

Supporting Information

Selective Cleavage of Inert Aryl C-O Bonds to Arenes

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11. References

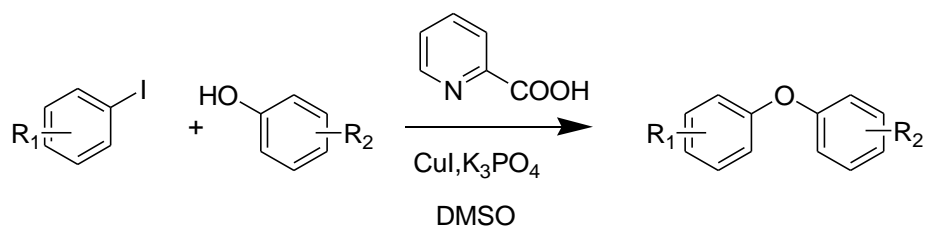
1. General experimental details

1.1 Materials

Toluene (A.R. grade) was purchased from Xilong Chemical CO., LTD, and used as received. LiAlH_4 (>98%, gray powder) was purchased from TCI, and KOtBu (99%) from Across. Phenol, anisole, dodecane, tetradecane were from Across. Diphenyl ether, 4-ethylanisole, 4-tert-butylanisole, 2-naphthol, 1,2,3,4-tetrahydronaphthalene, biphenyl, 4-hydroxydiphenyl 1,4-diphenoxybenzene were purchased from Alfa Aesar. 4-Ethylphenol, 2-ethylanisole, tert-butylbenzene was purchased from TCI. Benzene, dibenzofuran, benzofuran, 2-methoxynaphthalene, 2-ethylphenol, 4-ethylguaiacol, 2-hydroxydiphenyl, 2-methoxybiphenyl, 4-methoxybiphenyl, 1,2-dimethoxybenzene, 1,3-dimethoxybenzene, pyrocatechol, 1,2,3,4-tetrahydro-1-naphthol, sodium hydride, sodium ethoxide, sodium tert-butoxide, lithium t-butoxide diisobutyl aluminum hydride (1M solution in toluene), triethylsilane, sodium borohydride, potassium borohydride, potassium hydroxide, 1,8-diazabicyclo[5.4.0]undec-7-ene were purchased from J&K. Anhydrous copper iodide, pyridine-2-carboxylic acid (picolinic acid), anhydrous K_3PO_4 , phenols were also from J&K. Di-2-methoxyphenyl ether, di-4-tert-butylphenyl ether, di-4-ethylphenylether, 2-phenoxy-1-phenethanol, 2-(2-methoxyphenoxy)-1-phenylethanol, and 2-phenoxy-1-phenylpropane-1, 3-diol were synthesized by ourselves as follows.

1) Synthesis of diarylethers

General procedure for the synthesis of diarylethers was based on a reported route (S1).



Typically, a 100 mL round bottom flask was charged with copper (I) iodide (1mmol), picolinic acid (pyridine-2-carboxylic acid, 2 mmol), aryl iodide (10 mmol), phenol (12 mmol), potassium phosphate (20 mmol), DMSO (30ml) and a magnetic stir bar. The reaction flask was sealed with a septum in an argon atmosphere and the reaction mixture was stirred at 100 °C until complete reaction. The reaction mixture was cooled and diluted with a saturated aqueous solution of ammonium chloride (100 ml) and water (100 ml). The crude product was extracted with methylene chloride (2 × 100 ml). The combined organic extracts were successively washed with a 5% aqueous solution of potassium hydroxide (100 ml), brine (100 ml) and dried over anhydrous sodium sulfate.

The crude product was purified by flash column chromatography.

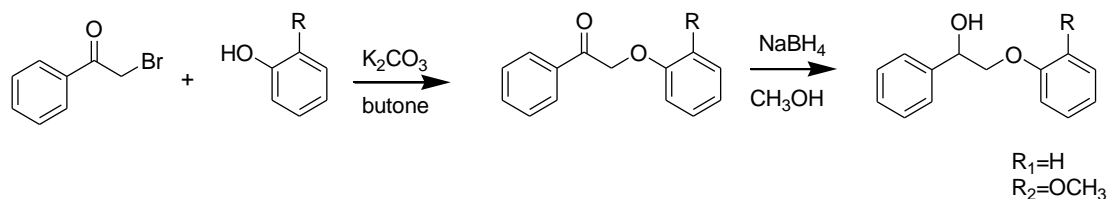
Di-2-methoxyphenyl ether was synthesized according to the general procedure using 2-iodoanisole (2.34 g, 10 mmol), guaiacol (2-methoxyphenol, 1.49 g, 12 mmol), potassium phosphate (4.24 g, 20 mmol), copper (I) iodide (190 mg, 1 mmol), pyridine-2-carboxylic acid (246 mg, 2 mmol) and DMSO (30 ml). The crude product was purified by flash column chromatography (eluent: petro to petro acetate, 10:1) to give di-2-methoxyphenyl ether as a white solid in 65% yield. ^1H NMR (400MHz, CDCl_3): δ 7.03-7.07 (m, 2H), 6.96-6.98 (m, 2H), 6.81-6.87 (m, 4H), 3.85 (s, 6H). ^{13}C { ^1H } NMR (100 MHz, CDCl_3): δ 150.6 (C), 146.1 (C), 123.9 (CH), 120.9 (CH), 118.9 (CH), 112.6 (CH), 56.2 (CH_3).

Di-4-tert-butylphenyl ether was synthesized using the similar procedure as above. ^1H NMR (400 MHz, CDCl_3): δ 7.32 (d, J = 8 Hz, 4H), 6.93 (d, J = 8 Hz, 4H), 1.31 (s, 18H). ^{13}C { ^1H } NMR (100 MHz, CDCl_3): δ 155.6 (C), 146.2 (C), 126.9 (CH), 118.7 (CH), 34.7 (C), 31.9 (CH_3).

Di-4-ethylphenyl ether was synthesized using the similar procedure as above. ^1H NMR (400 MHz, CDCl_3): δ 7.13 (d, J = 8 Hz, 4H), 6.91 (d, J = 8 Hz, 4H), 2.61(q, J=8 Hz, 2H), 1.22 (t, J=8 Hz, 3H). ^{13}C { ^1H } NMR (100 MHz, CDCl_3): δ 155.6 (C), 138.9 (C), 129.1 (CH), 118.7 (CH), 28.3 (CH_2), 15.8(CH_3).

2) Synthesis of β -O-4 lignin-type dimers

General procedure for the synthesis of β -O-4 lignin-type dimers was similar to a reported procedure (S2).



Typically, bromoacetophenone (5 mmol) and phenols (6 mmol) were dissolved in 50 ml butone, mixed with K_2CO_3 (7.5 mmol) and stirred overnight with a reflux condenser. The reaction mixture was cooled and diluted with water (100 ml). The crude product was extracted with methylene chloride (2 \times 100 ml). The combined organic extracts were washed with brine (100 ml) and dried over anhydrous sodium sulfate. The crude product was resolved in methanol, and treated with small portions of sodium borohydride (5.5 mmol) and stirred for 2 h. A saturated solution of ammonium sulfate (100 ml) followed by methylene chloride (2 \times 100 ml) was added to the reaction mixture. The organic layer was separated, washed with water (2 \times 100 ml) and dried over anhydrous sodium sulfate. The crude product was purified by flash column chromatography.

2-phenoxy-1-phenylethanol was synthesized using the similar procedure as above. ^1H NMR (400 MHz, CDCl_3) δ 7.46-6.97(m, 7H), 6.95-6.80 (m, 3H), 5.10 (dd, J = 12, 4 Hz, 1H), 4.10 (dd, J = 12, 4 Hz, 1 H), 4.00 (t, J=12 Hz, 1H), 2.85(br.s, 1H). ^{13}C { ^1H } NMR (100 MHz, CDCl_3) δ 159.1 (C), 140.4 (C), 130.2 (CH), 129.2 (CH),

128.8(CH), 126.9(CH), 122.0(CH), 121.2(CH), 116.0(C), 115.3(CH), 74.9 (CH), 73.3(CH).

2-(2-methoxyphenoxy)-1- phenylethanol was synthesized using the similar procedure as above. ^1H NMR (400 MHz, CDCl_3) δ 7.43-7.28(m, 5H), 6.96-6.87(m, 3H), 5.09 (dd, $J = 12, 4$ Hz, 1H), 4.15 (dd, $J = 12, 4$ Hz, 1 H), 3.98 (t, $J=12$ Hz, 1H), 2.0(br.s, 1H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 159.1 (C), 140.4 (C), 130.2(CH), 129.2 (CH), 128.8(CH), 126.9(CH), 122.0(CH), 121.2 (CH), 116.0(C), 115.3(CH), 74.9 (CH), 73.3(CH).

3) Synthesis of 2-phenoxy-1-phenylpropane-1, 3-diol

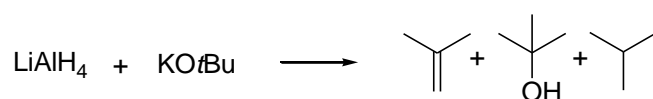
2-Phenoxy-1-phenylpropane-1, 3-diol was synthesized based on a reported procedure (S3). ^1H NMR and ^{13}C NMR spectra are as follows. ^1H NMR (400 MHz, CDCl_3): δ 7.41-7.20(m, 7H), 6.98-6.86(m, 3H), 5.02 (dd, $J = 12, 4$ Hz, 1H), 4.39(m, 1 H), 3.91 (m, 1H), 3.52(dd, $J=12,4$ Hz, 1H). ^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) major diastereomer: δ 158.5(C), 140.2(C), 130.1(CH), 129.0(CH), 128.6(CH), 127.3(CH), 122.4(CH), 116.9(CH), 83.3(CH), 74.2(CHOH), 61.5(CH_2OH); minor diastereomer: 158.0(C), 140.8(C), 130.0(CH), 128.9(CH), 128.3(CH), 126.7(CH), 122.3(CH), 117.1(CH), 82.3(CH), 74.4(CHOH), 61.6(CH_2OH).

1.2 General procedures for deoxygenation of aryl C-O containing compounds

The water- and O_2 -sensitive manipulations were conducted under an argon atmosphere in a glovebox. The deoxygenation reactions were conducted in a 35 mL vial with Teflon-lined screw cap (supplied by Synthware Company) and Teflon-coated magnetic stir bar. In a glovebox, a 35 mL screw cap vial was loaded with the corresponding substrate (1 mmol, 1 equiv.), base (2.5-5 equiv.) and a magnetic stirring bar, followed by syringe addition of 5 mL (or 8 mL) of toluene and hydride source (2.5-5 equiv.). The reaction vial was sealed with the Teflon-lined screw cap and heated at a desired temperature and time. After cooling to room temperature, n-dodecane or n-tetradecane (internal standard for GC) was added to the reaction solution, and the liquid was separated. Toluene (3×2.5 mL) was used to clean the tube. The combined substrate was centrifuged and then subjected to GC/FID, GC/MS for qualitative and quantitative identification.

In order to isolate the products, ethyl acetate (3×2.5 mL) was used to clean the tube. The combined mixture were centrifuged and then the solvent was removed under vacuum. The crude product was purified by flash column chromatography (the eluent was petro).

1.3 Reaction of KO^tBu and LiAlH_4 in toluene



In a glovebox, KO^tBu (2.5 mmol), LiAlH_4 (5 mmol.) and toluene (5 mL) were loaded in a 35 mL vial with a

magnetic stirring bar. Then the vial was sealed with a Teflon-lined screw cap and heated at 180 °C for 24h. After cooling to room temperature, n-dodecane (internal standard for GC analysis) was added to the reaction solution, and the liquid solution was separated via centrifugation for GC/FID and GC/MS identification. It was demonstrated that 2-methylpropane, 2-methylprop-1-ene and 2-butanol were detected in the liquid solution, indicating that 2-methylpropane, 2-methylprop-1-ene and 2-butanol in the following reaction solutions were from the reaction of KO^tBu and LiAlH₄.

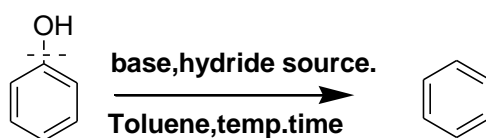
1.4 Characterization

The liquid products were analyzed by GC on an Agilent 6890/7890B gas chromatography equipped with an HP-5 25 m x 0.20 mm ID x 0.33 μm capillary column (Agilent) or an HP-INNOWAX 19091N-133 (30 m x 0.25 mm ID x 0.25 μm) capillary column (Agilent) and an FID detector. The following GC temperature program was used: 50 °C hold for 2 min, ramp 20 °C/min to a final temperature of 260 °C, and hold for 8 min. Nitrogen was used as a carrier gas. The injector temperature was held at 250 °C.

The gas products were analyzed by GC on an Agilent 4890D Gas Chromatography equipped with a carbon sieves packing column and TCD detector for CO, O₂, H₂ and hydrocarbons. Argon was used as the carrier gas. The following GC temperature program was used: 80 °C hold for 4 min, ramp 20 °C/min to a final temperature of 180 °C, and hold for 3 min. The injector temperature was held at 250 °C.

GC-MS analyses were performed on a Shimadzu QP-2010 gas chromatography equipped with a DB-5 30 m × 0.25 mm × 0.25 μm capillary column (Agilent). The GC was directly interfaced to an Agilent 5973 mass selective detector (EI, 70 eV). The following GC temperature program was used: 50 °C hold for 2 min, ramp 20 °C/min to a final temperature of 250 °C, and hold for 20 min. Nitrogen was used as a carrier gas. The injector temperature was held constant at 250 °C.

¹H-NMR spectra were acquired on a 400 MHz Varian Unity instrument. ¹³C-NMR spectra were acquired on a 100 MHz Varian Unity instrument. Chemical shifts were reported in ppm relative to a peak of a residual CHCl₃ (CDCl₃, δ 7.26 ppm for ¹H and 77 ppm for ¹³C).

2. Table S1. Reductive cleavage of C-O bond in phenol under different conditions

Entry	Hydride source(equiv.)	Base(equiv.)	Temp.(°C)	Time(h)	Yield (%)
1	NaBH ₄ (5)	KOtBu (2.5)	180	24	0
2	NaH (5)	KOtBu (2.5)	180	24	<1
3	DIBAL (5)	KOtBu (2.5)	180	24	5
4	Et ₃ SiH (5)	KOtBu (2.5)	180	24	0
5	KBH ₄ (5)	KOtBu (2.5)	180	24	0
6	LiAlH ₄ (5)	DBU (2.5)	180	24	0
7	LiAlH ₄ (5)	KOH (2.5)	180	24	67
8	LiAlH ₄ (5)	NaOEt (2.5)	180	24	51
9	LiAlH ₄ (5)	NaOtBu (2.5)	180	24	56
10	LiAlH ₄ (5)	LiOtBu (2.5)	180	24	4
11	LiAlH ₄ (5)	KOtBu (2.5)	180	24	80
12	LiAlH ₄ (2.5)	KOtBu (2.5)	180	24	65
13	LiAlH ₄ (2.5)	KOtBu (5)	180	24	50
14	LiAlH ₄ (5)	KOtBu (2.5)	140	24	11
15	LiAlH ₄ (5)	KOtBu (2.5)	140	32	14
16	LiAlH ₄ (5)	KOtBu (2.5)	160	24	25
17	LiAlH ₄ (5)	KOtBu (2.5)	180	32	82

3. Dependence of the unreacted phenol amount and benzene yield on reaction time

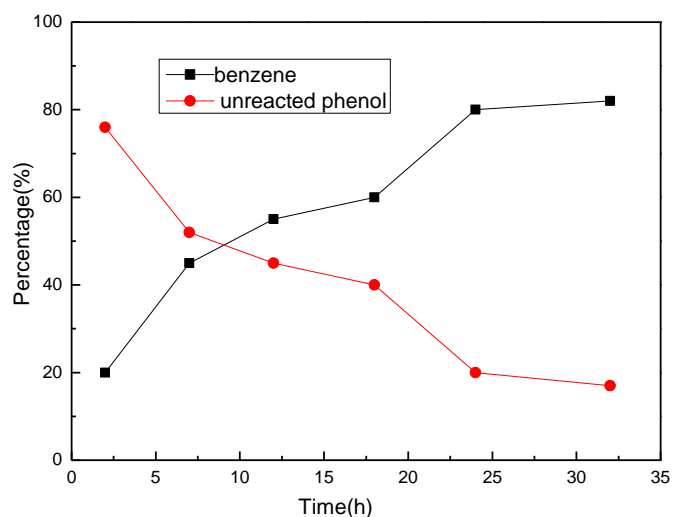


Figure S1 Dependence of the unreacted phenol amount and benzene yield on reaction time.

