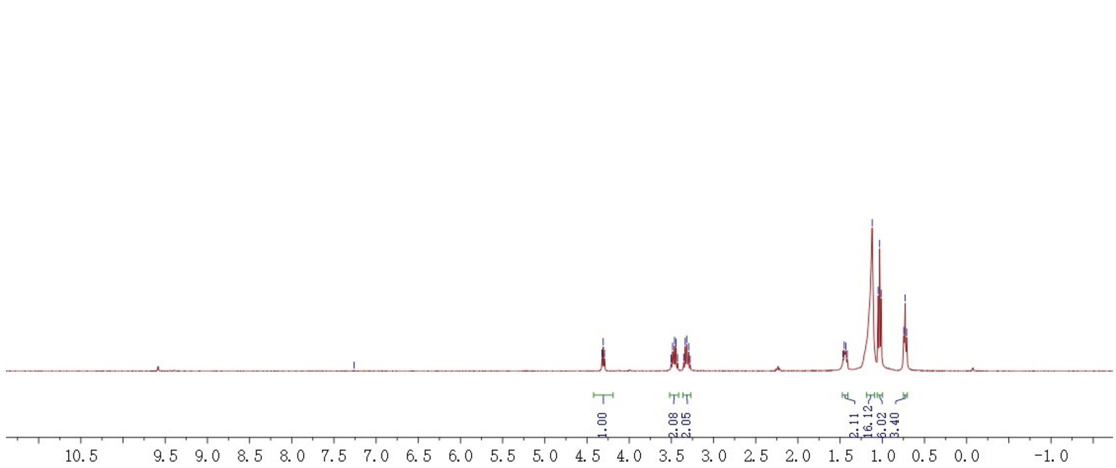
^{1}H NMR

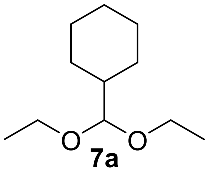




6a

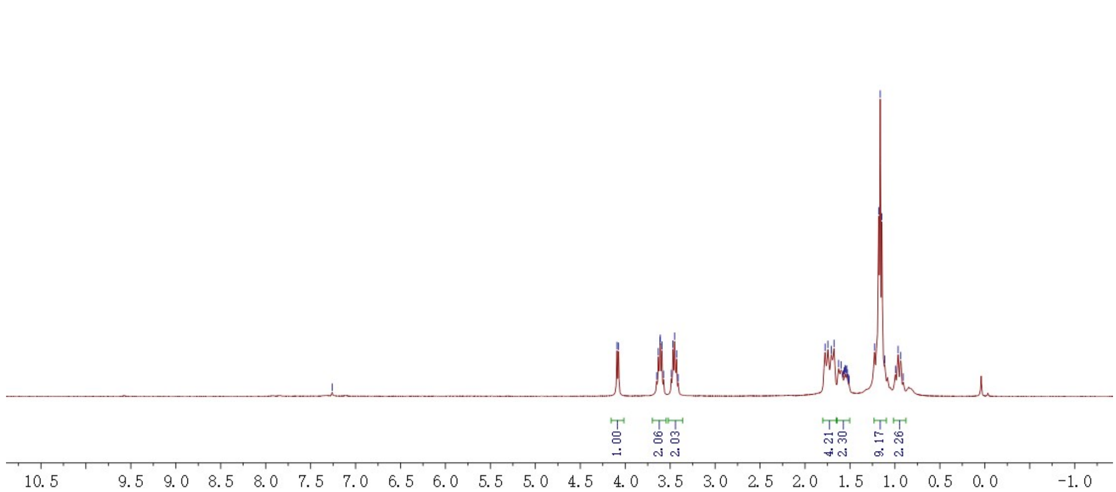
[1]H NMR

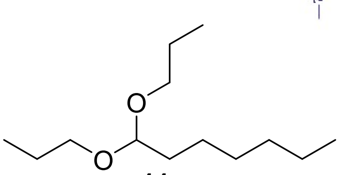




7a

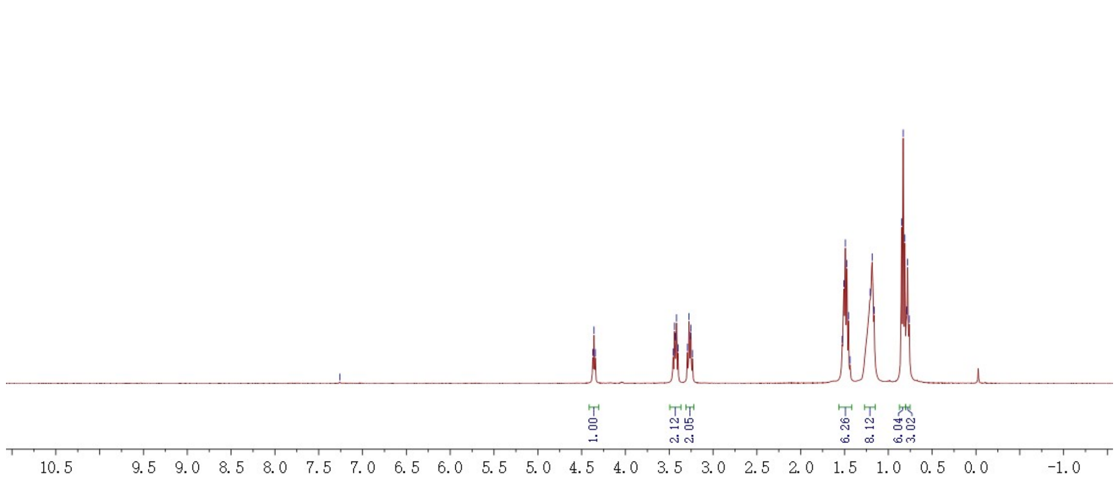
[1]H NMR

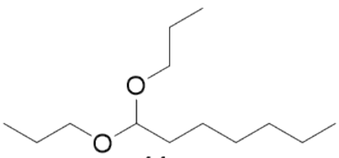




11a