4. GC spectra of CH₄+H₂ mixture and the gas phase of the anisole reduction.

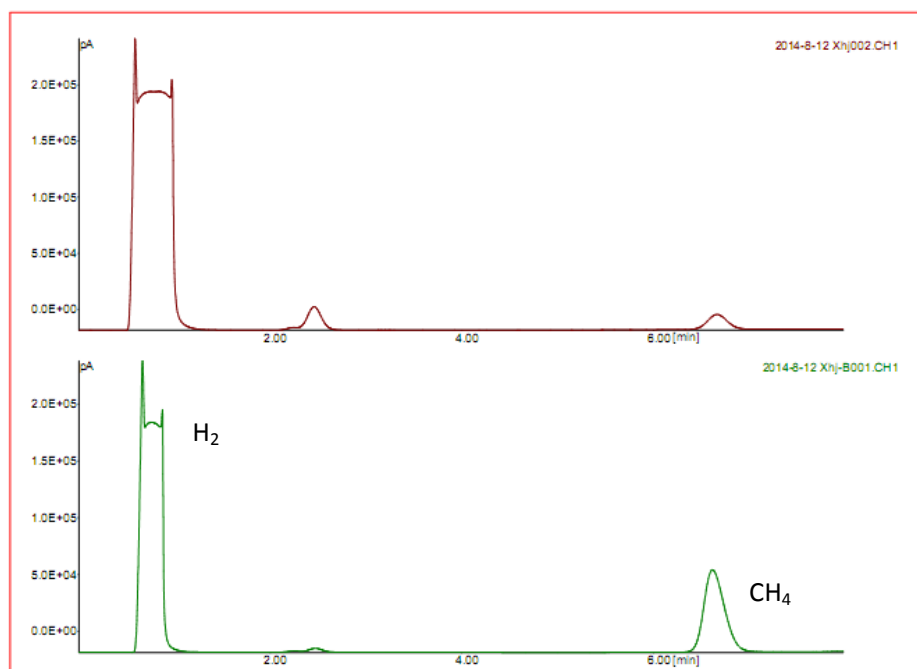


Figure S2 GC spectra of CH₄+H₂ mixture (bottom) and the gas phase of the anisole reduction (top).

5. EPR spectra of the reaction solution

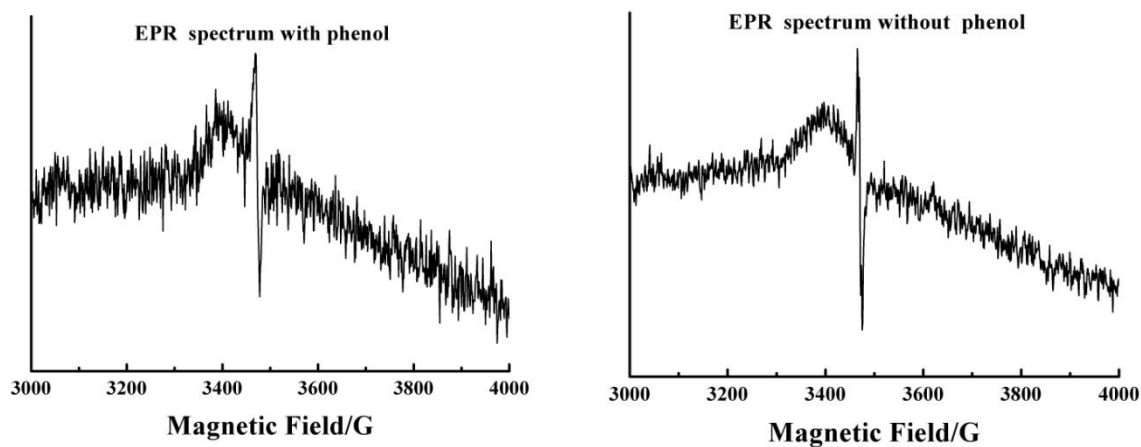
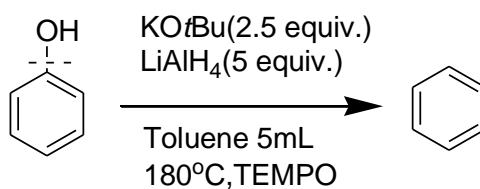


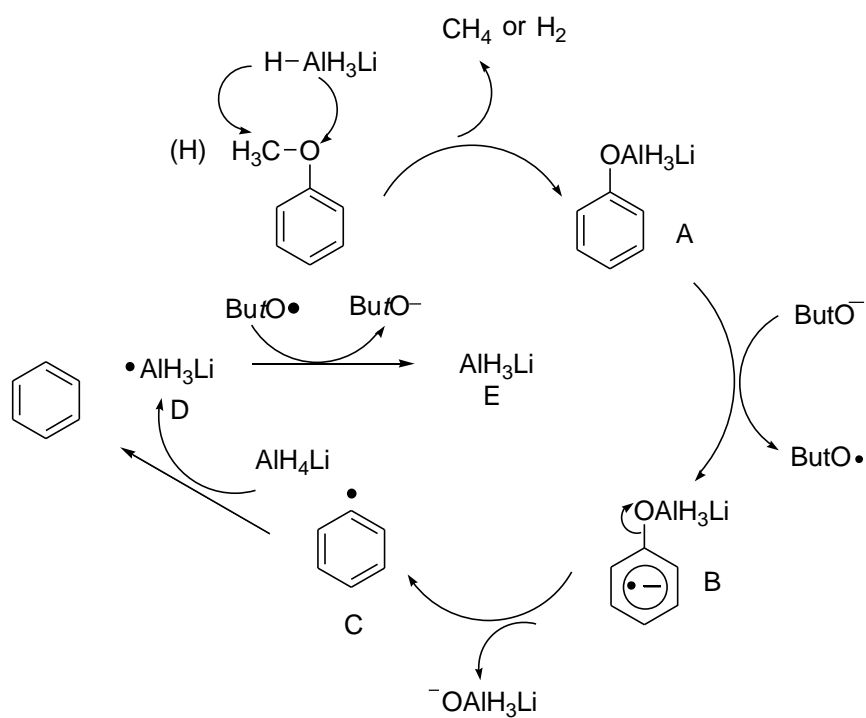
Figure S3. EPR spectra of: (left) reaction solution of phenol reduced by LiAlH_4 in the presence of $\text{KO}t\text{Bu}$ in toluene at 180°C for 4h; (right) reaction solution of $\text{LiAlH}_4/\text{KO}t\text{Bu}$ in toluene at 180°C for 4h.

6. Table S2. Effect of radical scavenger TEMPO on the reduction of phenol.



TEMPO/ equiv.	Benzene yield/%
0	80
1	3.2
2.5	0

7. Scheme S1. Tentative mechanism for the LiAlH_4 and $\text{KO}t\text{Bu}$ -catalyzed deoxygenation



Scheme S1. Tentative mechanism for the LiAlH_4 and $\text{KO}t\text{Bu}$ -reduced deoxygenation of phenols and aryl ethers.

8. NMR spectra of the as-synthesized starting materials in experimental section

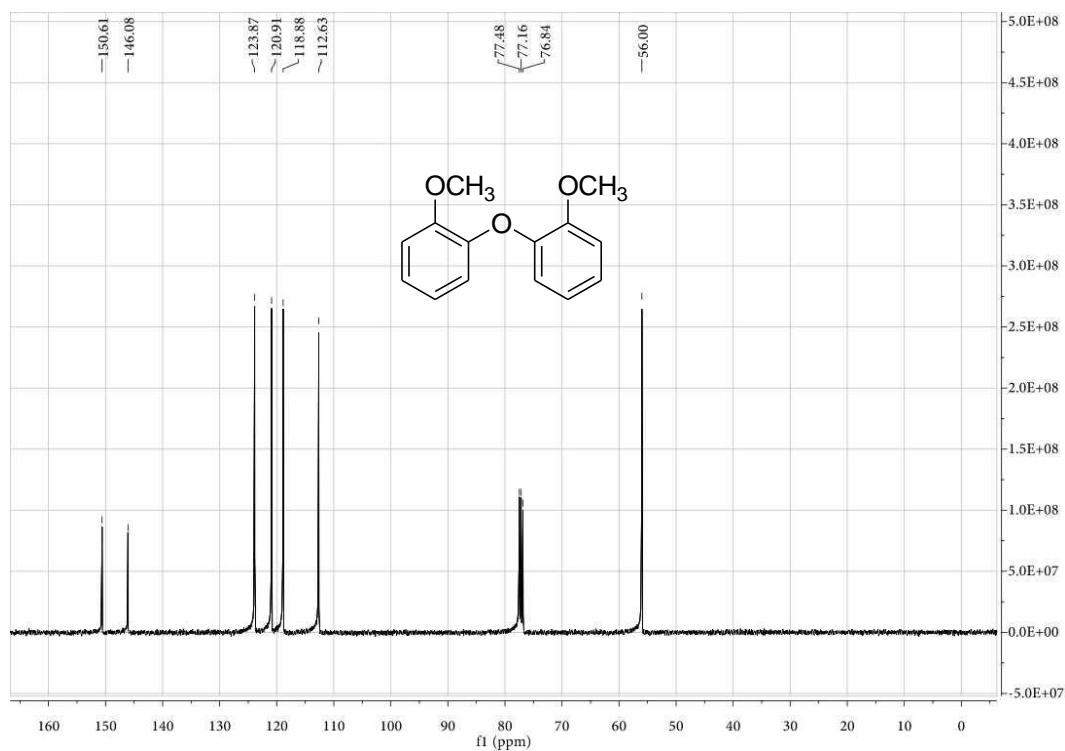
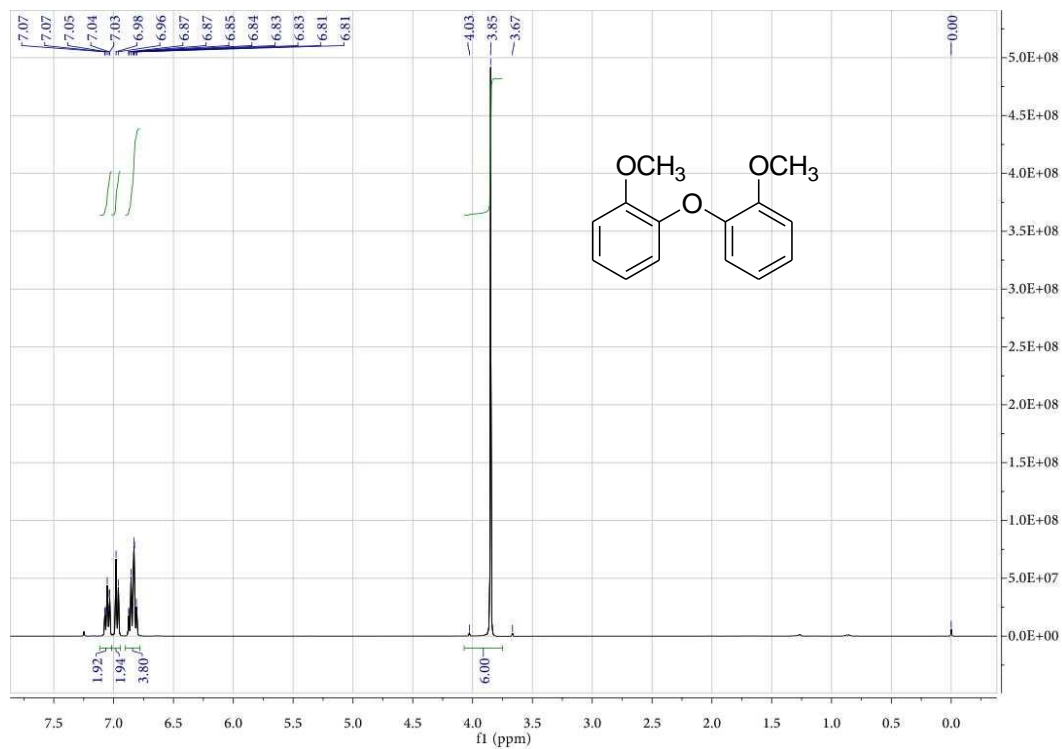


Figure S4. ¹H (top) and ¹³C (bottom) NMR spectra of di-2-methoxyphenyl ether.

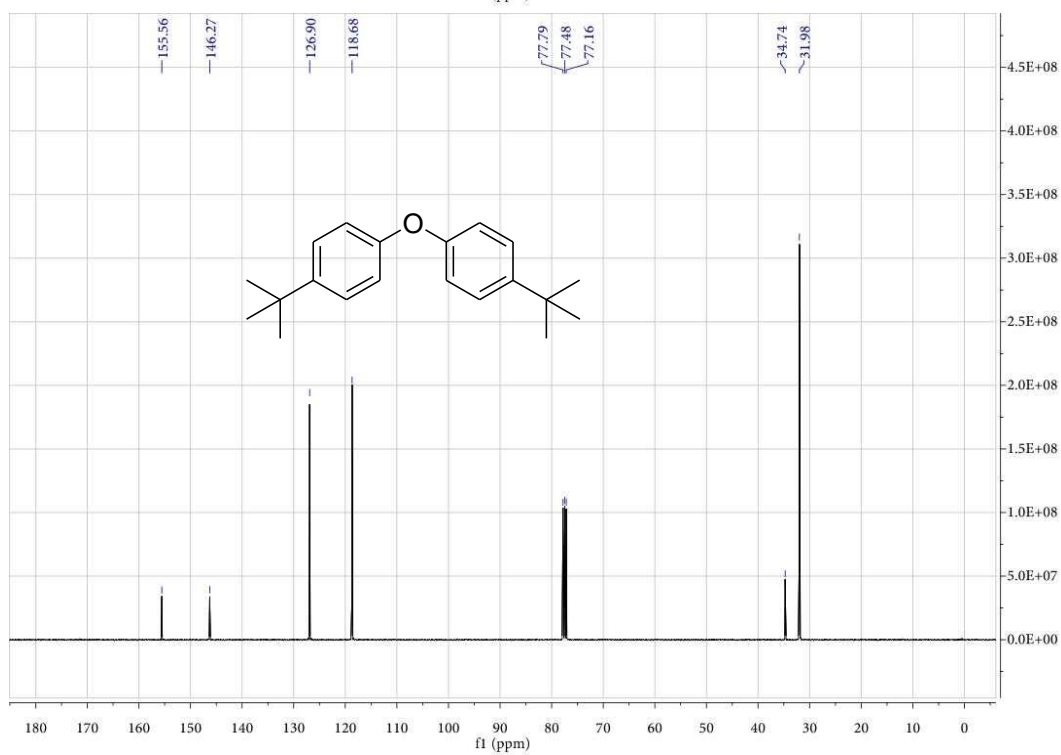
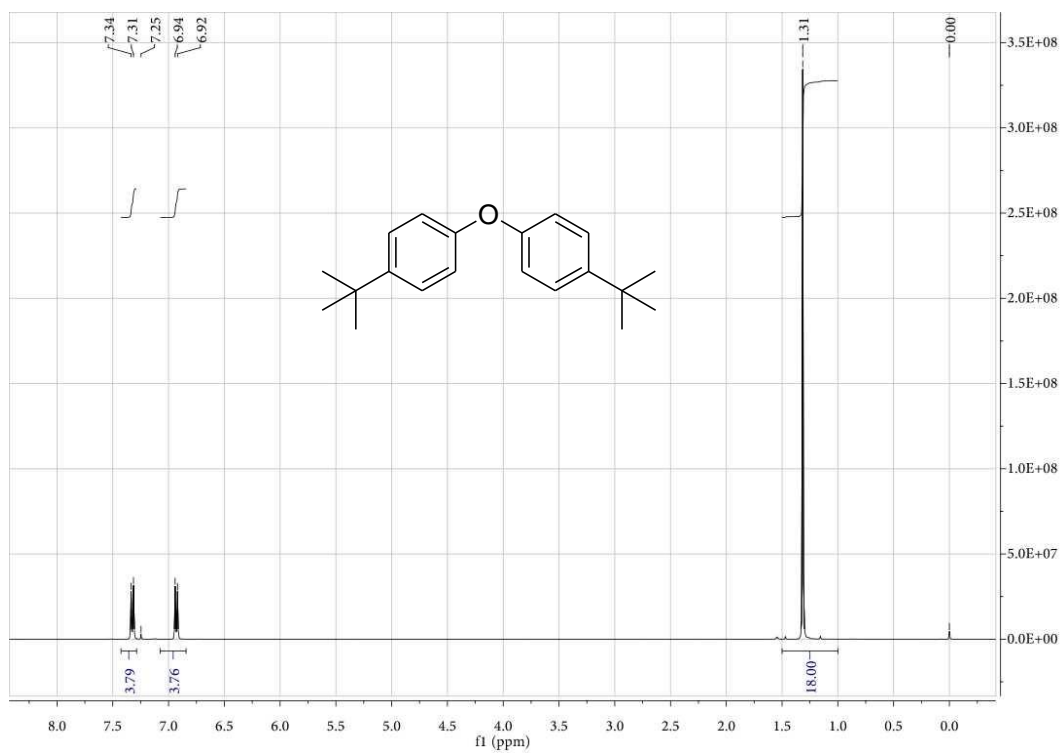


Figure S5. ¹H (top) and ¹³C (bottom) NMR spectra of di-4-tert-butylphenyl ether.

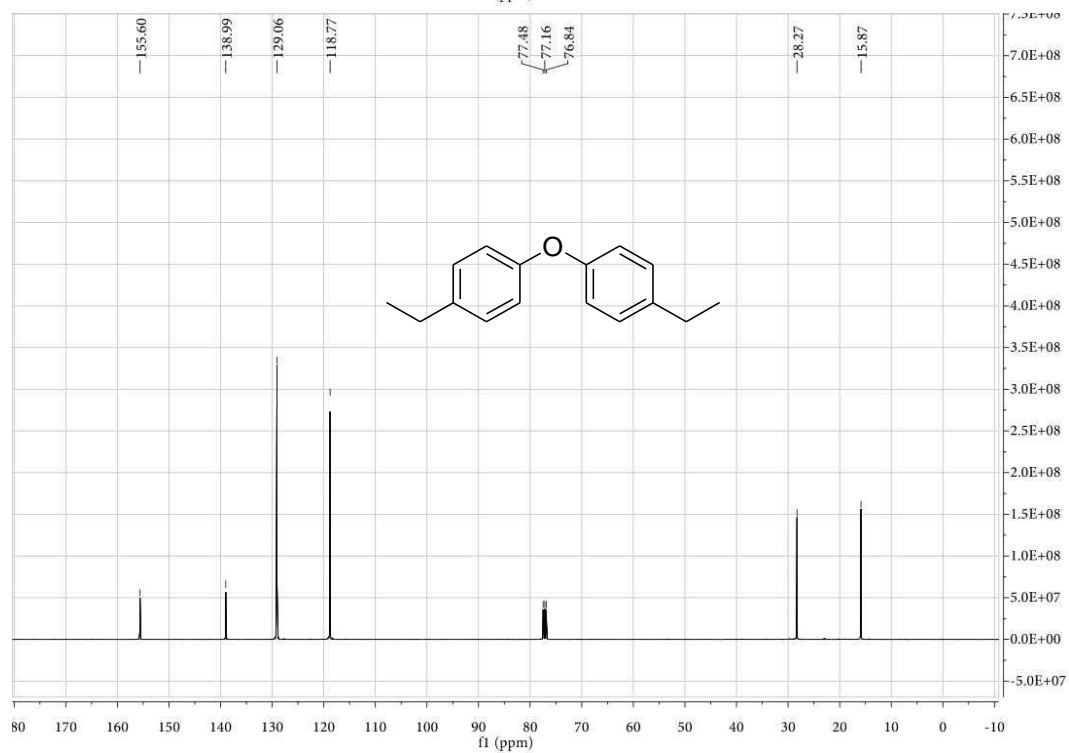
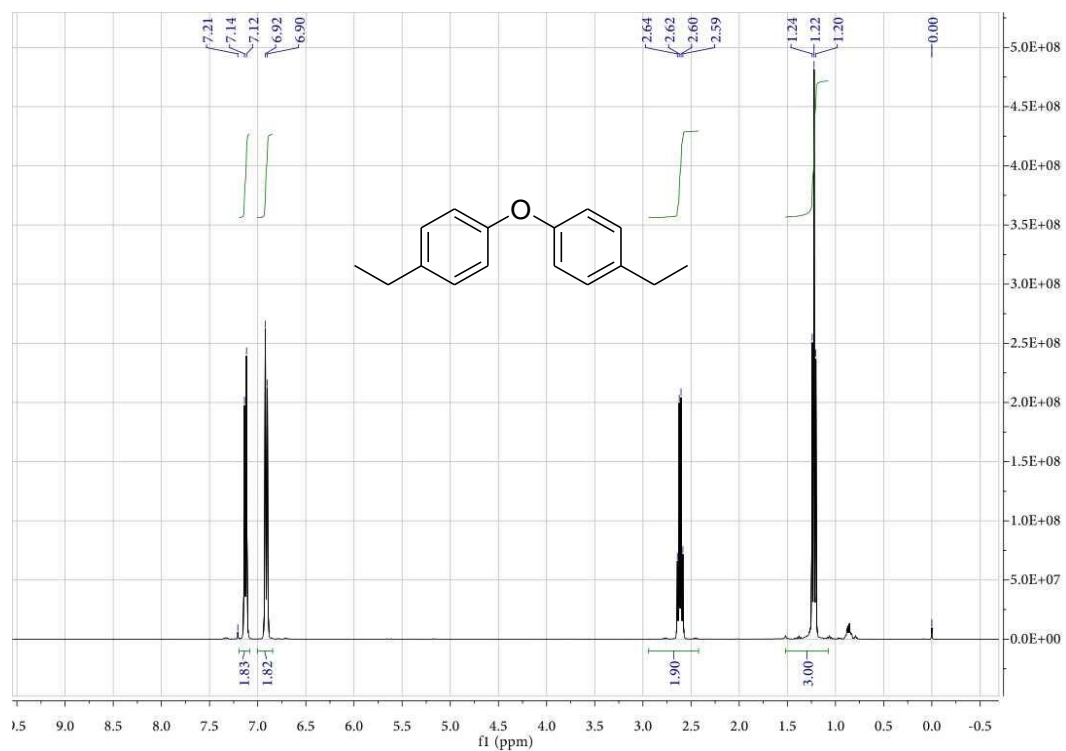


Figure S6. ¹H (top) and ¹³C (bottom) NMR spectra of di-4-ethylphenyl ether

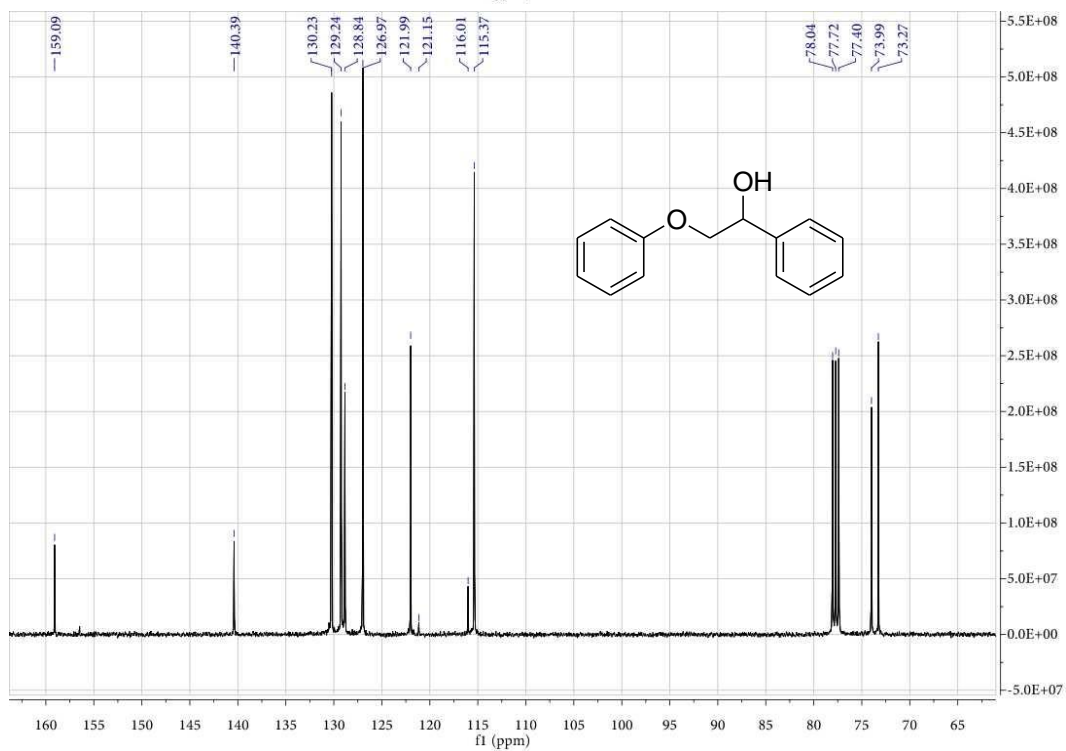
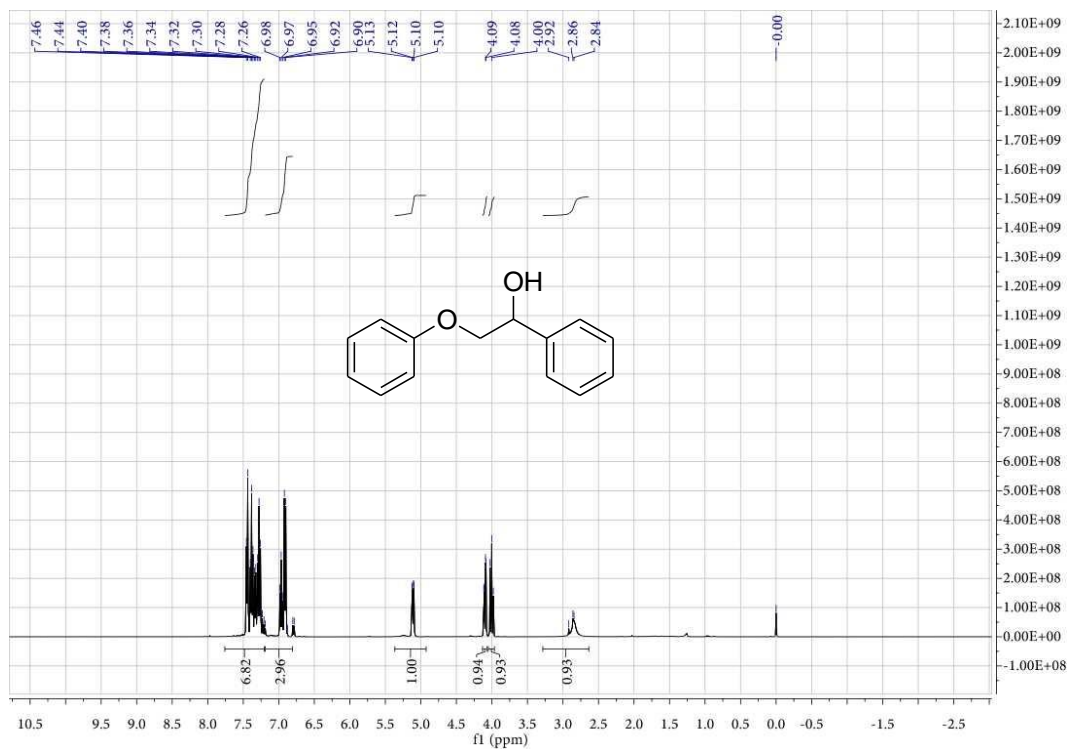


Figure S7. ^1H (top) and ^{13}C (bottom) NMR spectra of 2-phenoxy-1-phenethanol.

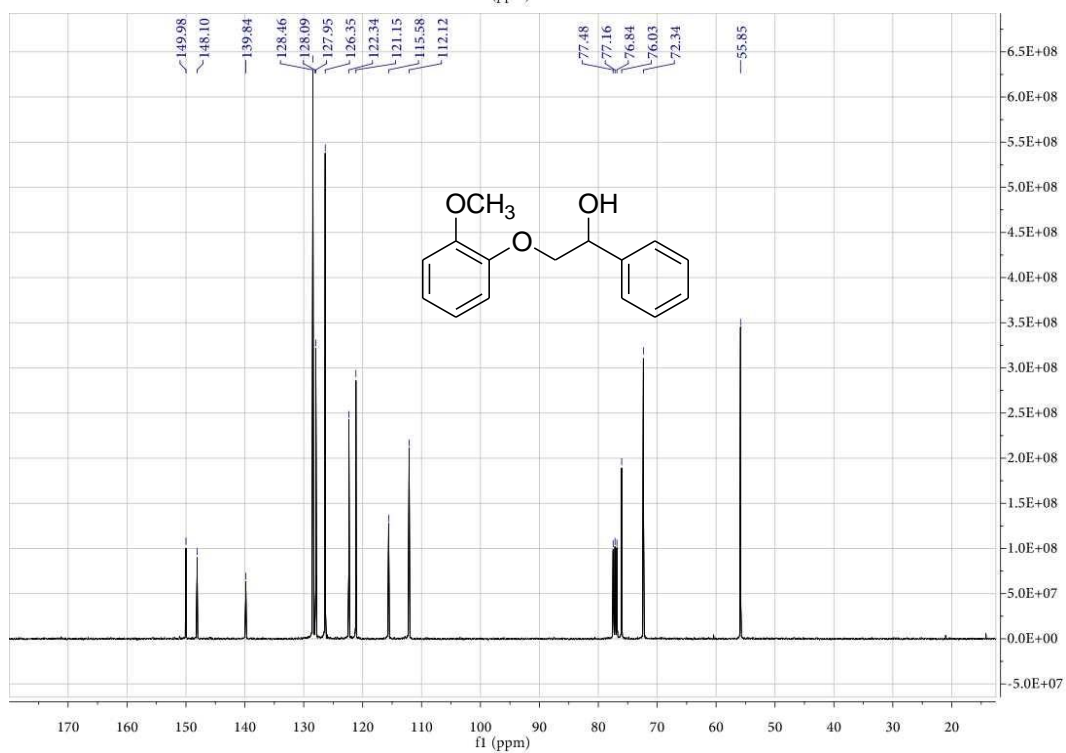
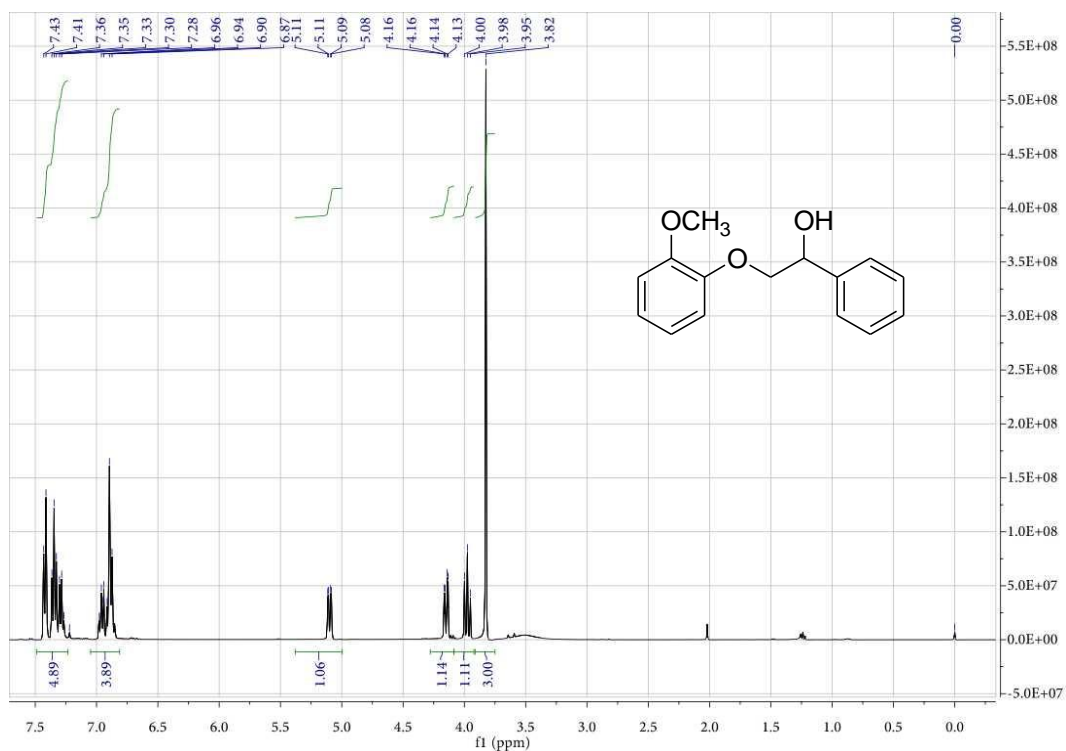


Figure S8. ¹H (top) and ¹³C (bottom) NMR spectra of 2-(2-methoxyphenoxy)-1-phenylethanol.