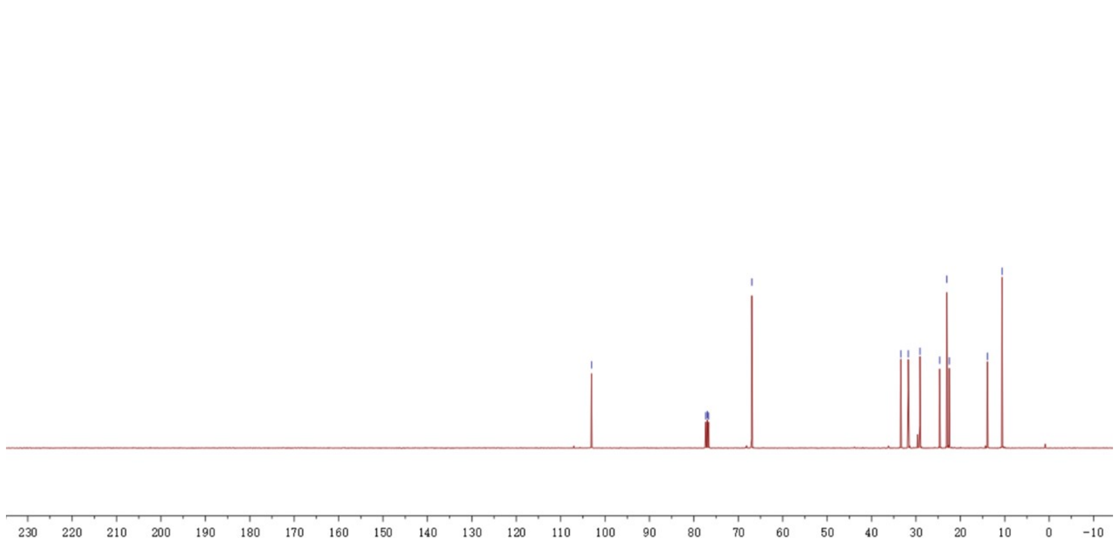
^{1}H NMR

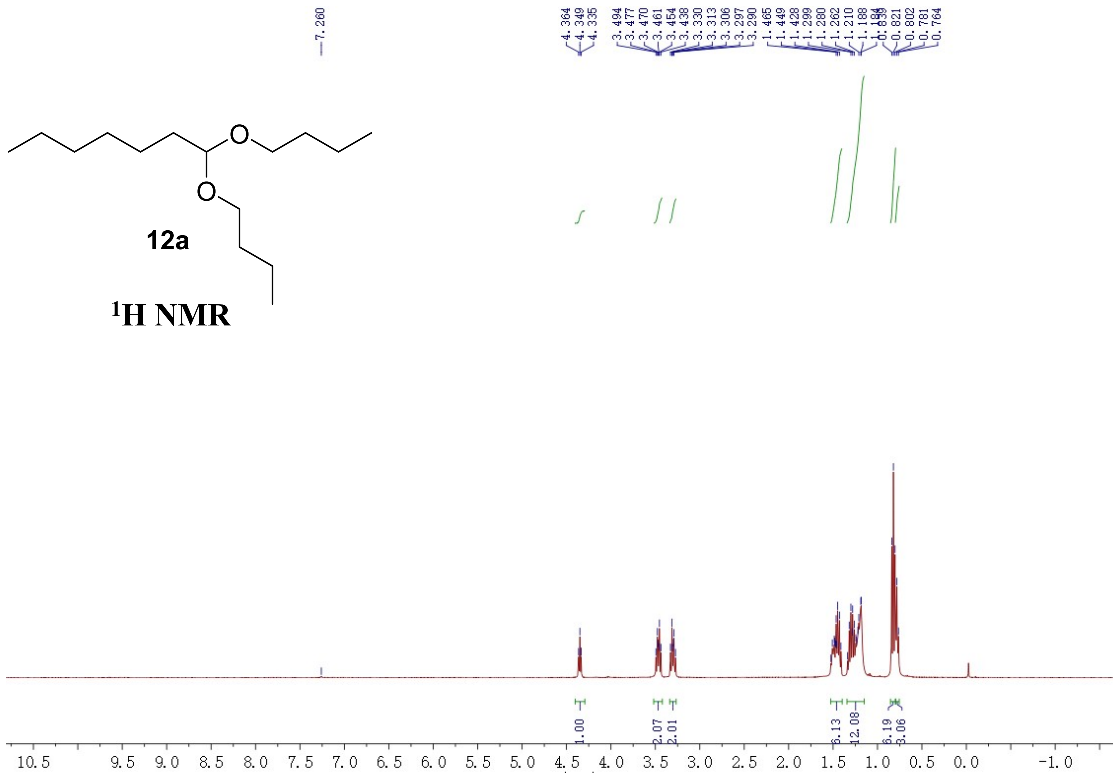




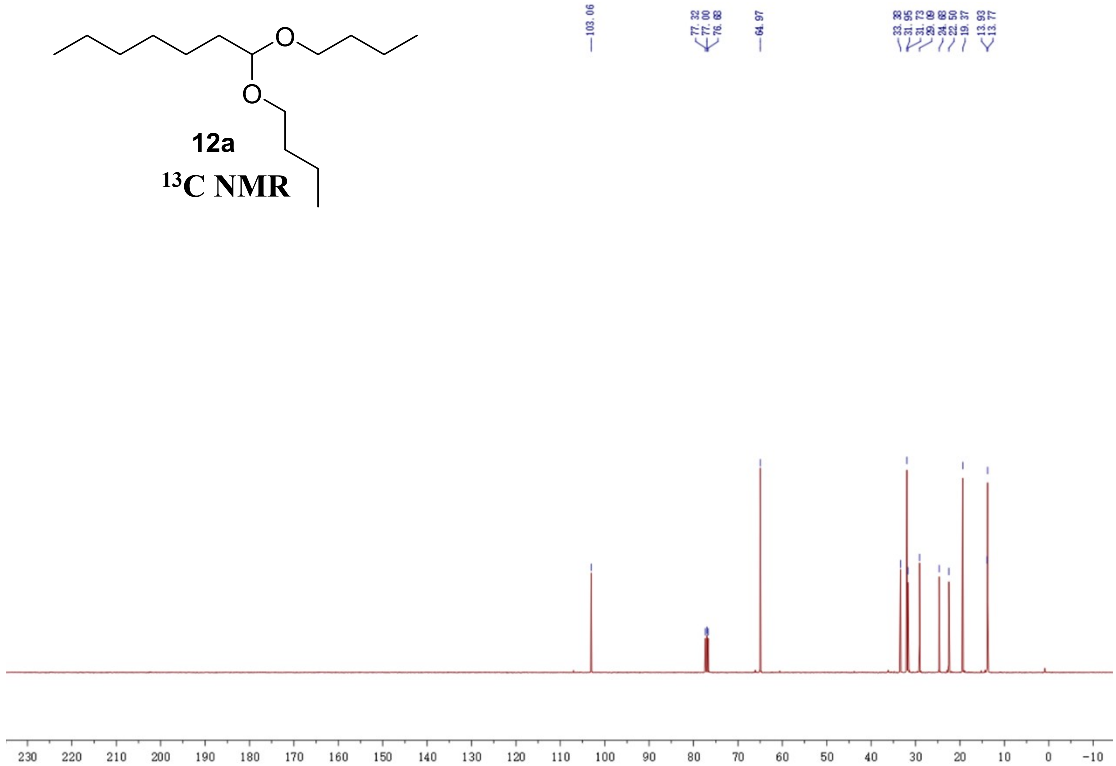
11a

^{13}C NMR

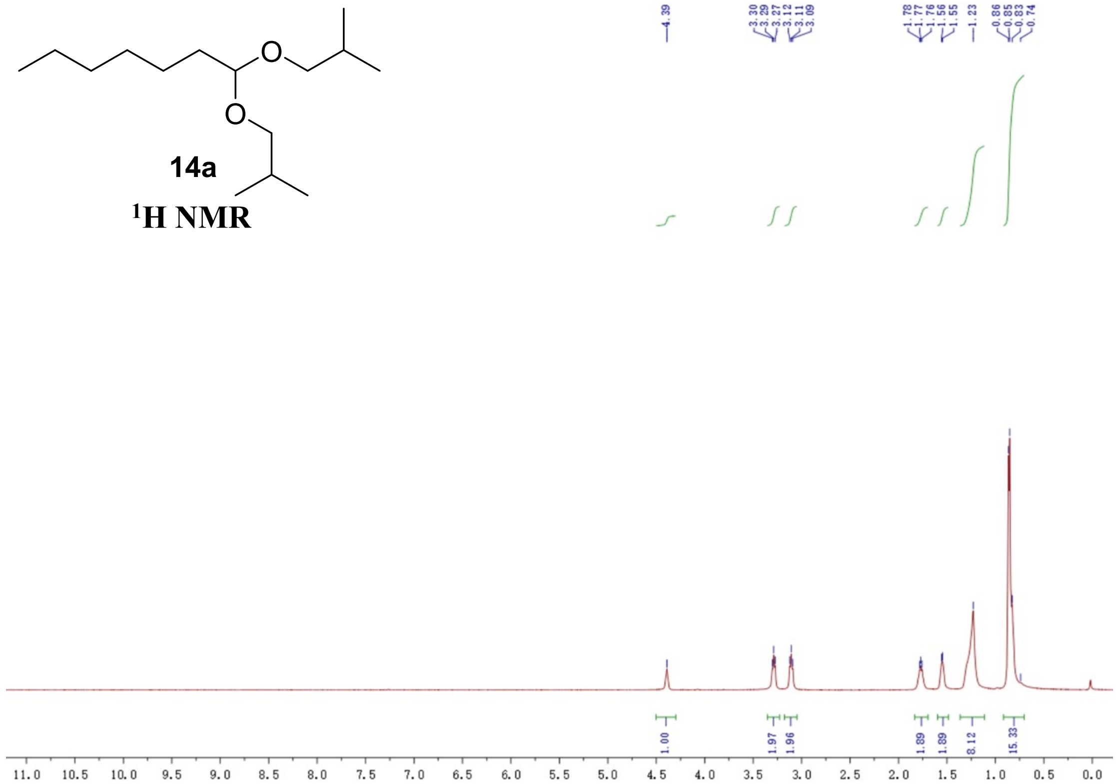




12a
1H NMR

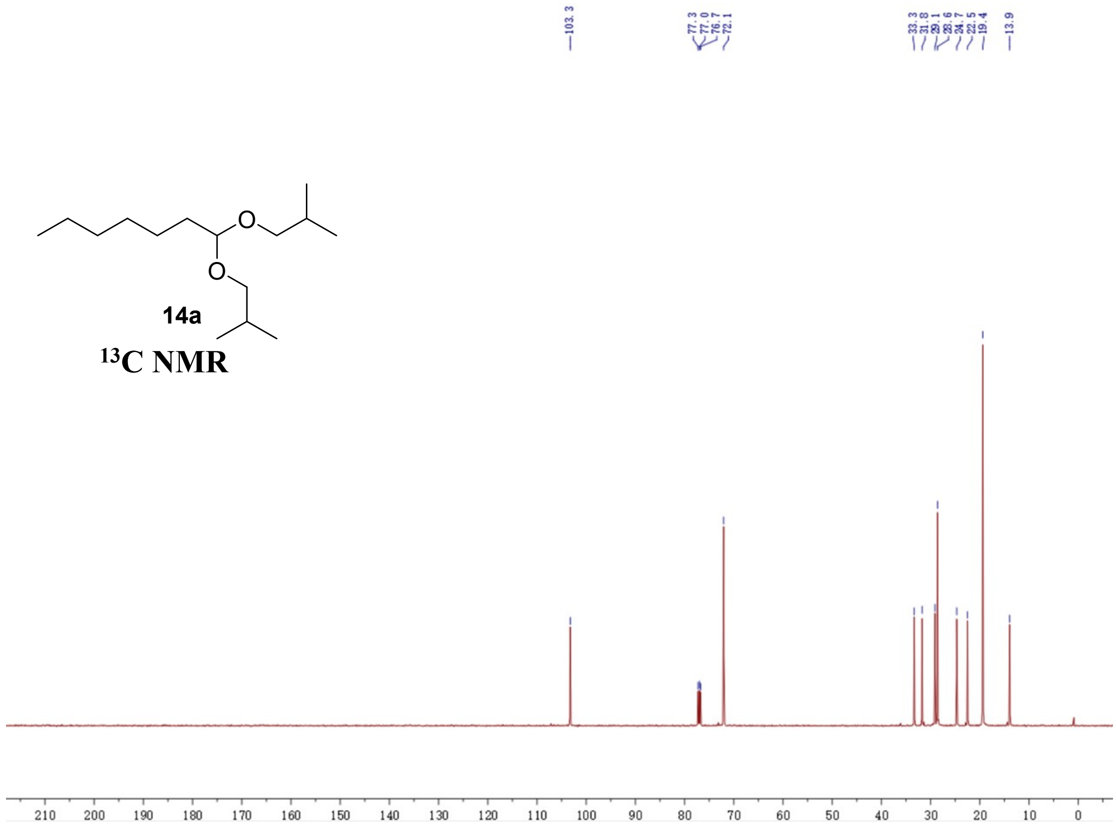


12a
13C NMR



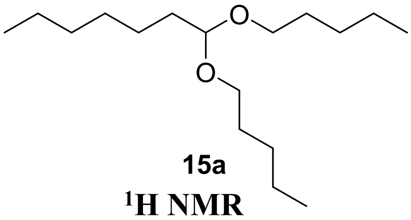
14a

^{1}H NMR



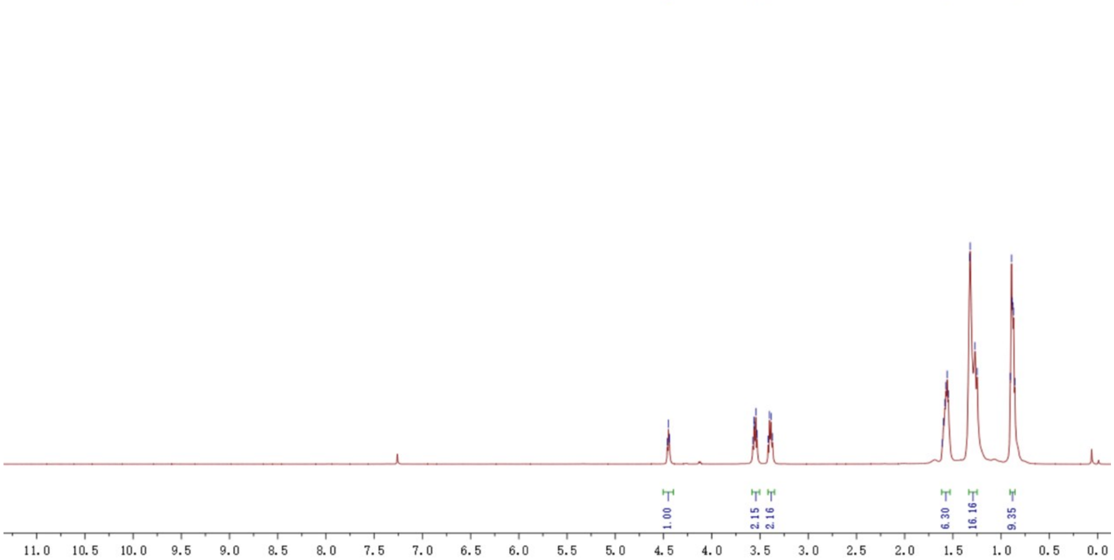
14a

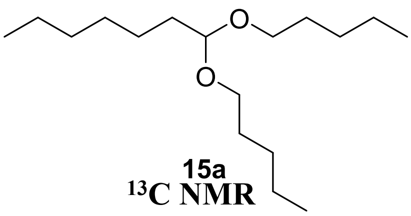
^{13}C NMR



15a

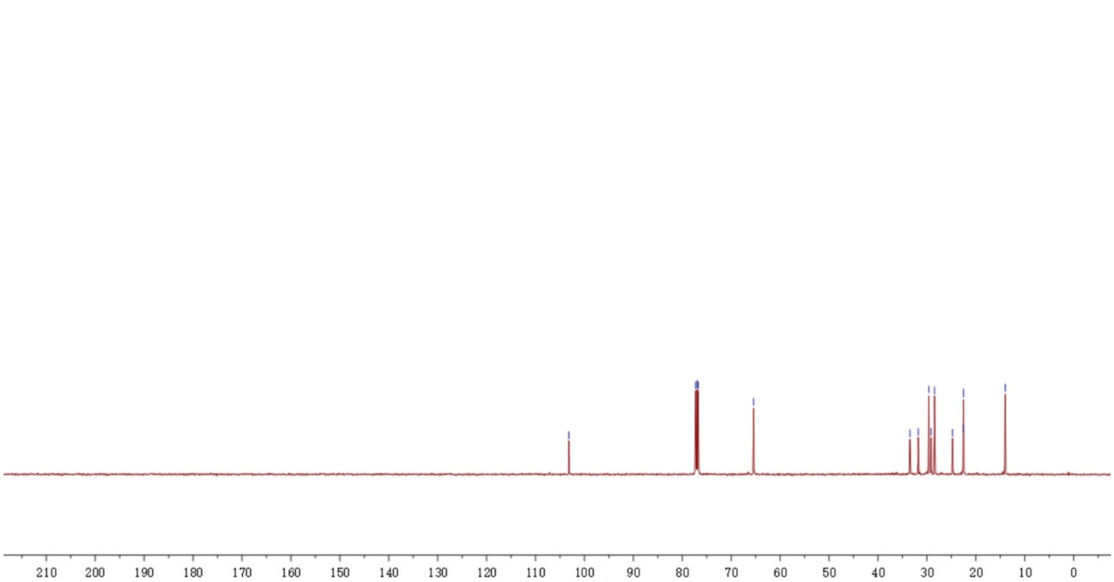
^{1}H NMR





15a

^{13}C NMR



10. GC data for Table 1

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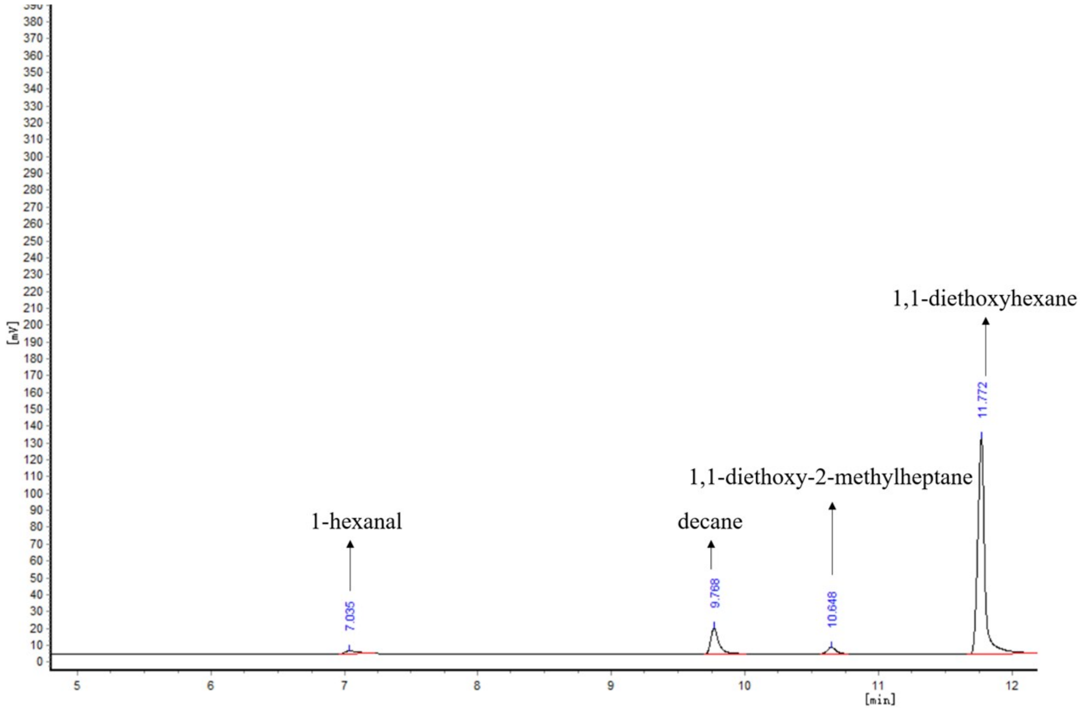