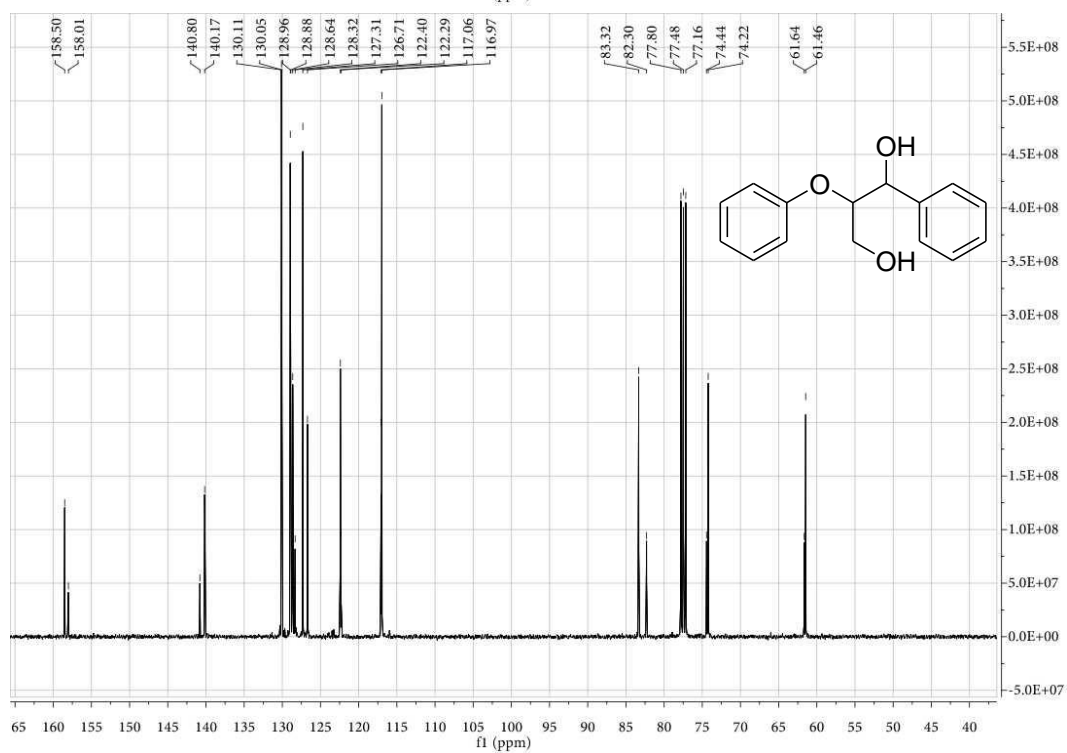
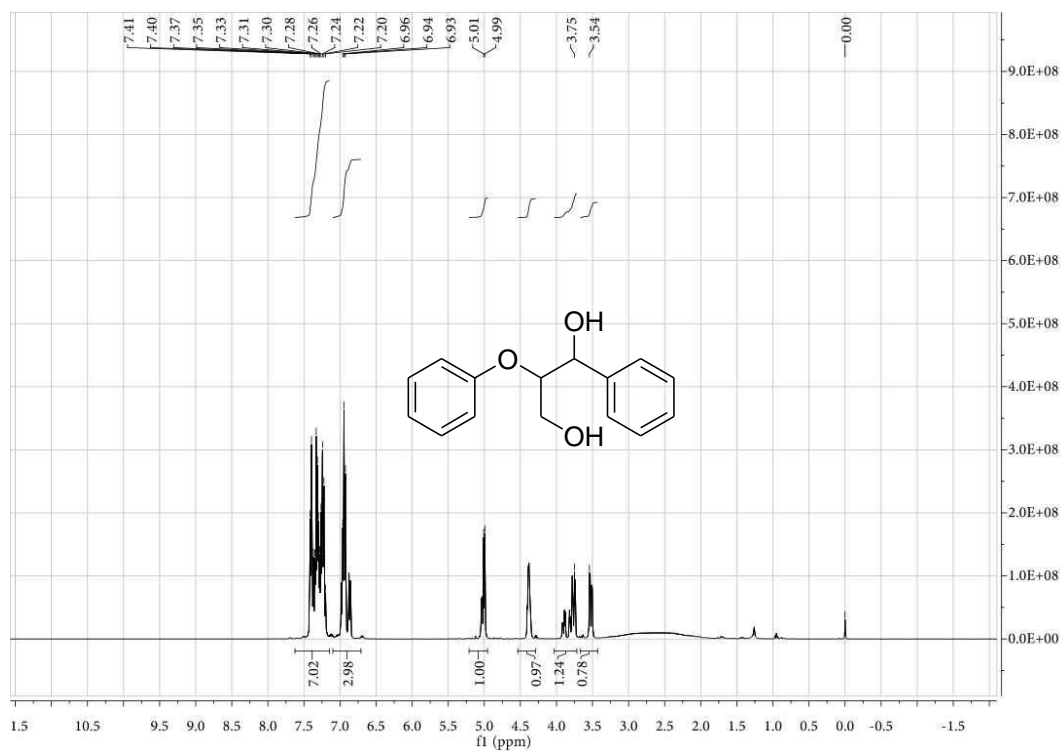
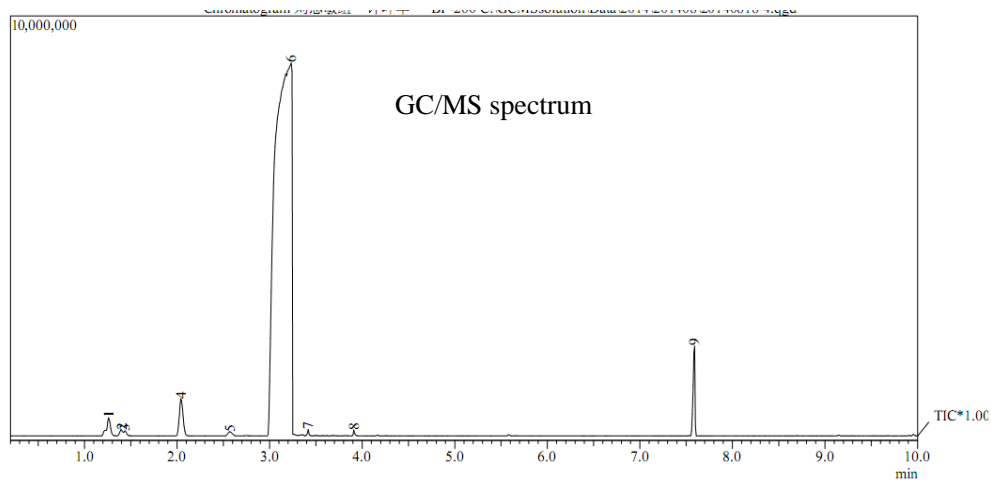
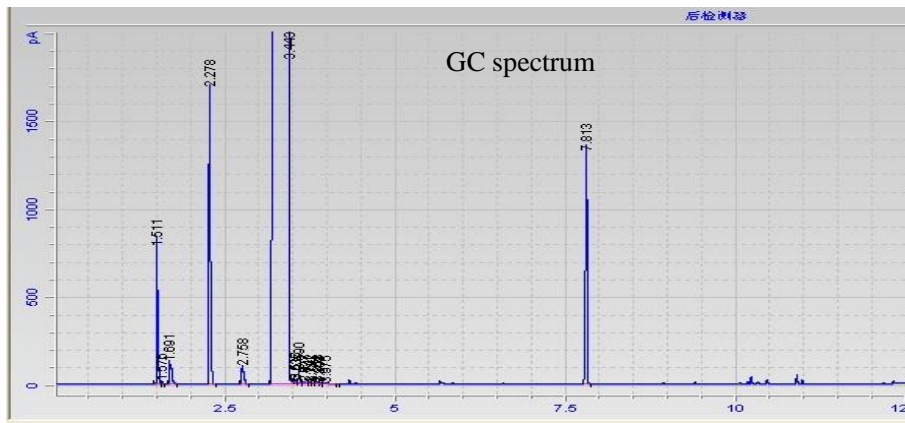
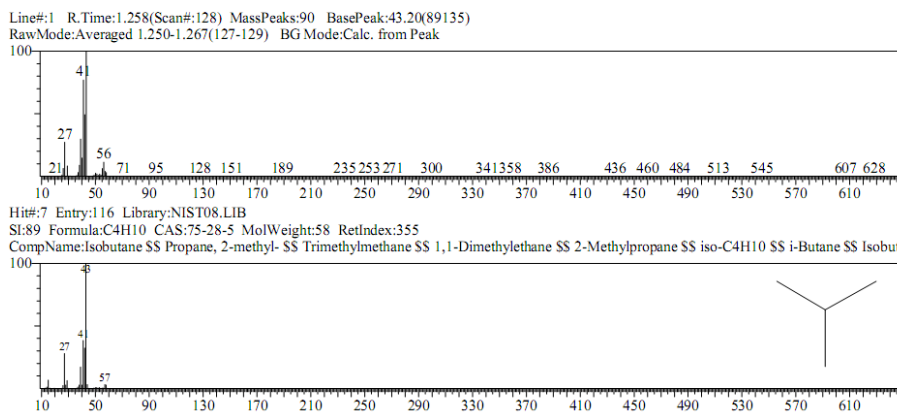


Figure S9. ¹H (top) and ¹³C (bottom) NMR spectra of 2-phenoxy-1-phenylpropane-1,3-diol.

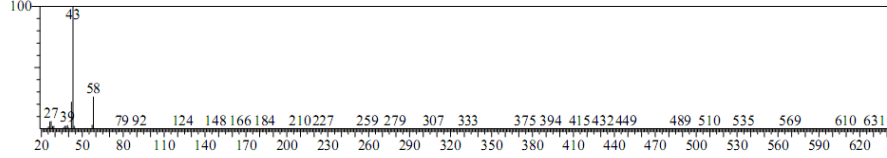
9. GC and GC-MS spectra of the reaction solutions.



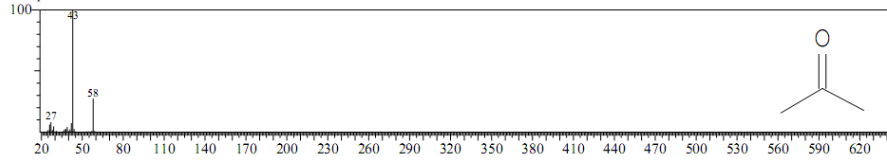
1. Isobutane, 2. Acetone (from syringe cleaning solvent), 3. tert-butanol, 4. Benzene, 5. Methylcyclohexane (from toluene solvent), 6. Toluene, 7. n-octane(impurity from internal standard), 8. Diactonealchol (from syringe cleaning solvent) 9. n-dodecane (internal standard).



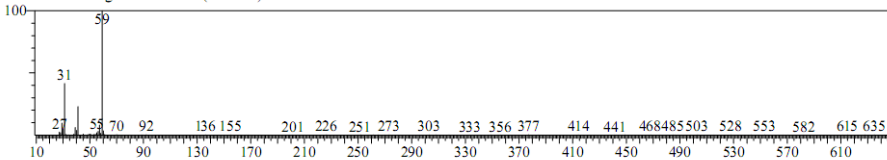
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RawMode:Averaged 1.392-1.408(144-146) BG Mode:Calc. from Peak



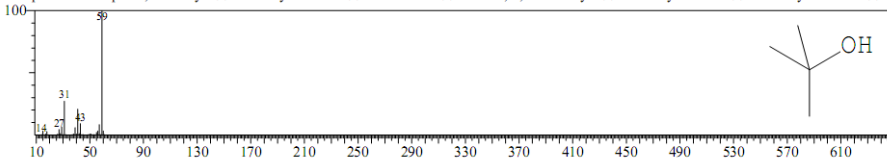
Hit#1 Entry:120 Library:NIST1.LIB
SI:94 Formula:C3H6O CAS:67-64-1 MolWeight:58 RetIndex:0
CompName:Acetone



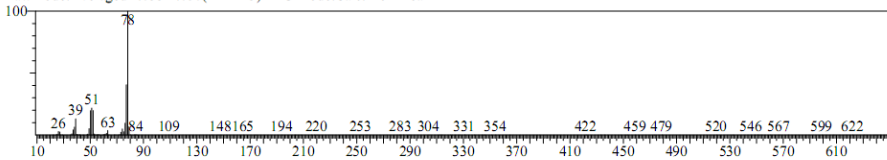
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RawMode:Averaged 1.425-1.442(148-150) BG Mode:Calc. from Peak



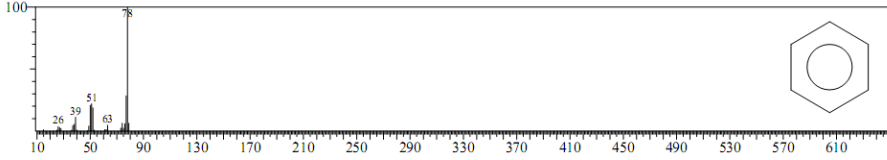
Hit#4 Entry:389 Library:NIST147.LIB
SI:92 Formula:C4H10O CAS:75-65-0 MolWeight:74 RetIndex:0
CompName:2-Propanol, 2-methyl- SS tert-Butyl Alcohol SS tert-Butanol SS Ethanol, 1,1-Dimethyl- SS Trimethylcarbinol SS Trimethylmethanol SS 1,



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RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak

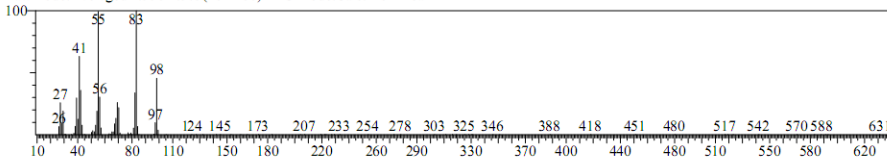


Hit#1 Entry:467 Library:NIST147.LIB
SI:97 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
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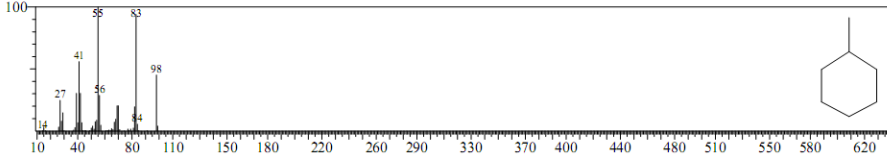


<< Target >>

Line#5 R.Time:2.567(Scan#:285) MassPeaks:92 BasePeak:83.20(13034)
RawMode:Averaged 2.558-2.575(284-286) BG Mode:Calc. from Peak



Hit#1 Entry:1584 Library:NIST08s.LIB
SI:95 Formula:C7H14 CAS:108-87-2 MolWeight:98 RetIndex:781
CompName:Cyclohexane, methyl- SS Cyclohexylmethane SS Hexahydroptoluene SS Methylcyclohexane SS Sextone B SS Toluene hexahydride SS He



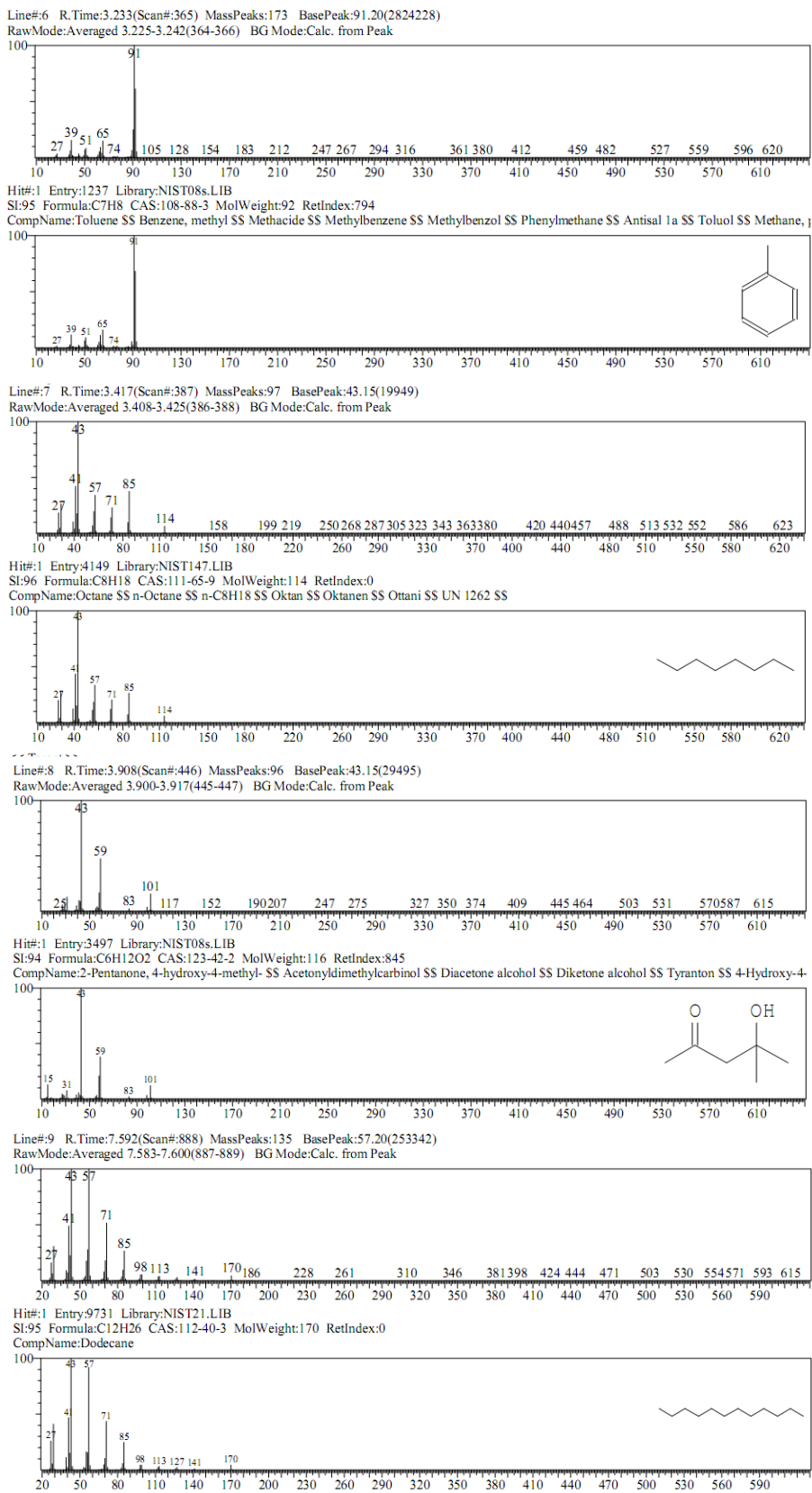
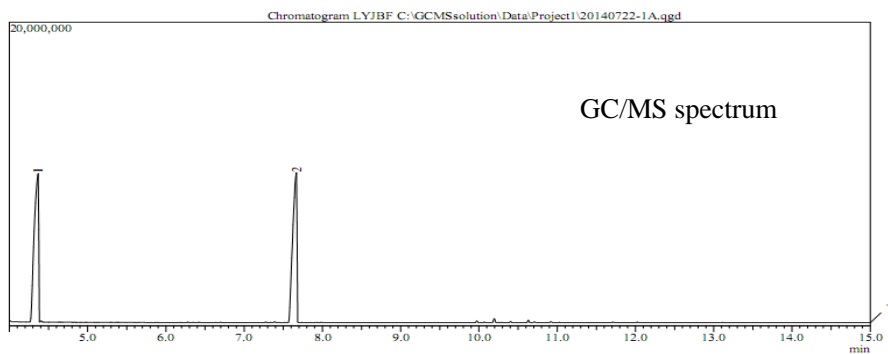
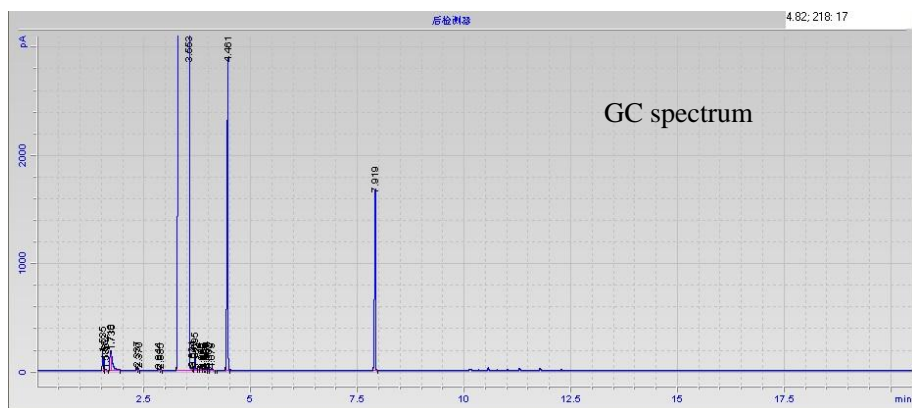
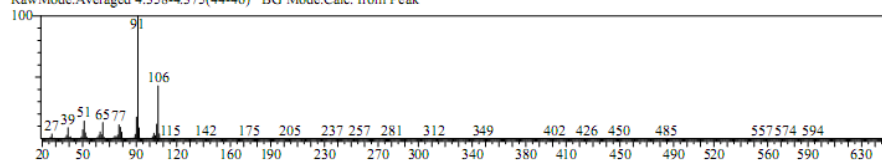


Figure S10. GC and GC/MS spectra of the reaction solution of phenol reduction.