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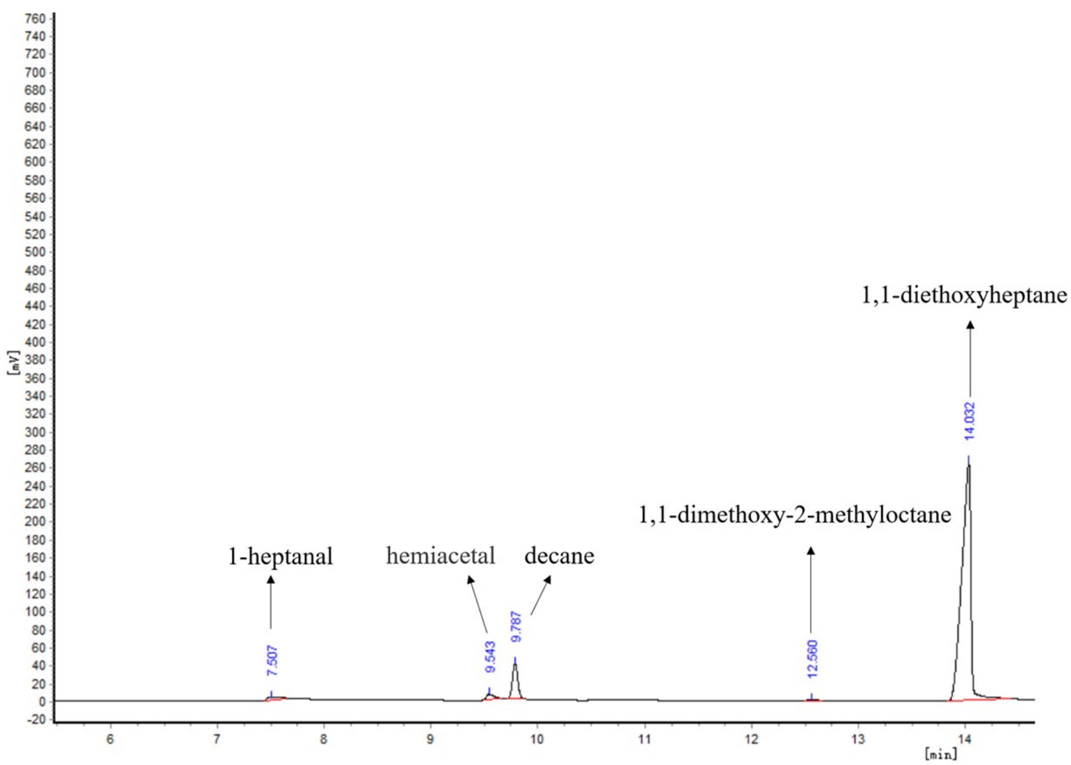

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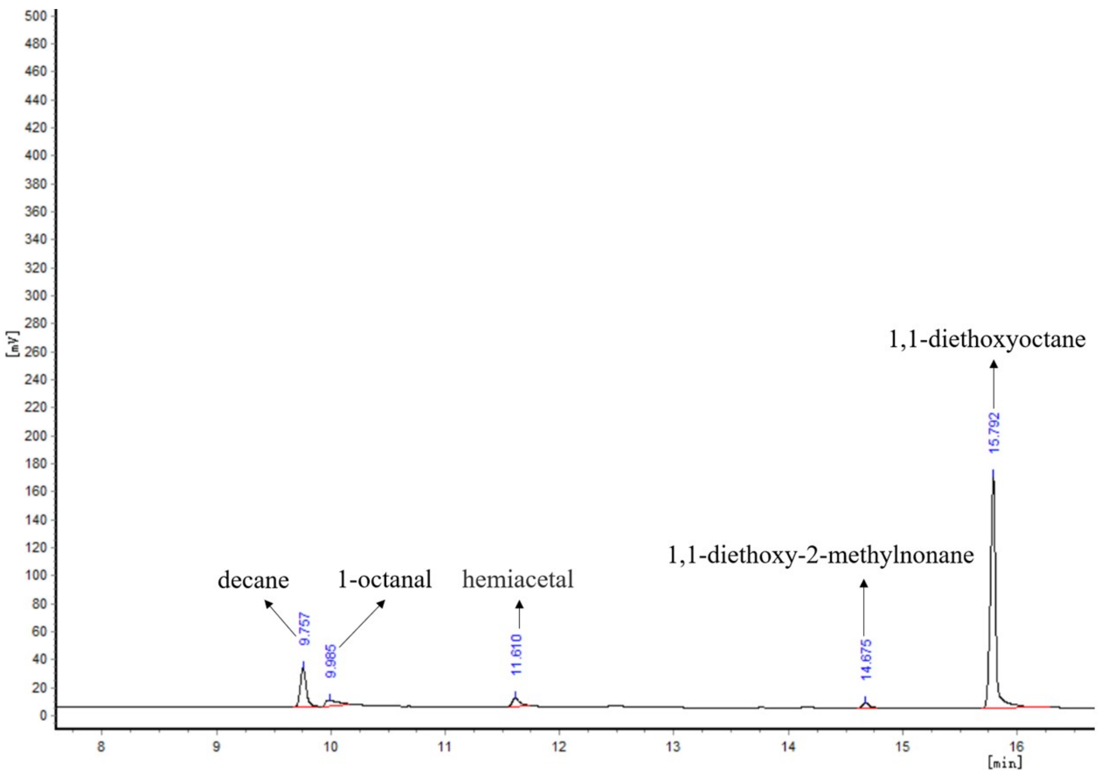

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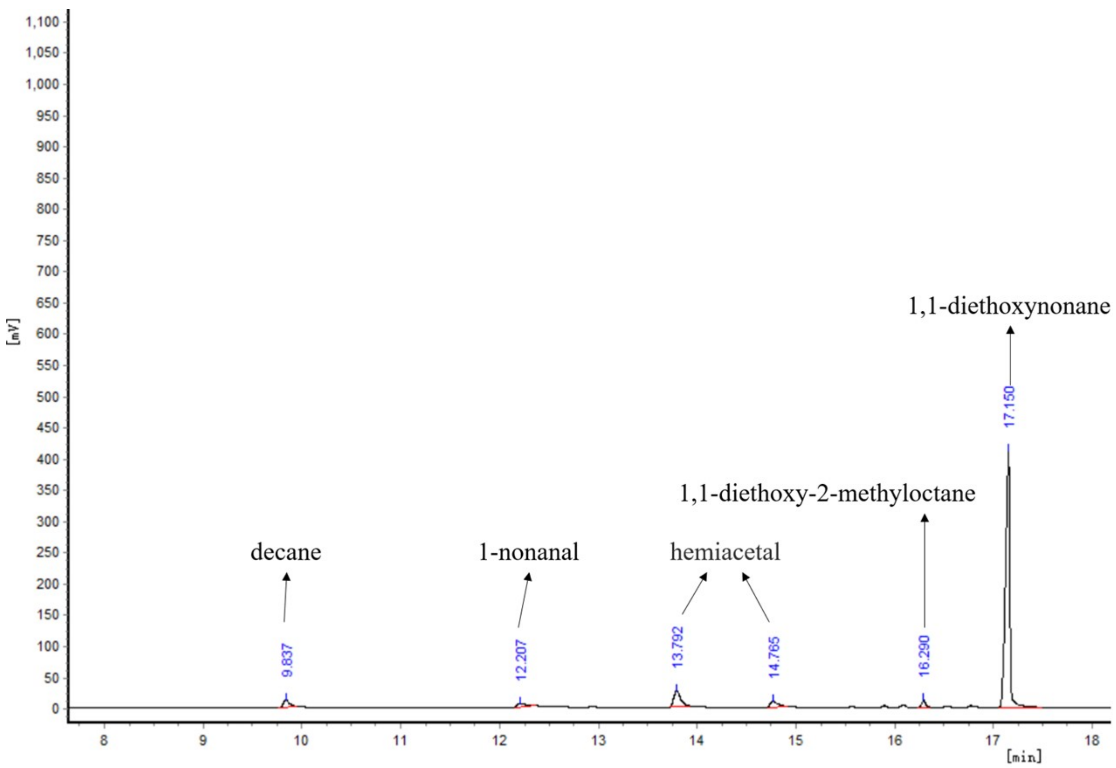

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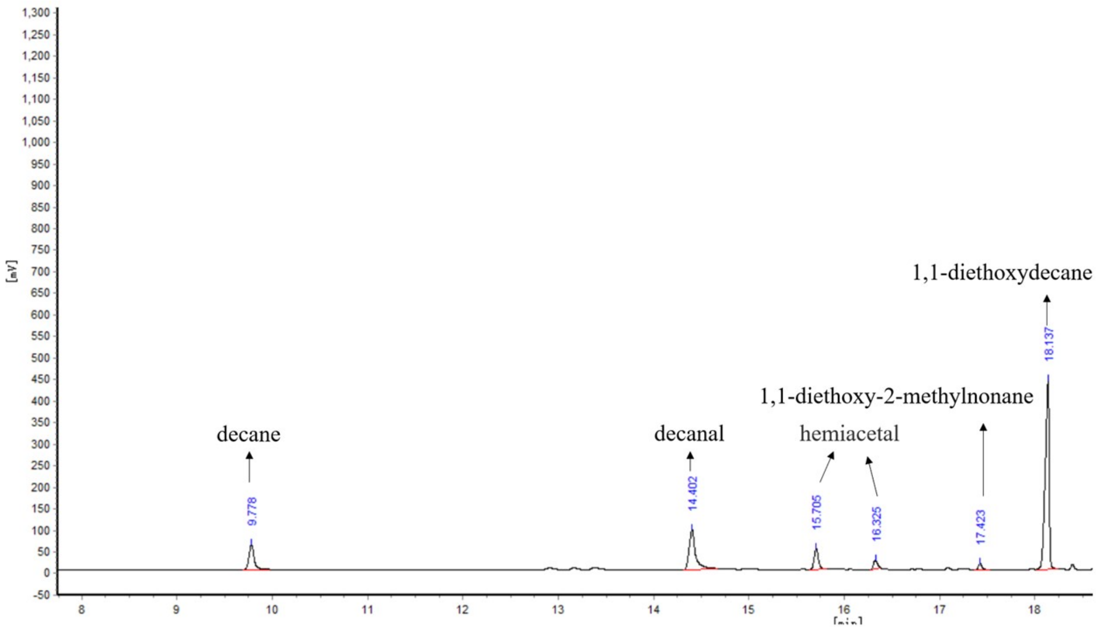

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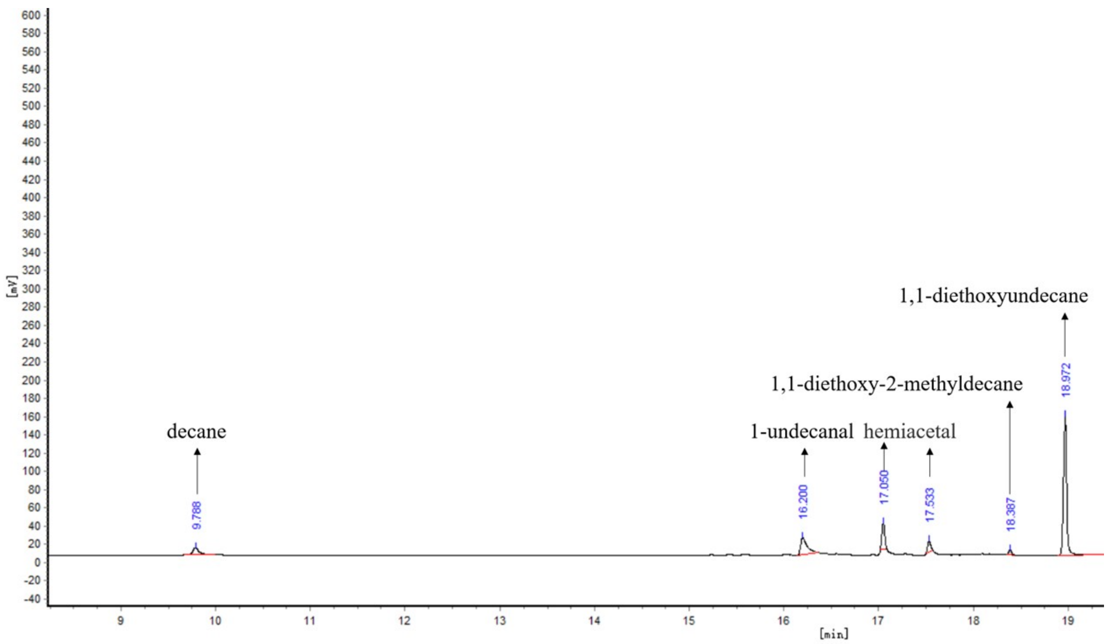

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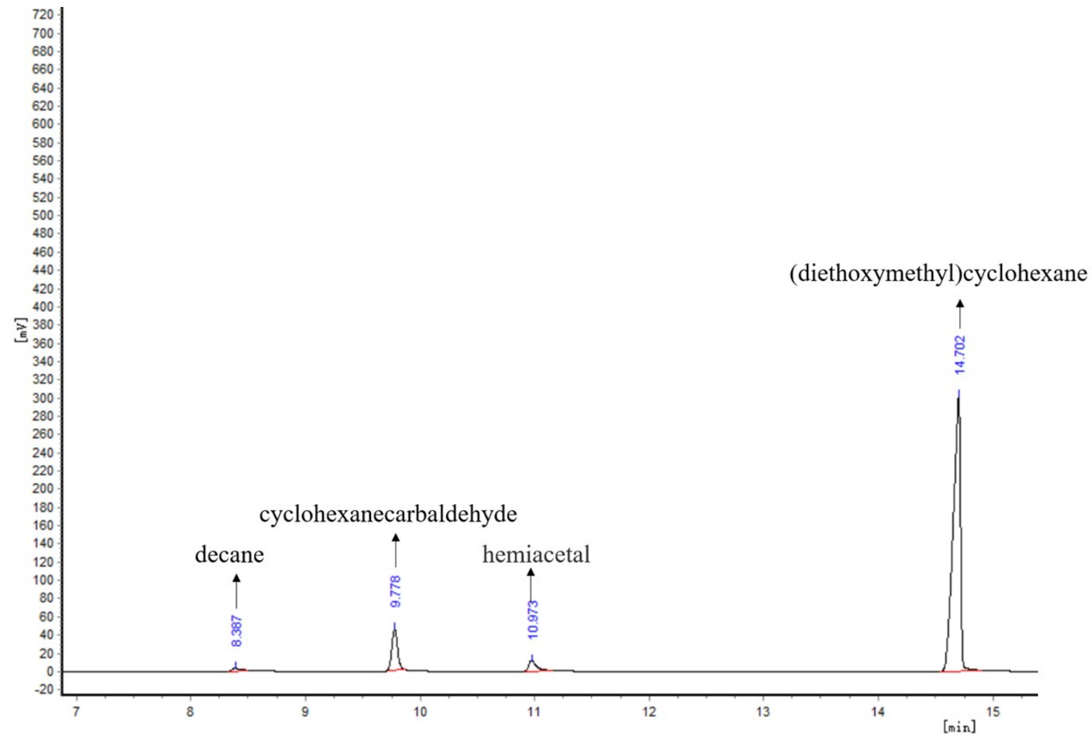

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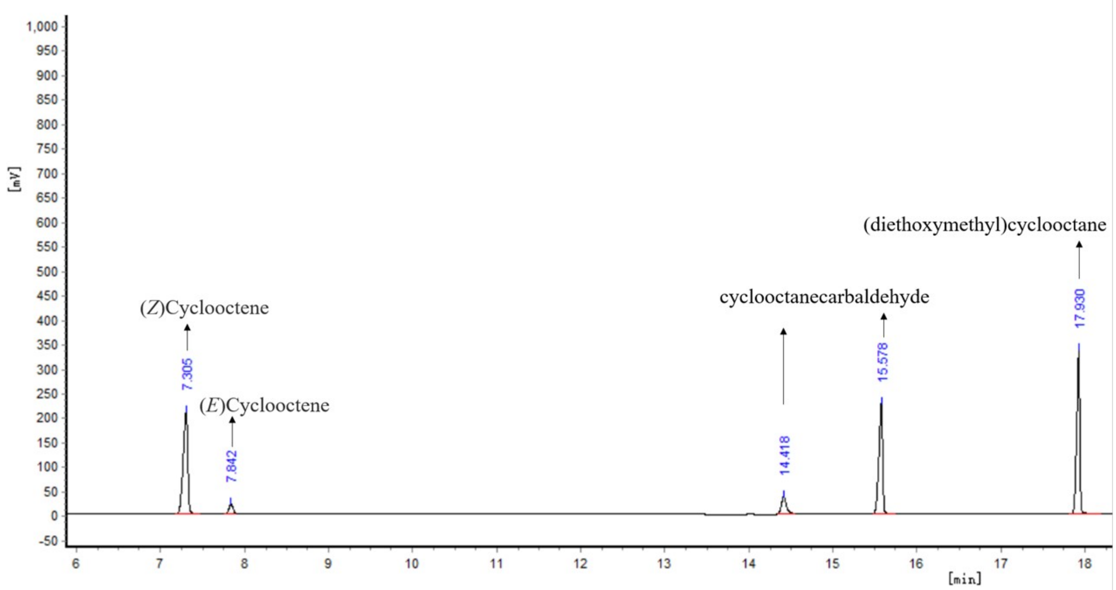