<< Target >>

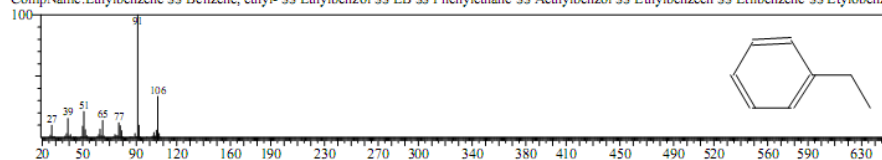
Line#:1 R.Time:4.367(Scan#:45) MassPeaks:130 BasePeak:91.15(2764102)
RawMode:Averaged 4.358-4.375(44-46) BG Mode:Calc. from Peak



Hit#:9 Entry:2360 Library:NIST08s.LIB

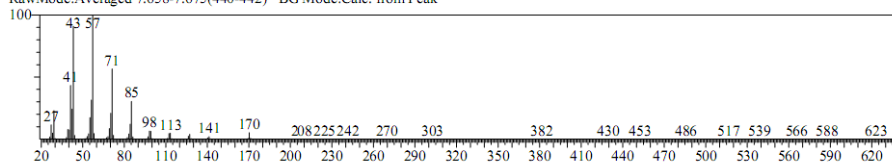
SI:94 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:893

CompName:Ethylbenzene SS Benzene, ethyl- SS Ethylbenzol SS EB SS Phenylethane SS Aethylbenzol SS Ethylbenzen SS Etilbenzene SS Etylobenz



Line#:2 R.Time:7.067(Scan#:441) MassPeaks:120 BasePeak:71.12(1242999)

RawMode:Averaged 7.658-7.675(440-442) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB

SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0

CompName:Dodecane

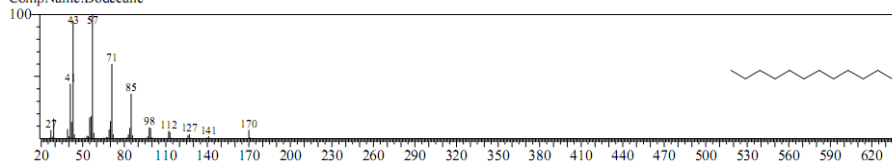
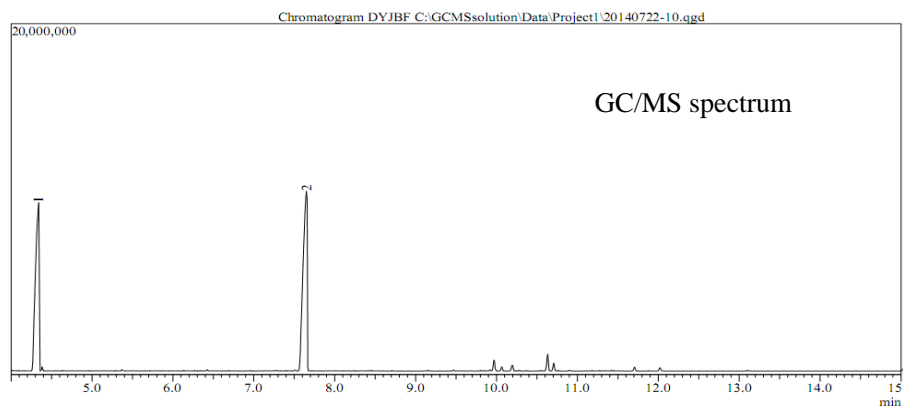
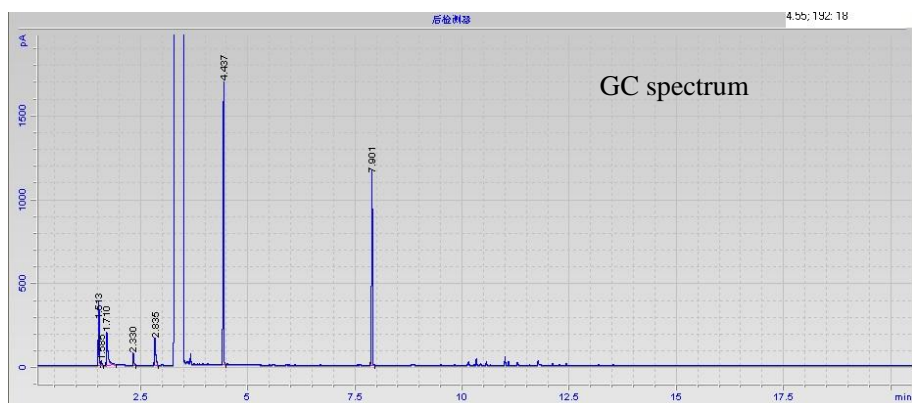
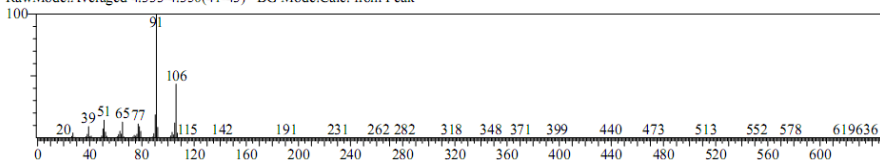


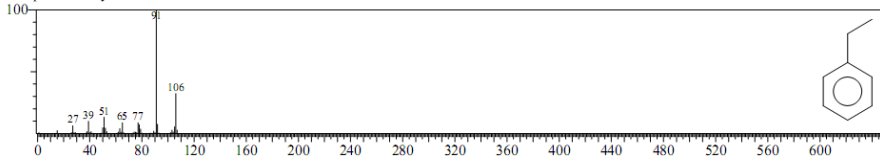
Figure S11. GC and GC/MS spectra of the reaction solution of 2-ethylphenol reduction.



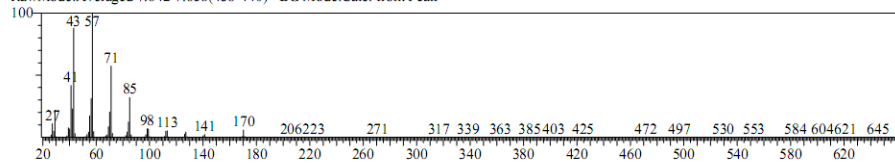
<< Target >>
 Line#:1 R.Time:4.342(Scan#:42) MassPeaks:136 BasePeak:91.15(2512746)
 RawMode:Averaged 4.333-4.350(41-43) BG Mode:Calc. from Peak



Hit#:13 Entry:2121 Library:NIST21.LIB
 SI:93 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
 CompName:Ethylbenzene



<< Target >>
 Line#:2 R.Time:7.650(Scan#:439) MassPeaks:141 BasePeak:57.15(1775378)
 RawMode:Averaged 7.642-7.658(438-440) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB
 SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
 CompName:Dodecane

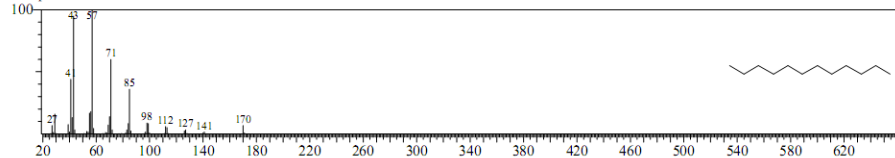
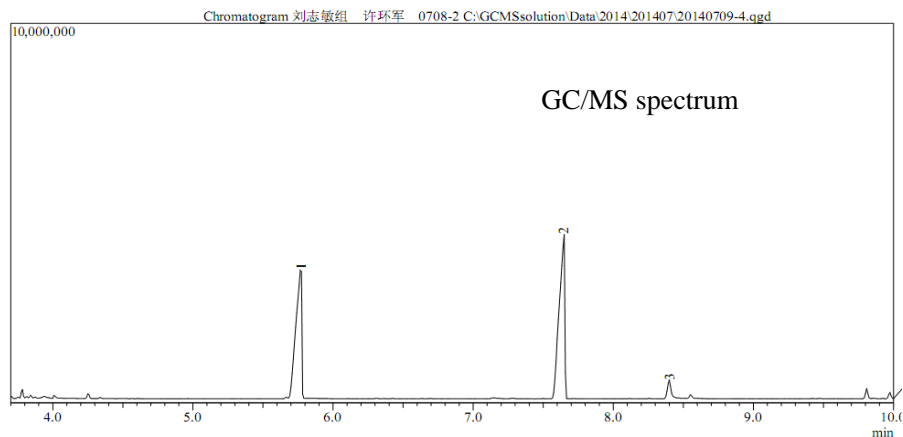
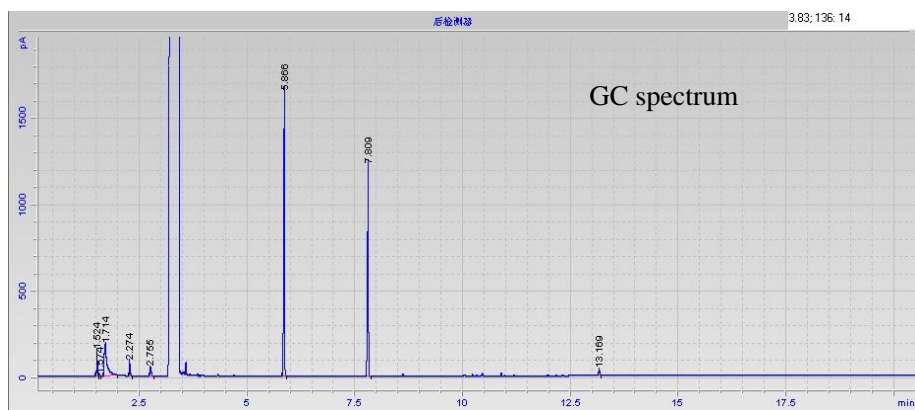
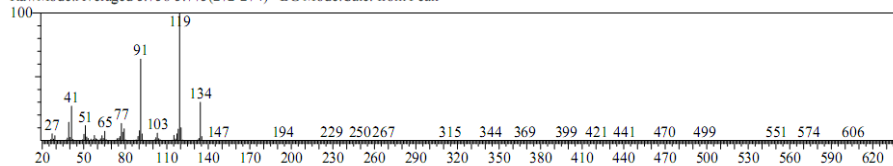


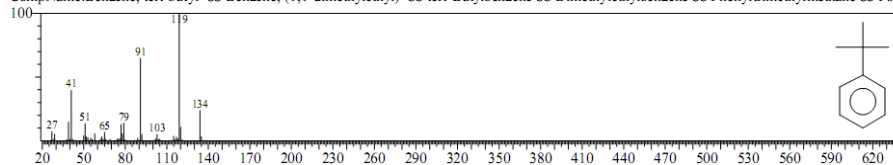
Figure S12. GC and GC/MS spectra of the reaction solution of 4-ethylphenol reduction.



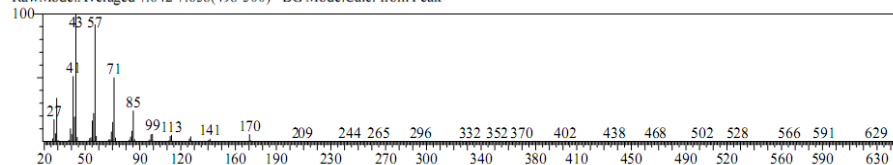
Line#:1 R.Time:5.767(Scan#:273) MassPeaks:150 BasePeak:119.30(810470)
RawMode:Averaged 5.758-5.775(272-274) BG Mode:Calc. from Peak



Hit#:1 Entry:8101 Library:NIST107.LIB
SI:95 Formula:C10H14 CAS:98-06-6 MolWeight:134 RetIndex:0
CompName:Benzene, tert-butyl- SS Benzene, (1,1-dimethylethyl)- SS tert-Butylbenzene SS Dimethylethylbenzene SS Phenyltrimethylmethane SS Pse



Line#:2 R.Time:7.650(Scan#:499) MassPeaks:147 BasePeak:43.20(547664)
RawMode:Averaged 7.642-7.658(498-500) BG Mode:Calc. from Peak



Hit#:1 Entry:9731 Library:NIST21.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane

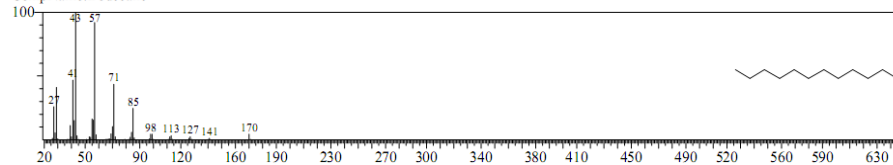


Figure S13. GC and GC/MS spectra of the reaction solution of 4-tert-butylphenol reduction.

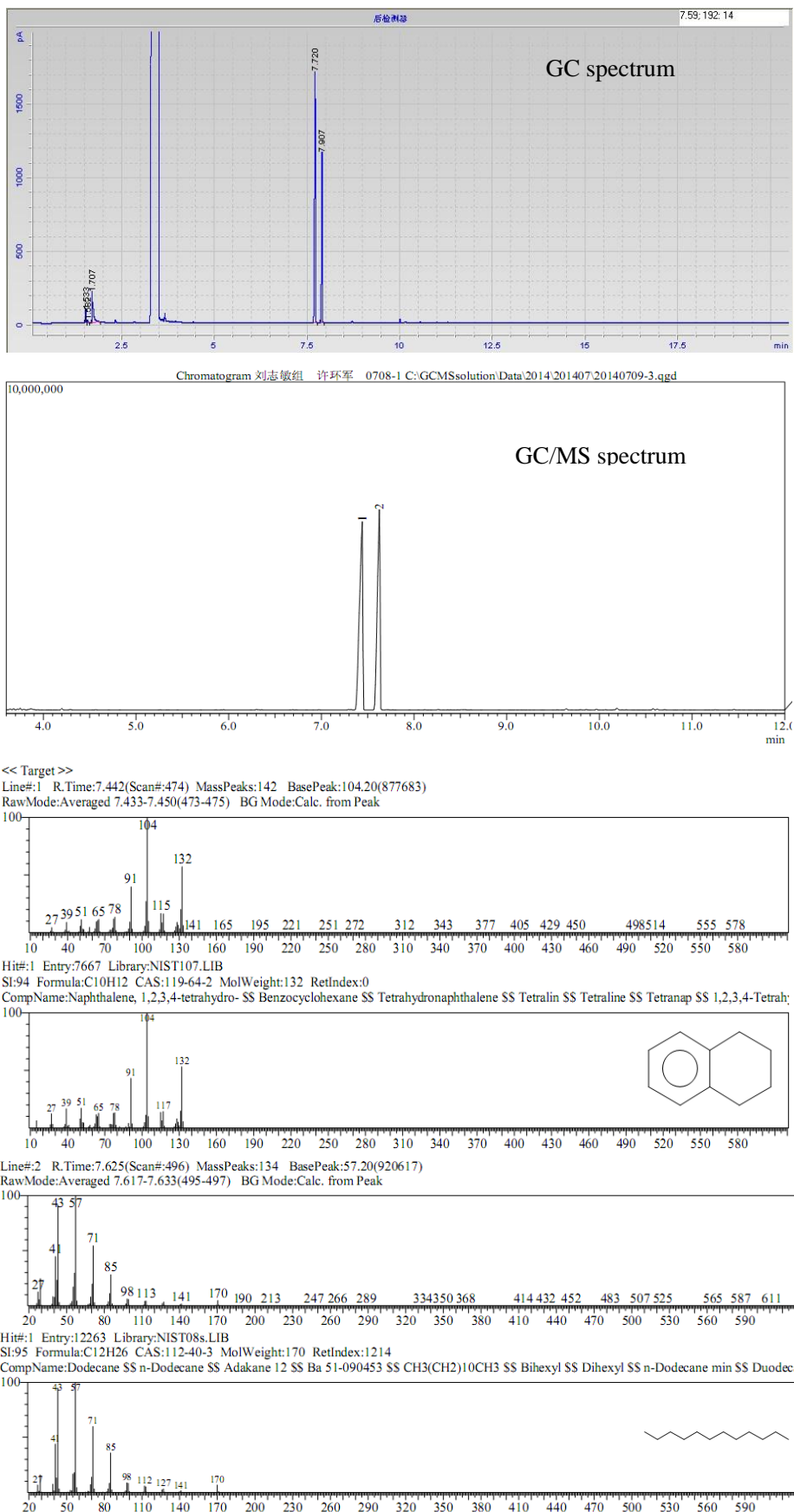
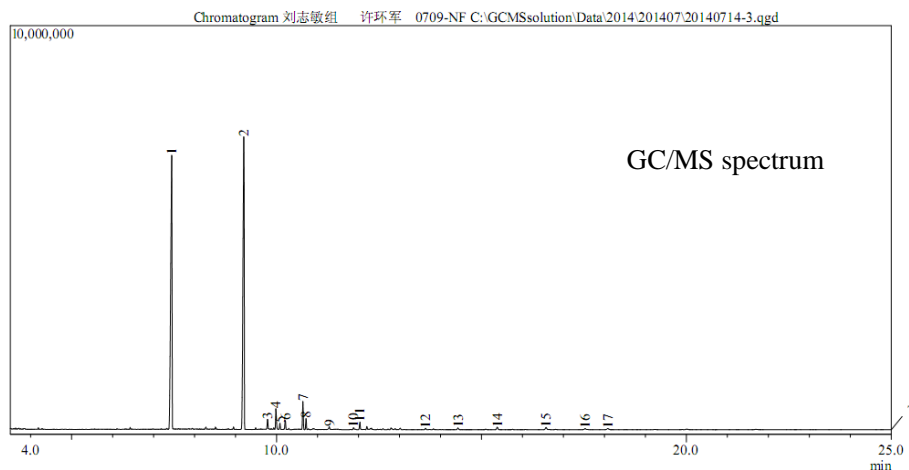
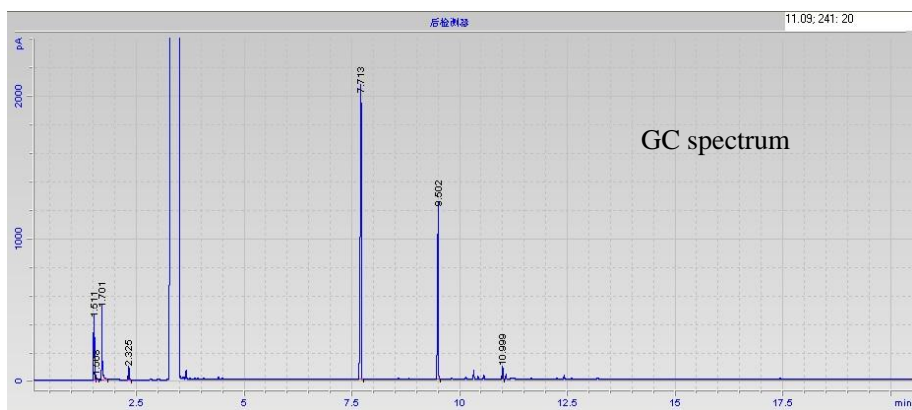
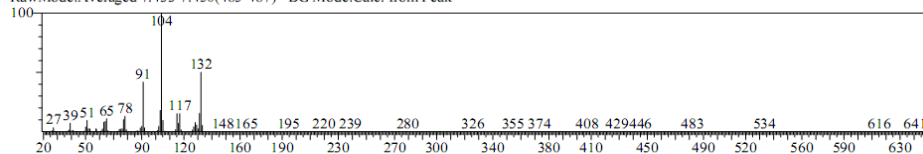


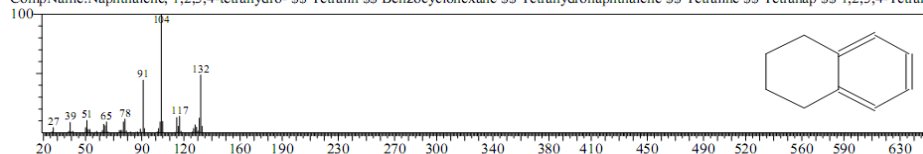
Figure S14. GC and GC/MS spectra of the reaction solution of 1,2,3,4-tetrahydro-1-naphthol reduction.



Line#:1 R.Time:7.442(Scan#:486) MassPeaks:142 BasePeak:104.10(1260748)
RawMode:Averaged 7.433-7.450(485-487) BG Mode:Calc. from Peak

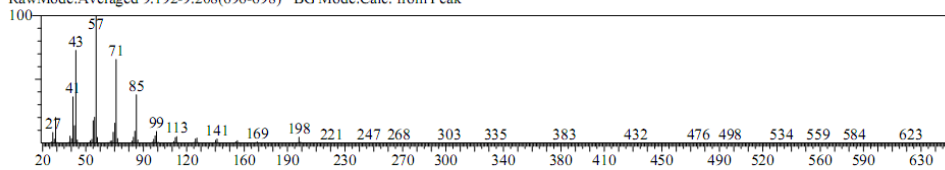


Hit#:1 Entry:5748 Library:NIST08s.LIB
SI:97 Formula:C10H12 CAS:119-64-2 MolWeight:132 RetIndex:1166
CompName:Naphthalene, 1,2,3,4-tetrahydro- SS Tetralin SS Benzocyclohexane SS Tetrahydronaphthalene SS Tetraline SS Tetranap SS 1,2,3,4-Tetrahydro-



<< Target >>

Line#:2 R.Time:9.200(Scan#:697) MassPeaks:155 BasePeak:57.10(1219921)
RawMode:Averaged 9.192-9.208(696-698) BG Mode:Calc. from Peak



Hit#:1 Entry:16430 Library:NIST08s.LIB
SI:97 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1413
CompName:Tetradecane SS n-Tetradecane SS

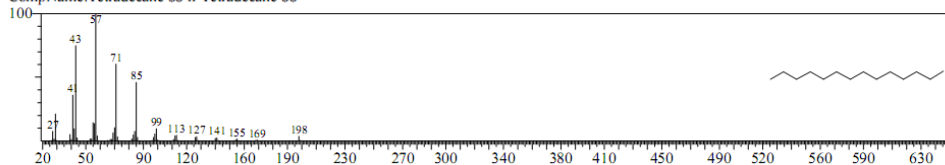


Figure S15. GC and GC/MS spectra of the reaction solution of 2-naphthol reduction.

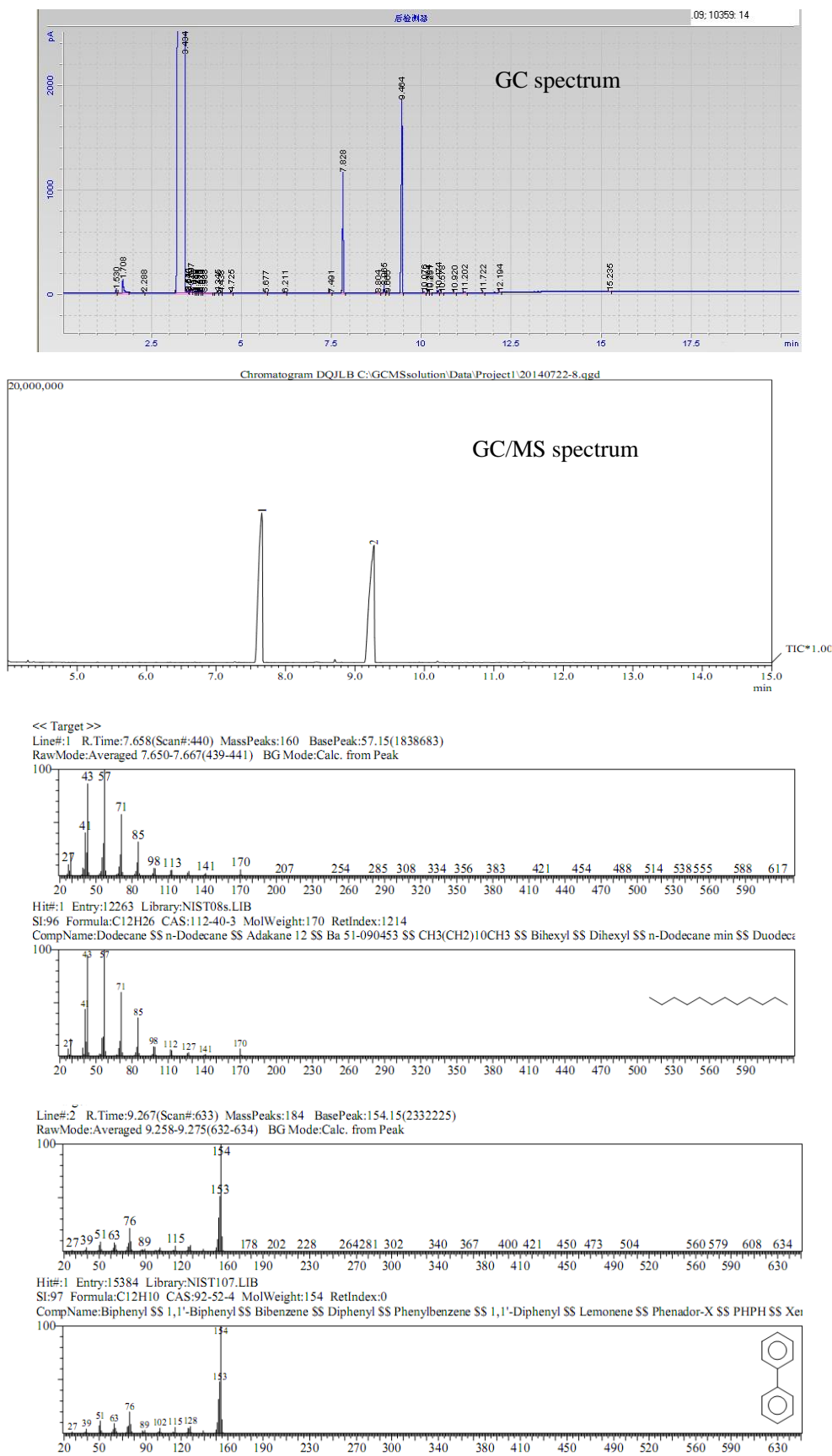
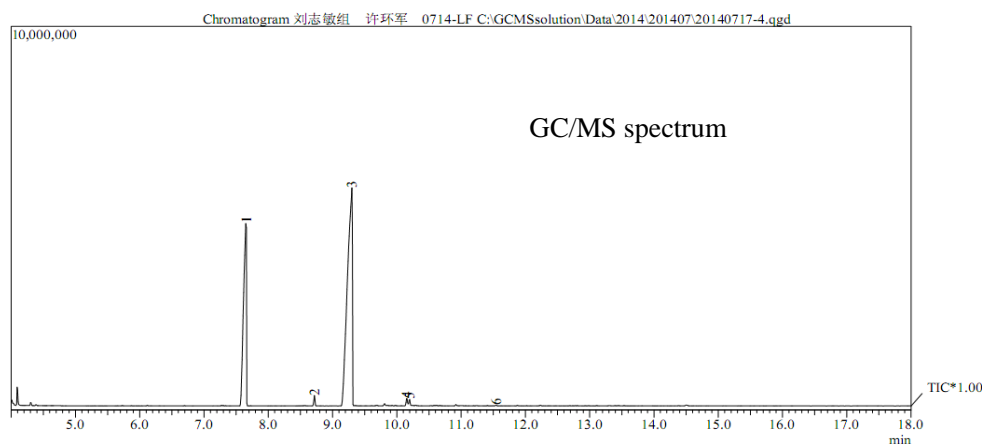
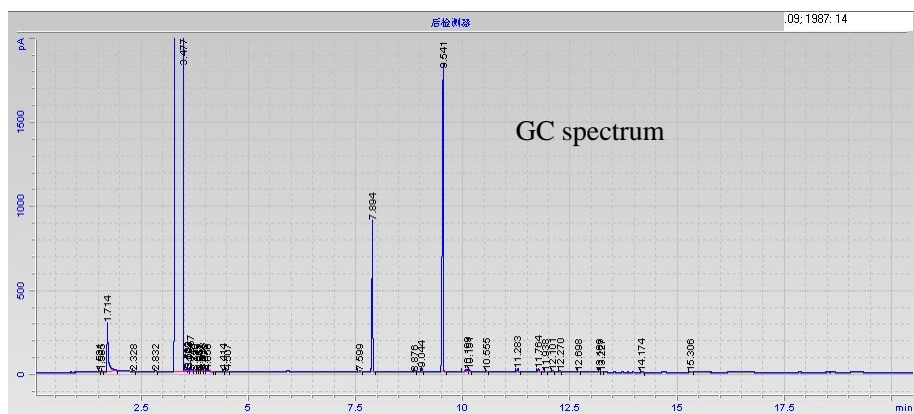
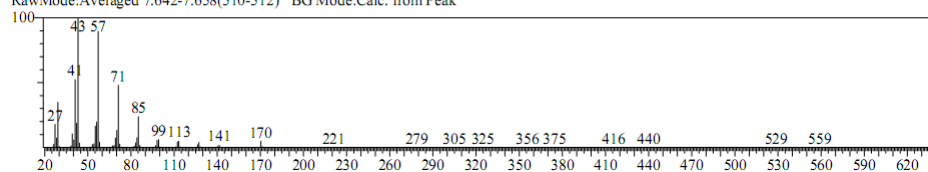


Figure S16. GC and GC/MS spectra of the reaction solution of 4-hydroxydiphenyl reduction.

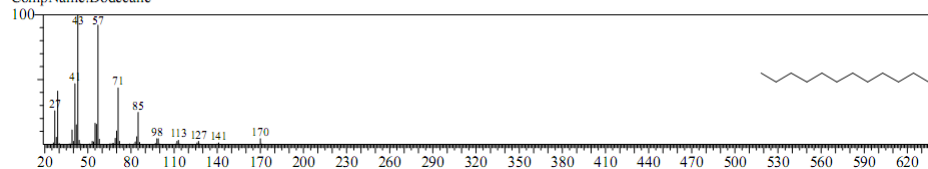


<< Target >>

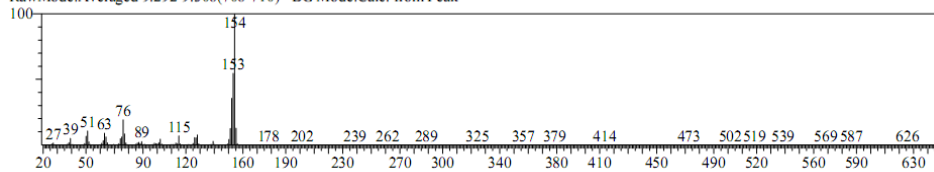
Line#:1 R.Time:7.650(Scan#:511) MassPeaks:132 BasePeak:43.20(846313)
RawMode:Averaged 7.642-7.658(510-512) BG Mode:Calc. from Peak



Hit#:1 Entry:9731 Library:NIST21.LIB
SI:97 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane



Line#:3 R.Time:9.300(Scan#:09) MassPeaks:172 BasePeak:154.20(1434257)
RawMode:Averaged 9.292-9.308(708-710) BG Mode:Calc. from Peak



Hit#:1 Entry:17580 Library:NIST08.LIB
SI:97 Formula:C12H10 CAS:92-52-4 MolWeight:154 RetIndex:1367
CompName:Biphenyl SS 1,1'-Biphenyl SS Bibenzene SS Diphenyl SS Phenylbenzene SS 1,1'-Diphenyl SS Lemonene SS Phenador-X SS PHPH SS Xer

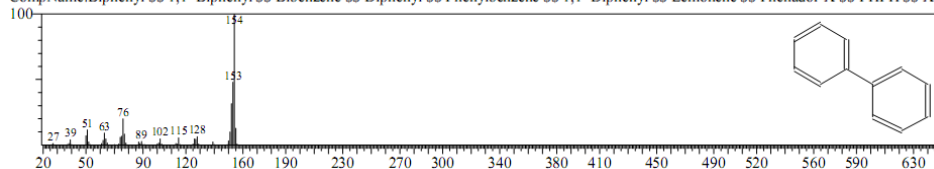
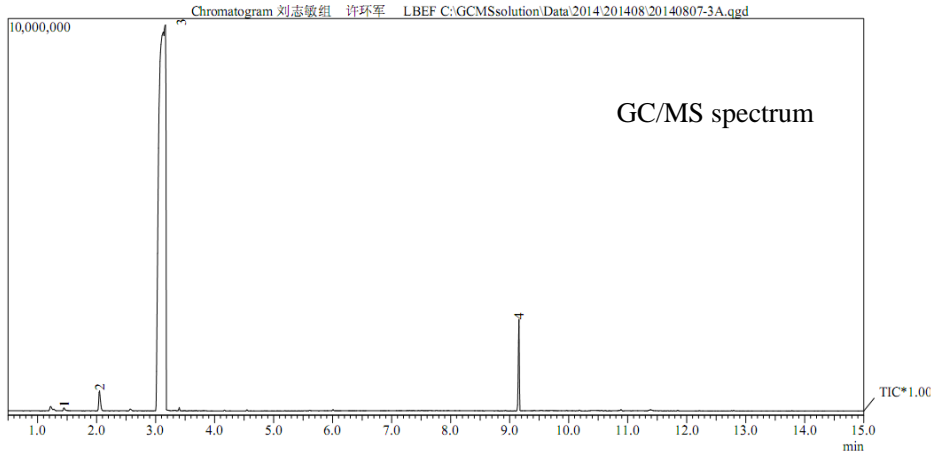
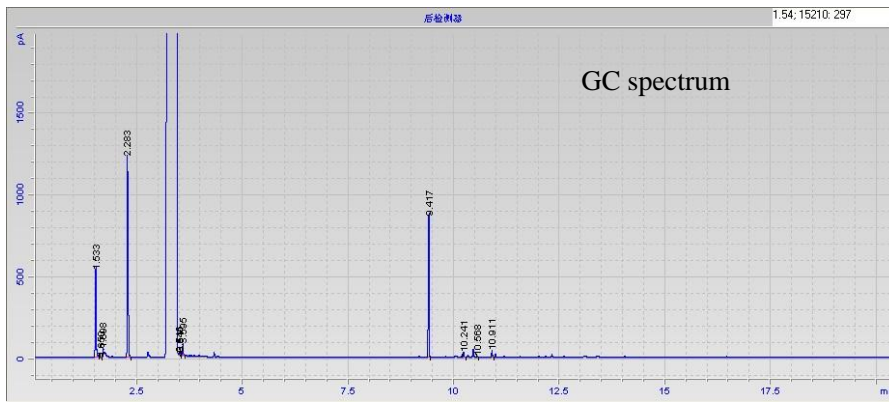
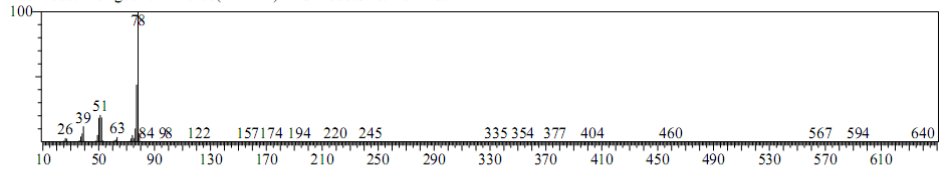


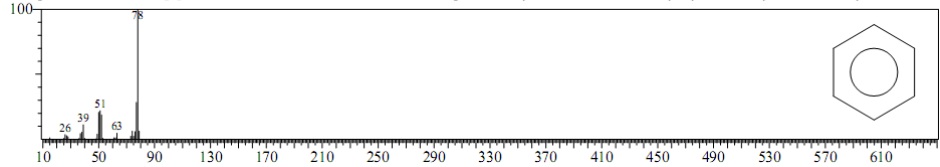
Figure S17. GC and GC/MS spectra of the reaction solution of 2-hydroxydiphenyl reduction.