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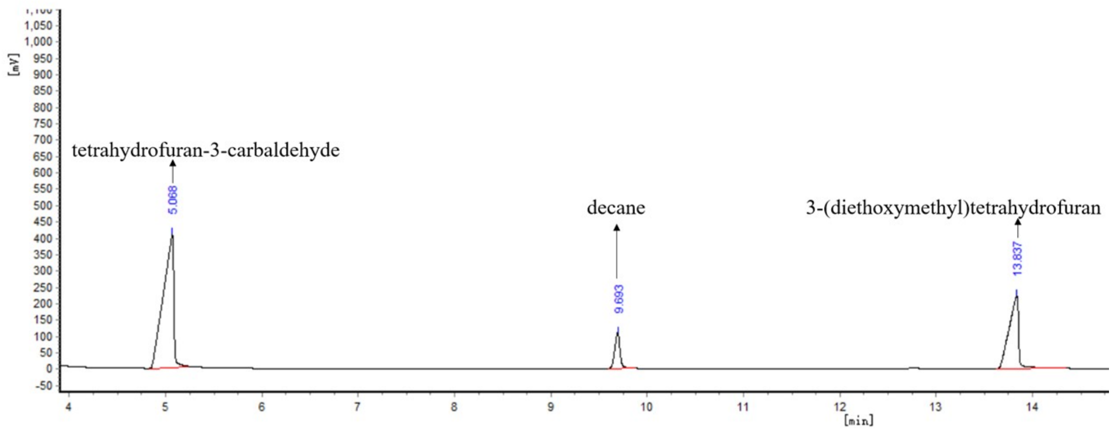

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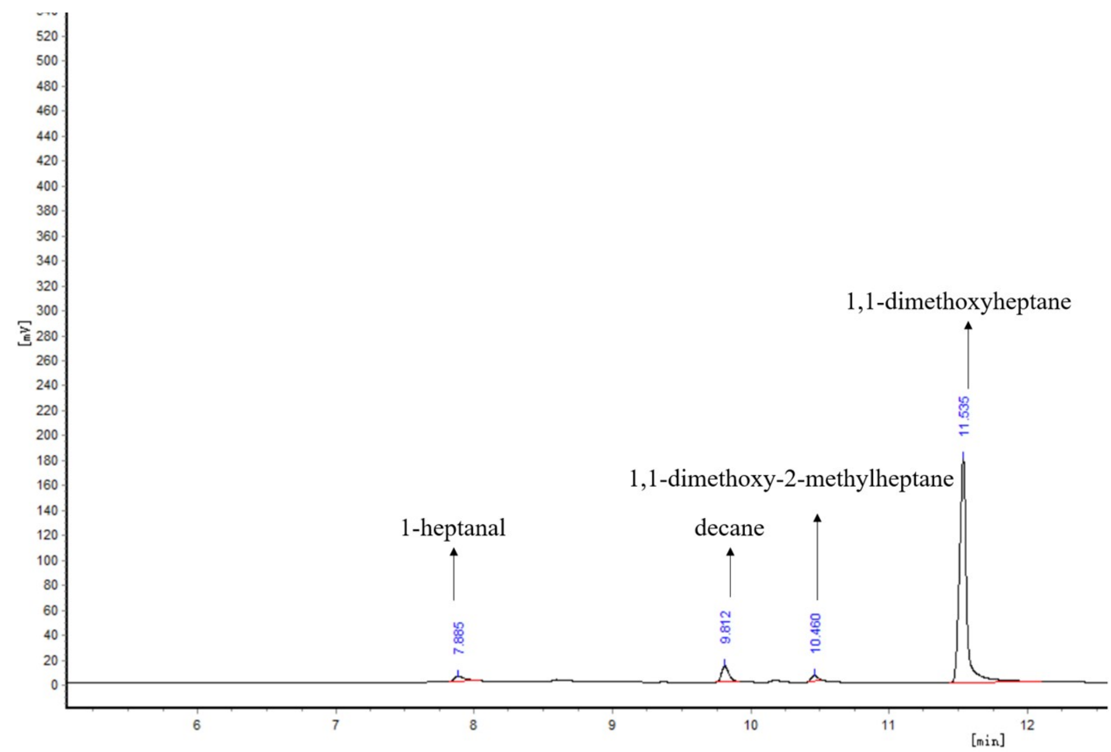

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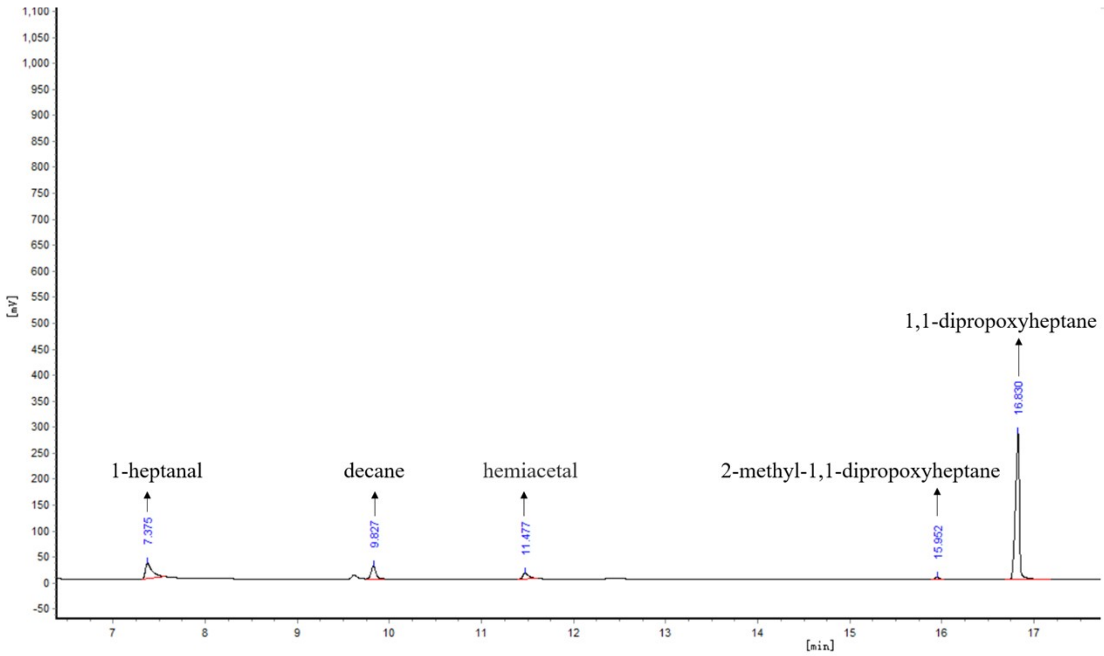

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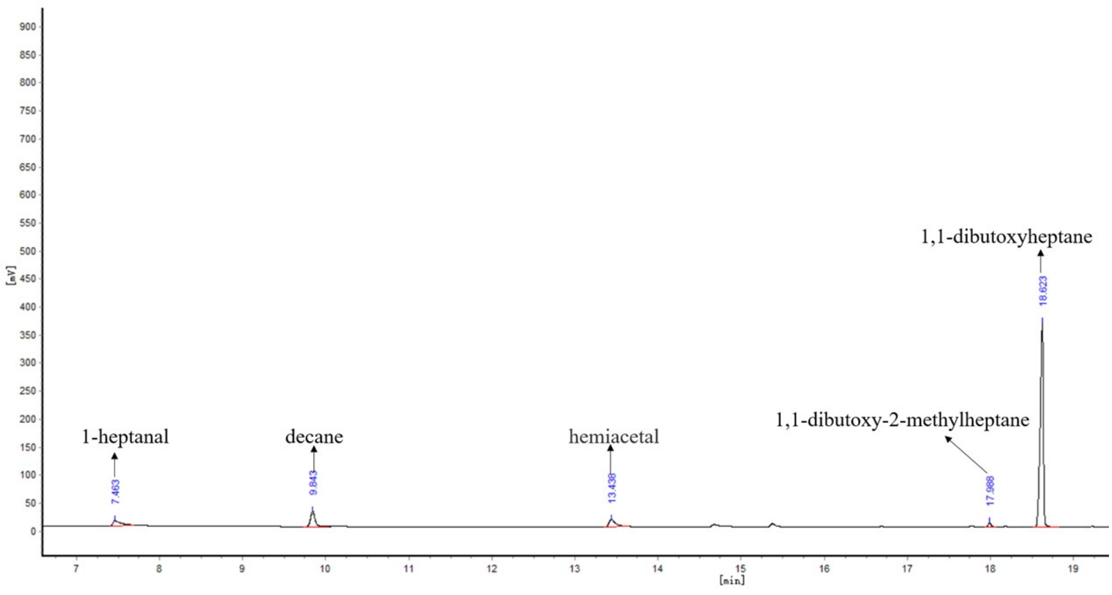