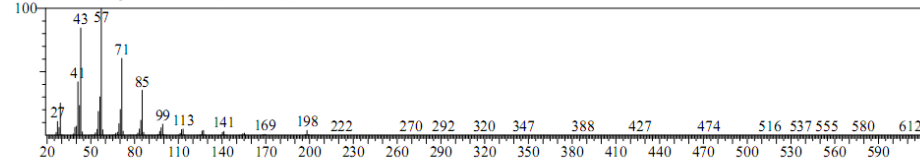
Line#2 R.Time:2.050(Scan#:223) MassPeaks:81 BasePeak:78.10(168398)
 RawMode:Averaged 2.042-2.058(222-224) BG Mode:Calc. from Peak



Hit#1 Entry:467 Library:NIST147.LIB
 SI:96 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
 CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



Line#4 R.Time:9.158(Scan#:1076) MassPeaks:135 BasePeak:57.15(267677)
 RawMode:Averaged 9.150-9.167(1075-1077) BG Mode:Calc. from Peak



Hit#1 Entry:12488 Library:NIST21.LIB
 SI:95 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:0
 CompName:Tetradecane

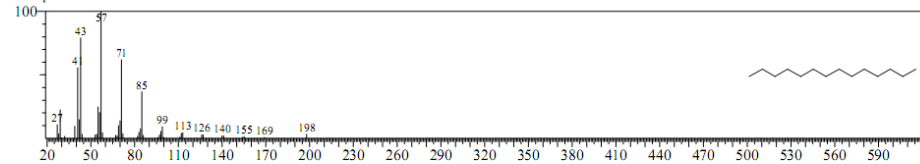
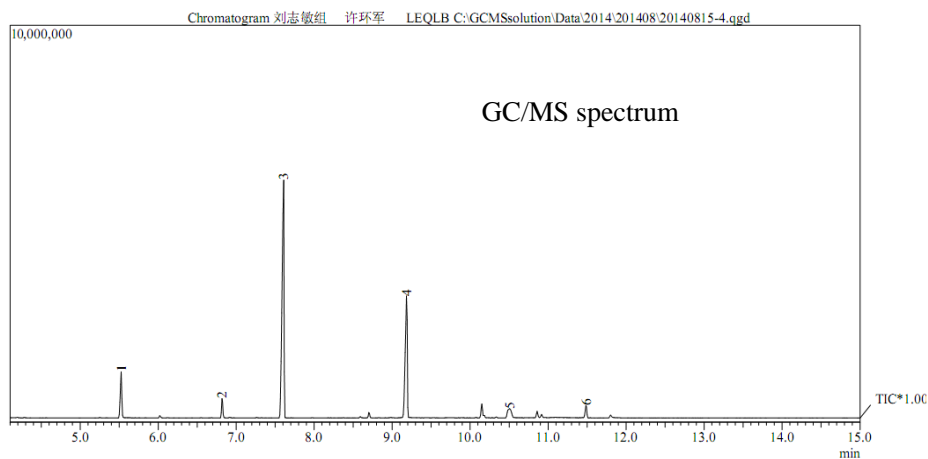
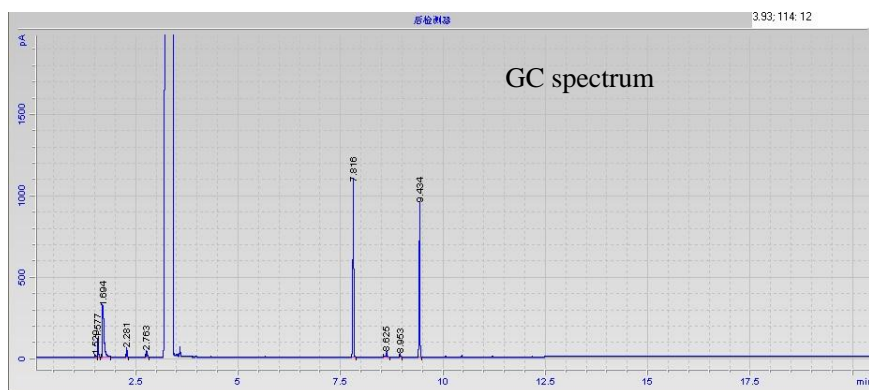
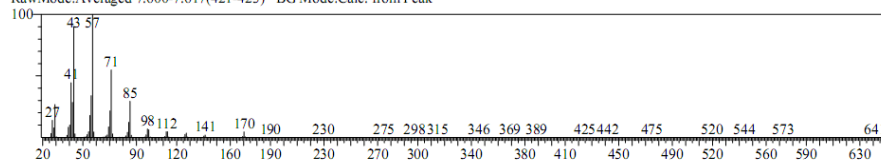


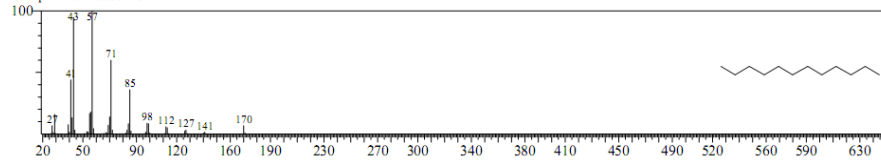
Figure S18. GC and GC/MS spectra of the reaction solution of catechol reduction.



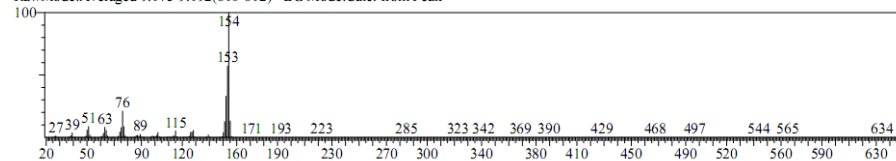
Line#3 R.Time:7.608(Scan#:422) MassPeaks:140 BasePeak:57.20(0.3402)
RawMode:Averaged 7.600-7.617(421-423) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane



Line#4 R.Time:9.183(Scan#:611) MassPeaks:144 BasePeak:154.20(742222)
RawMode:Averaged 9.175-9.192(610-612) BG Mode:Calc. from Peak



Hit#:1 Entry:17580 Library:NIST08.LIB
SI:97 Formula:C12H10 CAS:92-52-4 MolWeight:154 RetIndex:1367
CompName:Biphenyl SS 1,1'-Biphenyl SS Bibenzene SS Diphenyl SS Phenylbenzene SS 1,1'-Diphenyl SS Lemonene SS Phenador-X SS PHPH SS Xer

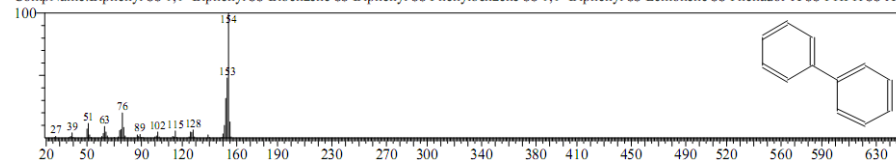
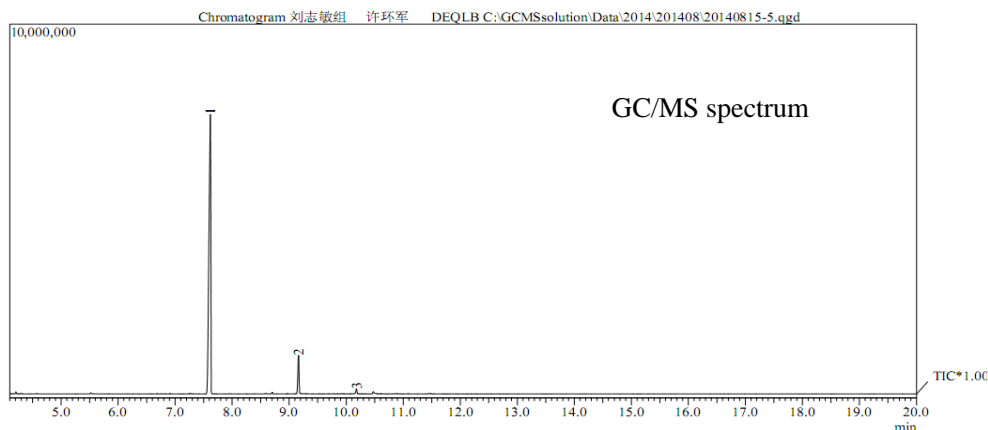
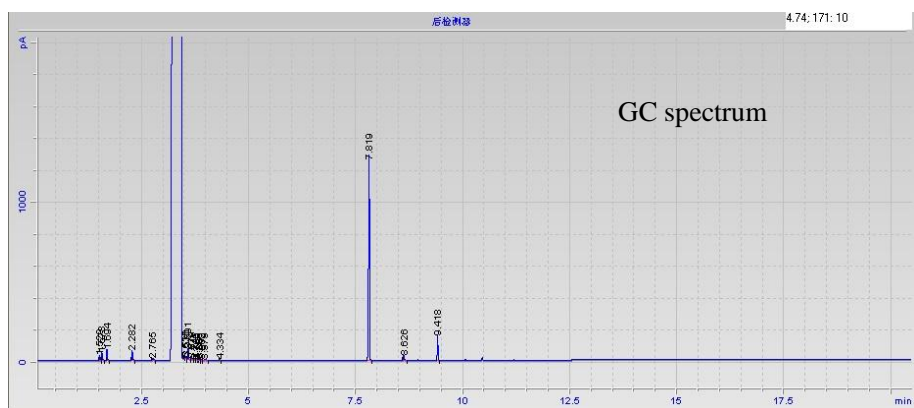
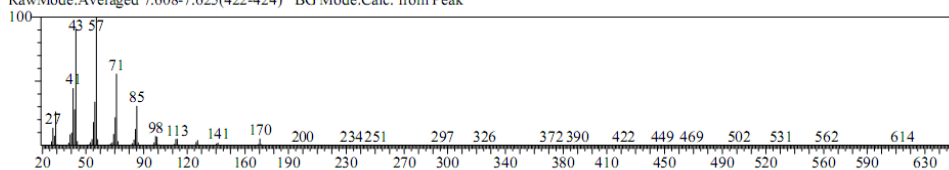


Figure S19. GC and GC/MS spectra of the reaction solution of 2,2'-bisphenol reduction.

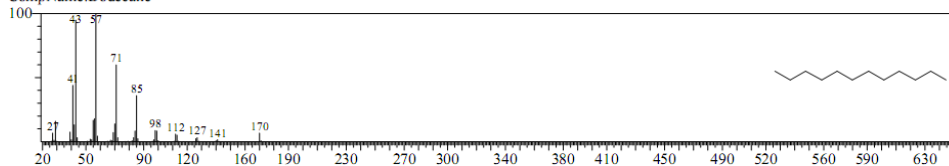


<< Target >>

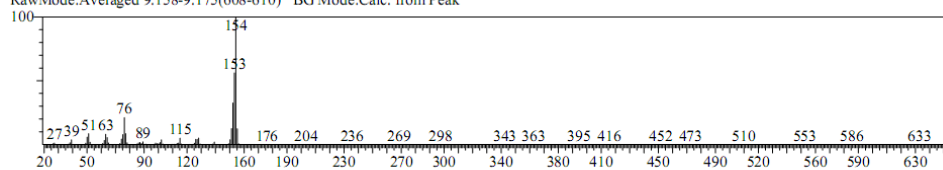
Line#:1 R.Time:7.617(Scan#:423) MassPeaks:142 BasePeak:57.20(1111960)
RawMode:Averaged 7.608-7.625(422-424) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane



Line#:2 R.Time:9.167(Scan#:609) MassPeaks:134 BasePeak:154.20(215869)
RawMode:Averaged 9.158-9.175(608-610) BG Mode:Calc. from Peak



Hit#:1 Entry:17580 Library:NIST08.LIB
SI:97 Formula:C12H10 CAS:92-52-4 MolWeight:154 RetIndex:1367
CompName:Biphenyl SS 1,1'-Biphenyl SS Bibenzene SS Diphenyl SS Phenylbenzene SS 1,1'-Diphenyl SS Lemonene SS Phenador-X SS PHPH SS Xer

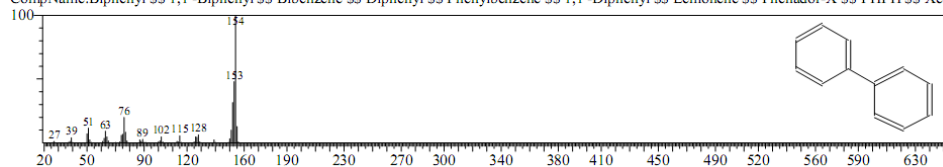
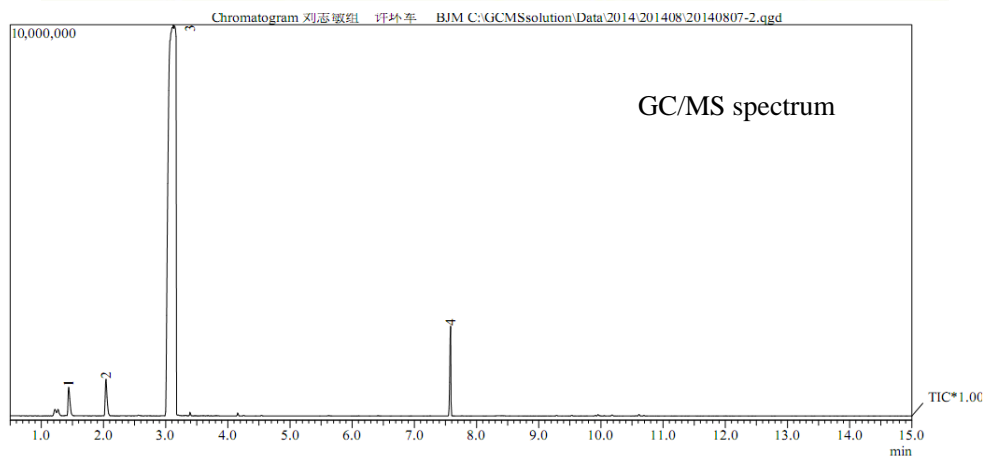
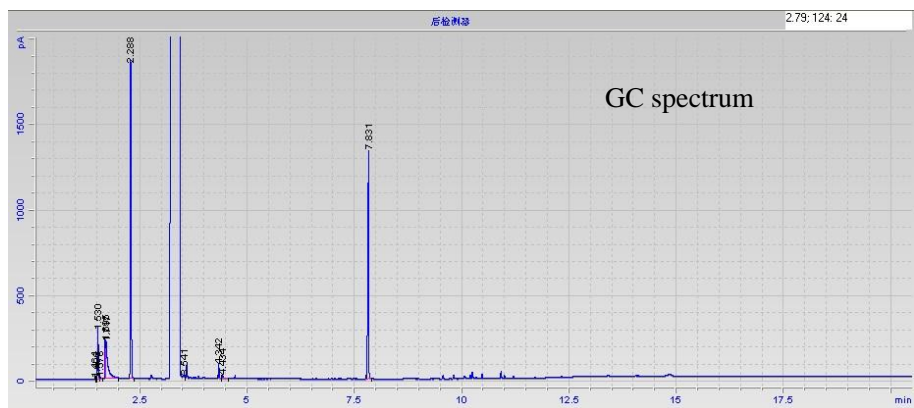
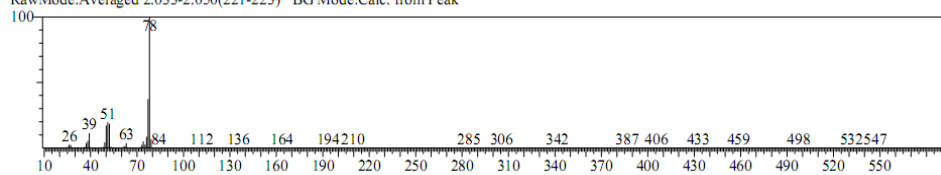


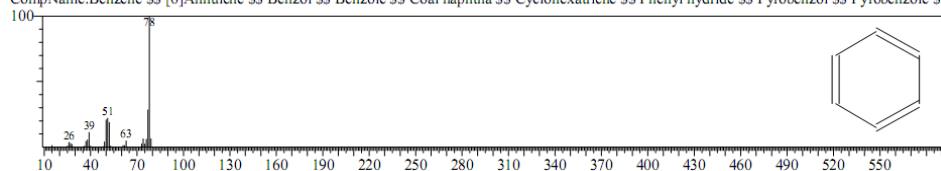
Figure S20. GC and GC/MS spectra of the reaction solution of 4,4'-bisphenol reduction.