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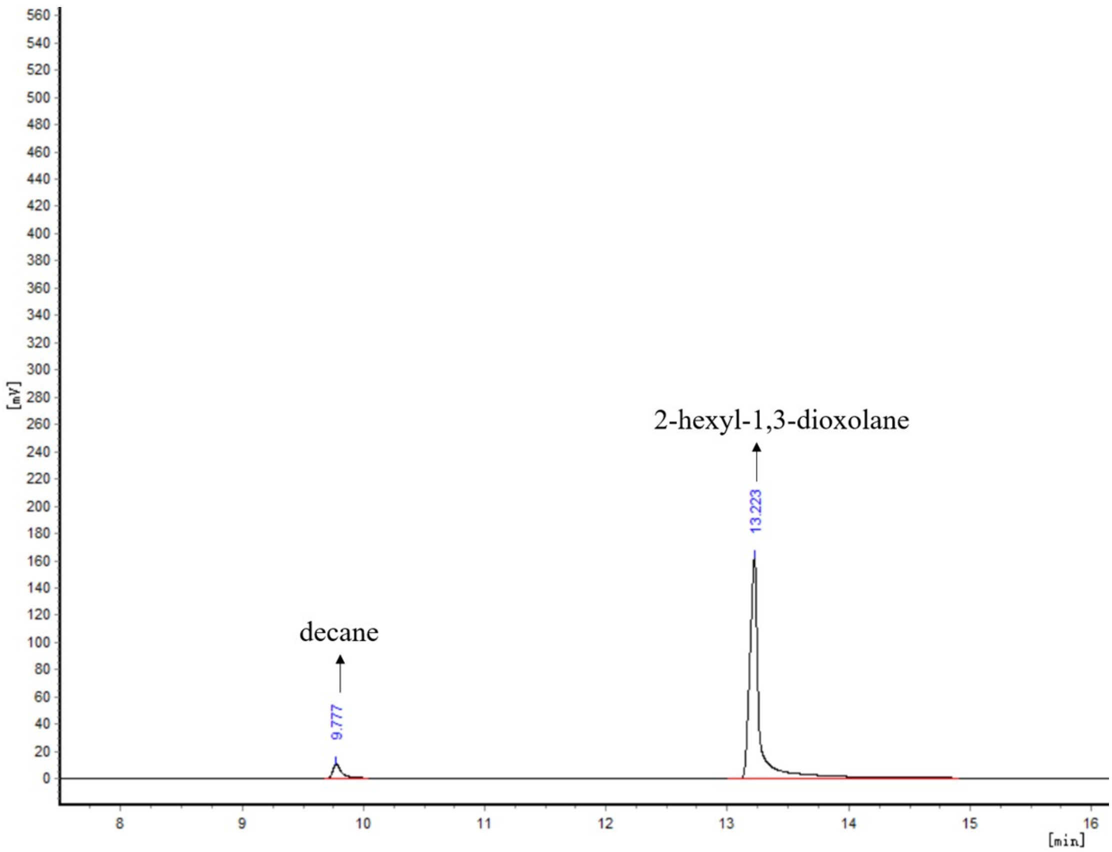

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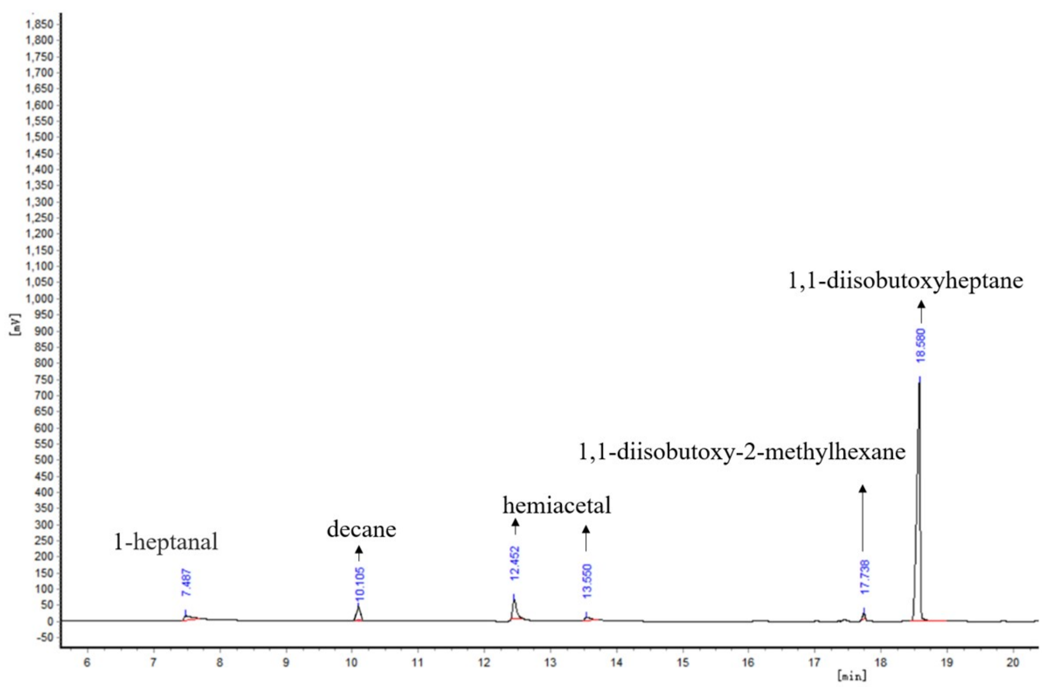

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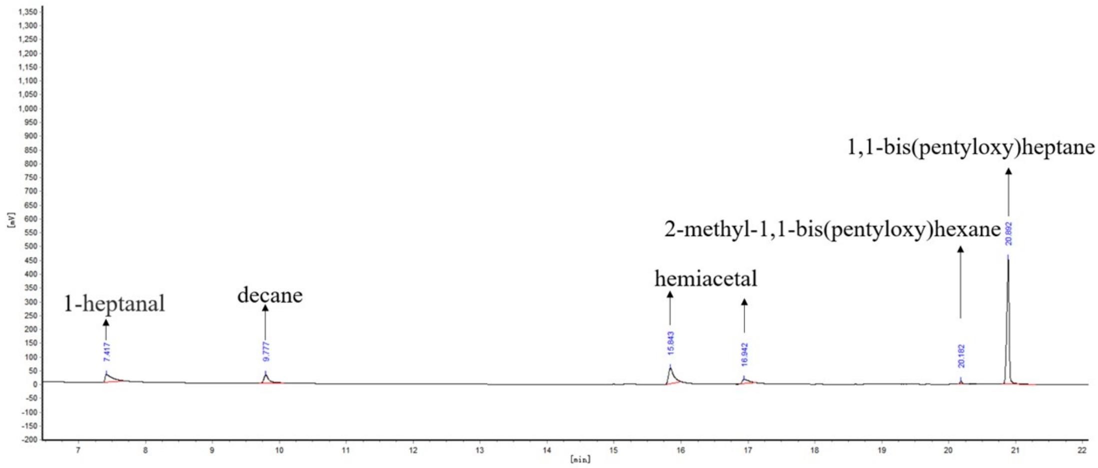

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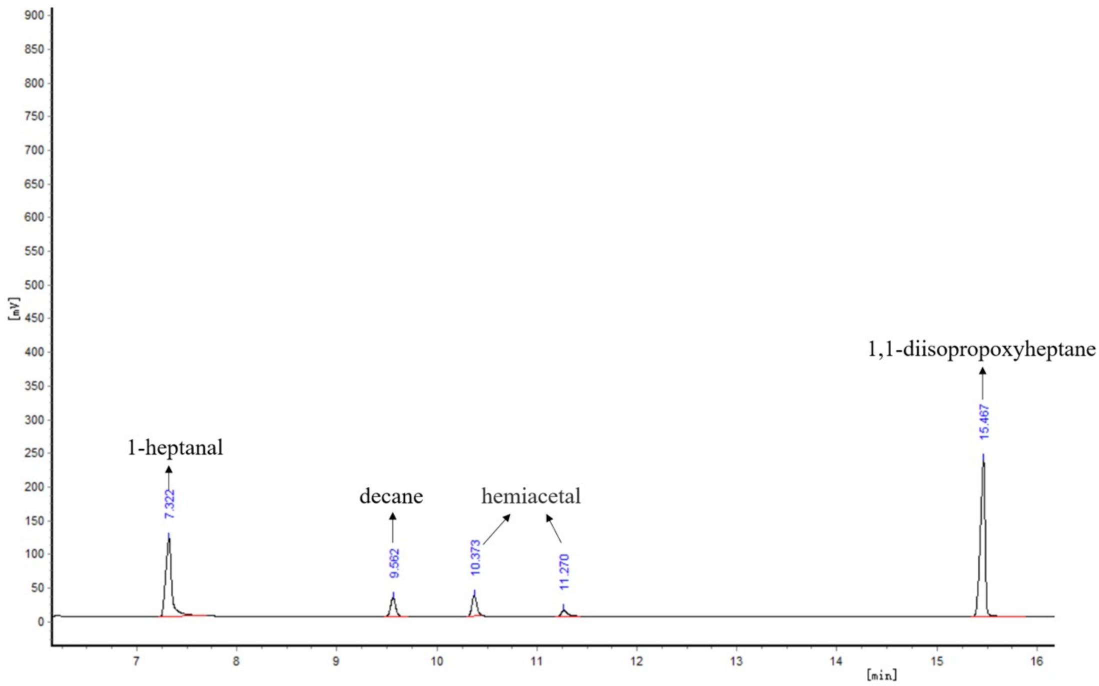

11. Standard orientation, imaginary frequencies of all stationary points

The DFT method with M062X(D3) functional at the basis set level of 6-311G (d, p) were performed using Gaussian 16 package.[5]

Structure 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.267393	0.038352	-0.000638
2	6	0	-2.015912	-0.410318	0.000464
3	1	0	-4.113366	-0.639643	-0.000511
4	1	0	-3.495473	1.100733	-0.001715
5	1	0	-1.849350	-1.486648	0.001486
6	6	0	-0.773702	0.455124	0.000473
7	1	0	-0.790353	1.116769	-0.874410
8	1	0	-0.790046	1.116289	0.875733
9	6	0	0.532499	-0.348320	0.000047
10	1	0	0.550532	-1.008056	0.877004
11	1	0	0.550249	-1.007603	-0.877256
12	6	0	1.788759	0.528265	0.000074
13	1	0	1.768013	1.187485	0.876457
14	1	0	1.767742	1.187931	-0.875966
15	6	0	3.089854	-0.279231	-0.000336
16	1	0	3.155561	-0.922431	-0.883436
17	1	0	3.966023	0.374821	-0.000309
18	1	0	3.155841	-0.922880	0.882415

0 imaginary frequencies

Structure 1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.038360	0.509055	0.000043
2	1	0	-3.028164	1.168659	-0.876121
3	1	0	-3.028249	1.168415	0.876392
4	6	0	-1.767365	-0.348015	-0.000015
5	1	0	-1.777398	-1.008398	0.876835
6	1	0	-1.777317	-1.008160	-0.877047

7	6	0	-4.325995	-0.319617	-0.000136
8	1	0	-4.381534	-0.964165	0.882708
9	1	0	-5.212613	0.320137	-0.000083
10	1	0	-4.381453	-0.963909	-0.883172
11	6	0	-0.473861	0.473900	0.000155
12	1	0	-0.463404	1.134039	0.876883
13	1	0	-0.463325	1.134273	-0.876396
14	6	0	0.795381	-0.384413	0.000099
15	1	0	0.786347	-1.044308	-0.876546
16	1	0	0.786275	-1.044528	0.876578
17	6	0	2.084202	0.440551	0.000258
18	1	0	2.130692	1.101986	0.874046
19	1	0	2.130856	1.102242	-0.873311
20	6	0	3.352640	-0.393625	0.000319
21	8	0	4.465014	0.066887	-0.000809
22	1	0	3.199335	-1.498399	0.001363

0 imaginary frequencies

Structure 1a

Center	Atomic	Atomic	Coordinates (Angstroms)		
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3	1	0	4.933309	-0.719760	-1.370282
4	6	0	6.190716	0.188948	0.132787
5	1	0	7.111696	-0.284513	-0.218368
6	1	0	6.159130	1.201594	-0.281517
7	1	0	6.258736	0.280287	1.221451
8	6	0	3.637864	0.012157	0.192539
9	1	0	3.560615	1.031475	-0.207852
10	1	0	3.659660	0.116921	1.285295
11	6	0	2.394531	-0.785731	-0.215070
12	1	0	2.468596	-1.803293	0.189867
13	1	0	2.375758	-0.894384	-1.306922
14	6	0	1.079743	-0.148355	0.248293

15	1	0	1.001093	0.863019	-0.164402
16	1	0	1.099112	-0.039951	1.340988
17	6	0	-0.154449	-0.951516	-0.167589
18	1	0	-0.115479	-1.961535	0.252624
19	1	0	-0.190935	-1.056841	-1.256611
20	6	0	-1.471420	-0.319423	0.261688
21	1	0	-1.503849	-0.168514	1.355032
22	8	0	-2.488837	-1.207961	-0.120890
23	8	0	-1.631516	0.941296	-0.375376
24	6	0	-3.806202	-0.830522	0.266954
25	1	0	-4.084283	0.109226	-0.223791
26	1	0	-3.840198	-0.668366	1.355705
27	6	0	-4.753902	-1.944981	-0.138072
28	1	0	-5.781865	-1.692175	0.135601
29	1	0	-4.711589	-2.104231	-1.217772
30	1	0	-4.481789	-2.880263	0.356316
31	6	0	-1.882384	2.059023	0.474952
32	1	0	-2.754130	1.865506	1.115084
33	1	0	-1.020929	2.235319	1.133812
34	6	0	-2.128962	3.271044	-0.404869
35	1	0	-2.993968	3.106050	-1.051202
36	1	0	-2.315754	4.156843	0.208336
37	1	0	-1.261788	3.464931	-1.039988

0 imaginary frequencies

Structure L11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.916216	0.390678	-2.800630
2	6	0	-0.473999	1.467756	-3.522681
3	6	0	0.098308	2.592562	-2.880880
4	6	0	0.209100	2.590434	-1.453652
5	6	0	-0.270547	1.468598	-0.707950
6	6	0	-0.814208	0.397499	-1.390721
7	1	0	0.480244	3.697995	-4.696039
8	1	0	-1.331192	-0.472080	-3.306424
9	1	0	-0.552536	1.461192	-4.604393
10	6	0	0.571885	3.710512	-3.614874

11	6	0	0.804337	3.718851	-0.826638
12	6	0	1.255371	4.784487	-1.568008
13	6	0	1.138110	4.785661	-2.976371
14	1	0	0.900207	3.730978	0.251669
15	1	0	1.706381	5.634287	-1.067838
16	1	0	1.497974	5.634064	-3.547091
17	6	0	0.886099	0.778844	1.386861
18	6	0	-0.166703	1.439309	0.782034
19	6	0	-1.130907	2.097471	1.608183
20	6	0	-0.985476	2.063676	3.033127
21	6	0	0.123794	1.383394	3.593050
22	6	0	1.045167	0.760447	2.792005
23	1	0	-2.377938	2.813674	-0.010027
24	6	0	-2.250045	2.785722	1.064499
25	6	0	-1.948060	2.716021	3.846561
26	1	0	0.245716	1.370597	4.670708
27	1	0	1.905289	0.264015	3.225075
28	6	0	-3.014790	3.374358	3.287183
29	6	0	-3.164436	3.405361	1.881961
30	1	0	-1.824025	2.684215	4.924039
31	1	0	-3.743982	3.869514	3.918166
32	1	0	-4.011171	3.922472	1.444861
33	8	0	-1.224135	-0.680730	-0.626332
34	8	0	1.819699	0.180827	0.563000
35	15	0	-2.147382	-1.956655	-1.181415
36	15	0	2.577497	-1.264577	0.943828
37	6	0	-4.153082	-0.540686	0.264573
38	6	0	-5.503873	-0.358613	0.143633
39	6	0	-5.934874	-1.051745	-1.029622
40	6	0	-4.830754	-1.631268	-1.589690

41	7	0	-3.721737	-1.324192	-0.800414
42	1	0	-3.455737	-0.166939	0.993967
43	1	0	-6.120714	0.217012	0.816740
44	1	0	-6.940670	-1.106780	-1.416356
45	1	0	-4.720557	-2.234652	-2.476336
46	6	0	-1.692207	-4.360063	0.022804
47	6	0	-1.394604	-4.906537	1.241504
48	6	0	-1.271123	-3.829695	2.172389
49	6	0	-1.501272	-2.662354	1.494566
50	7	0	-1.760400	-2.975966	0.165249
51	1	0	-1.860227	-4.821481	-0.936925
52	1	0	-1.274093	-5.958636	1.448096
53	1	0	-1.033077	-3.907683	3.222193
54	1	0	-1.475428	-1.637948	1.822317
55	6	0	3.183608	-1.574126	-1.814675
56	6	0	2.809424	-2.439523	-2.804798
57	6	0	1.940571	-3.417117	-2.225347
58	6	0	1.814013	-3.118502	-0.897303
59	7	0	2.580500	-1.982397	-0.628663
60	1	0	3.832963	-0.715733	-1.834808
61	1	0	3.129656	-2.389803	-3.834376
62	1	0	1.478036	-4.251754	-2.729120
63	1	0	1.254501	-3.603409	-0.112839
64	6	0	6.033675	0.626928	0.764417
65	6	0	6.383590	-0.561197	1.474039
66	6	0	5.241468	-1.301604	1.620128
67	1	0	6.694700	1.436439	0.494767
68	1	0	7.360689	-0.831037	1.843749
69	1	0	5.075421	-2.256158	2.093680
70	7	0	4.191689	-0.615130	1.019011

71	6	0	4.691668	0.572591	0.494153
72	1	0	4.034884	1.270370	0.003753

0 imaginary frequencies

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