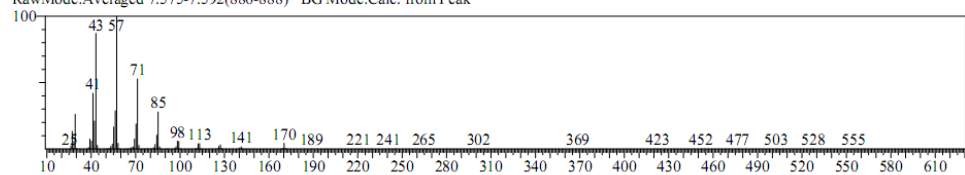
Line#:2 R. Time:2.042(Scan#:222) MassPeaks:77 BasePeak:78.10(32/197)
 RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak



Hit#:1 Entry:478 Library:NIST08.LIB
 SI:97 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:680
 CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S:



Line#:4 R. Time:7.583(Scan#:887) MassPeaks:109 BasePeak:57.15(282076)
 RawMode:Averaged 7.575-7.592(886-888) BG Mode:Calc. from Peak



Hit#:1 Entry:22005 Library:NIST107.LIB
 SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
 CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodec

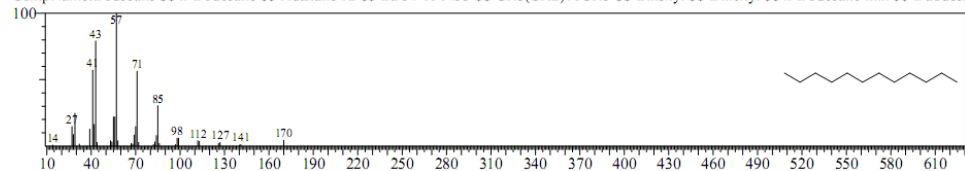


Figure S21. GC and GC/MS spectra of the reaction solution of anisole reduction.

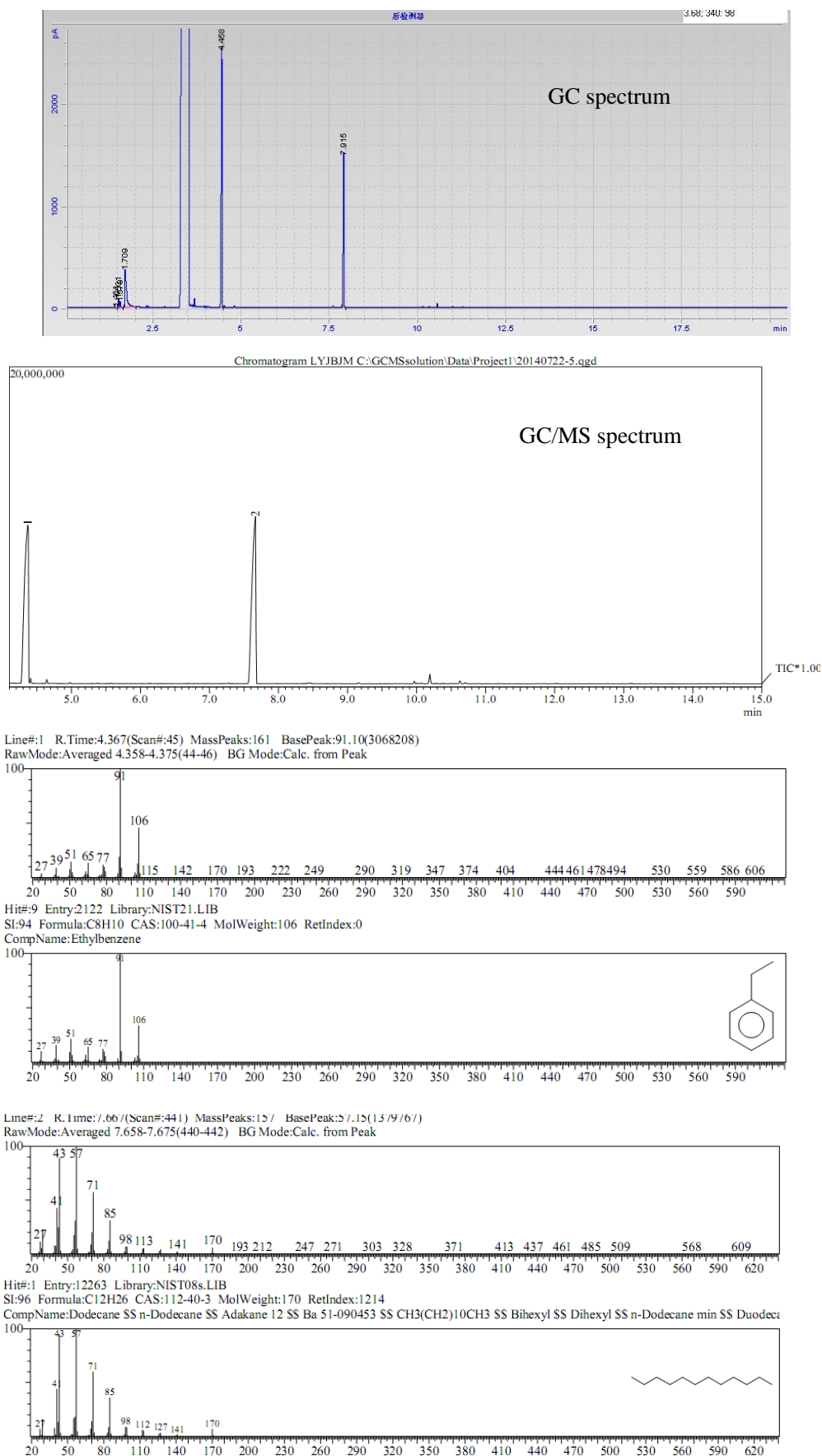
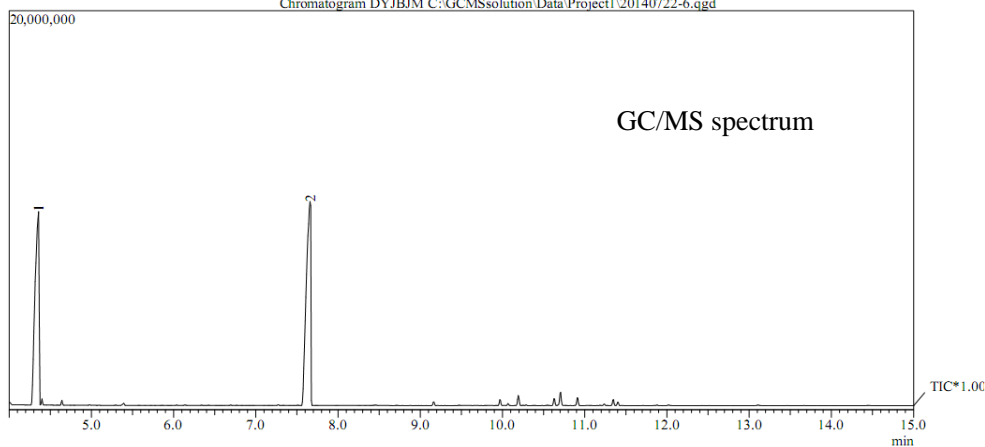
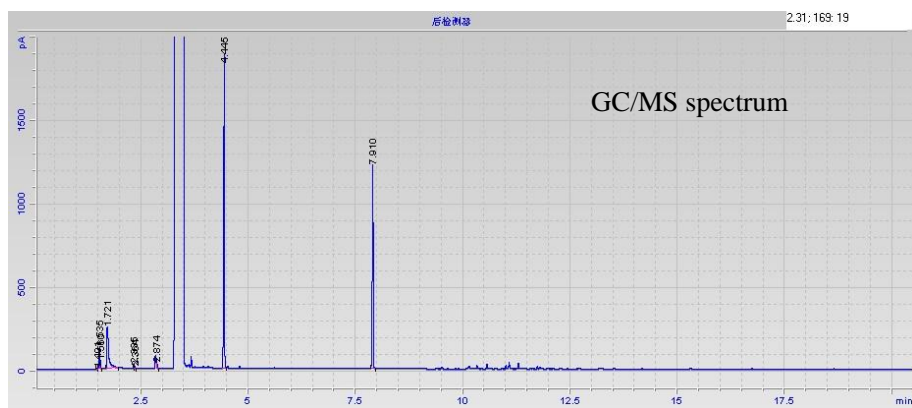
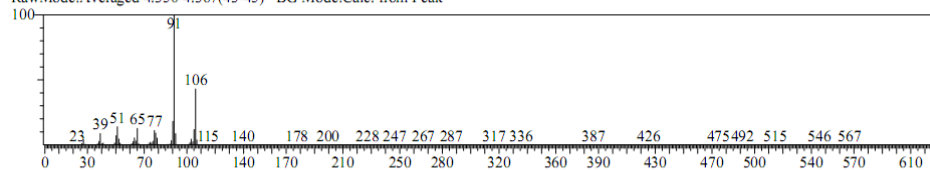


Figure S22. GC and GC/MS spectra of the reaction solution of 2-ethylanisole reduction.

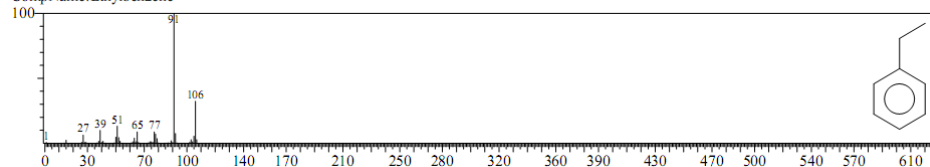


<< Target >>

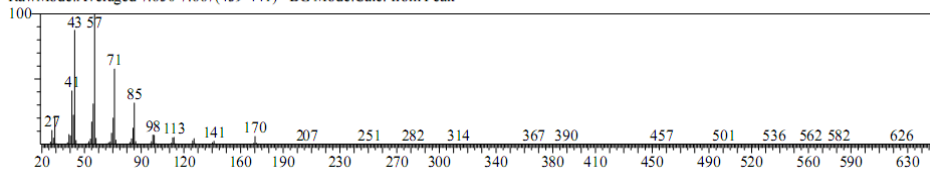
Line#:1 R.Time:4.358(Scan#:44) MassPeaks:149 BasePeak:91.10(2537739)
RawMode:Averaged 4.350-4.367(43-45) BG Mode:Calc. from Peak



Hit#:13 Entry:2121 Library:NIST21.LIB
SI:93 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
CompName:Ethylbenzene



Line#:2 R.Time:7.658(Scan#:440) MassPeaks:138 BasePeak:57.15(1802708)
RawMode:Averaged 7.650-7.667(439-441) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodecane

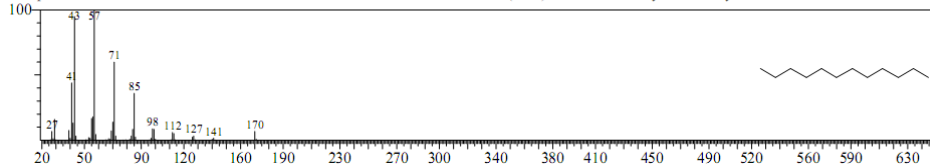


Figure S23. GC and GC/MS spectra of the reaction solution of 4-ethylanisole reduction.

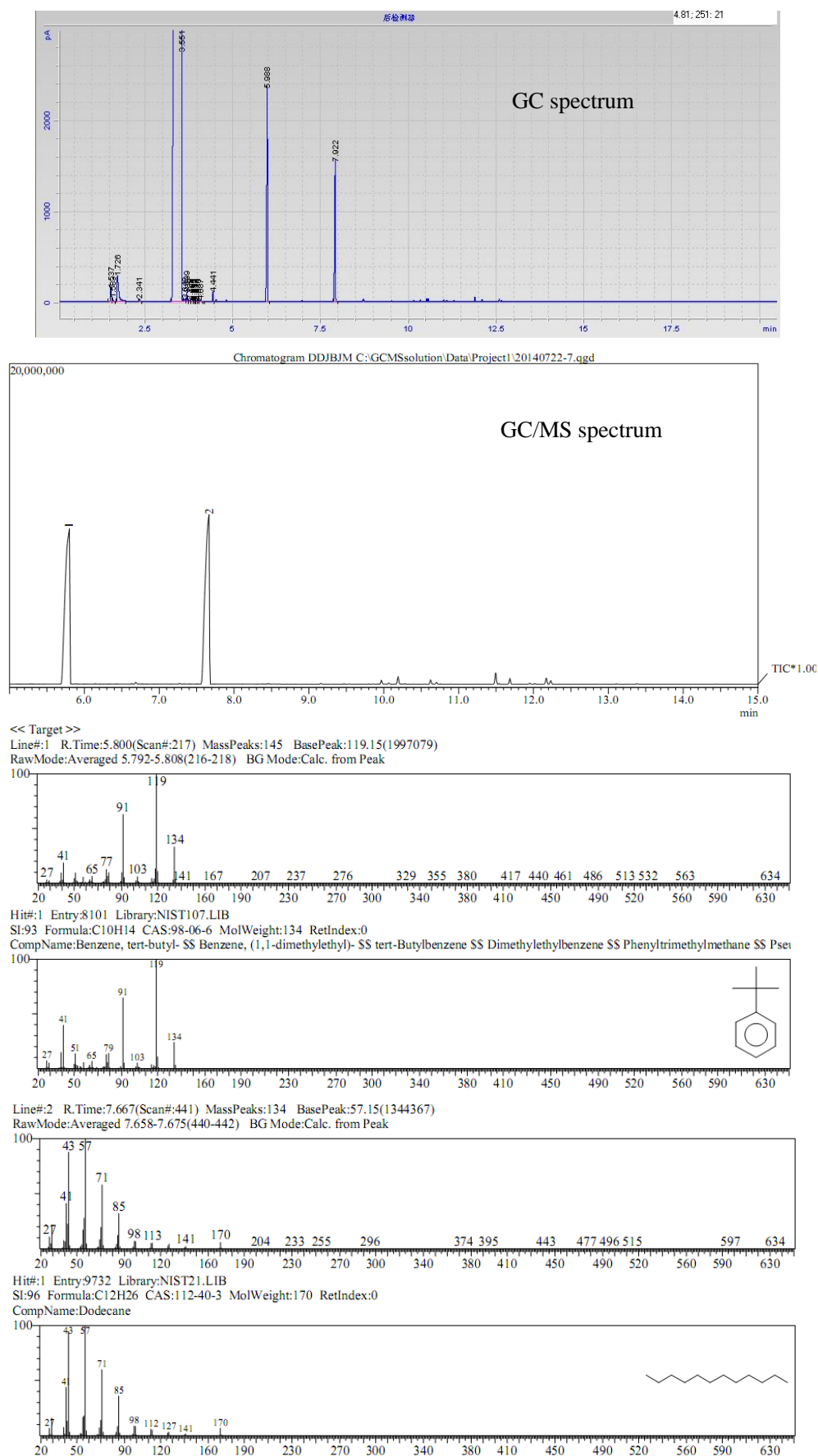
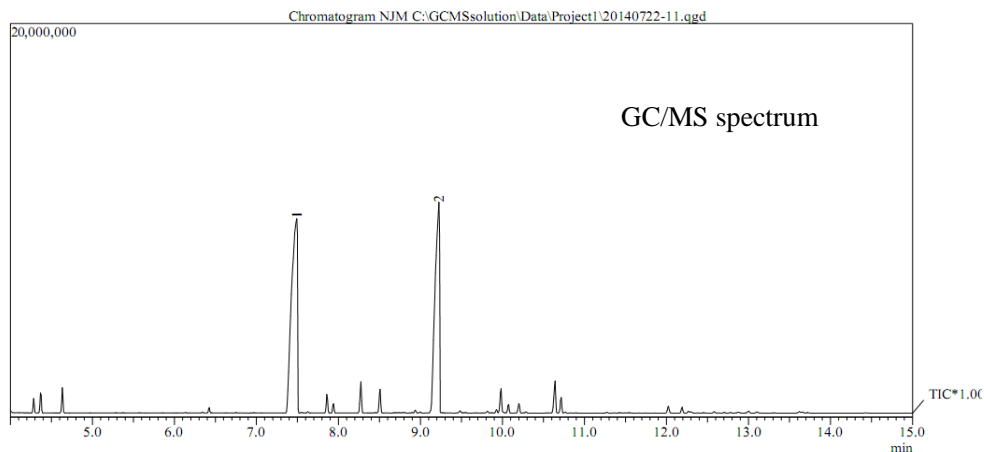
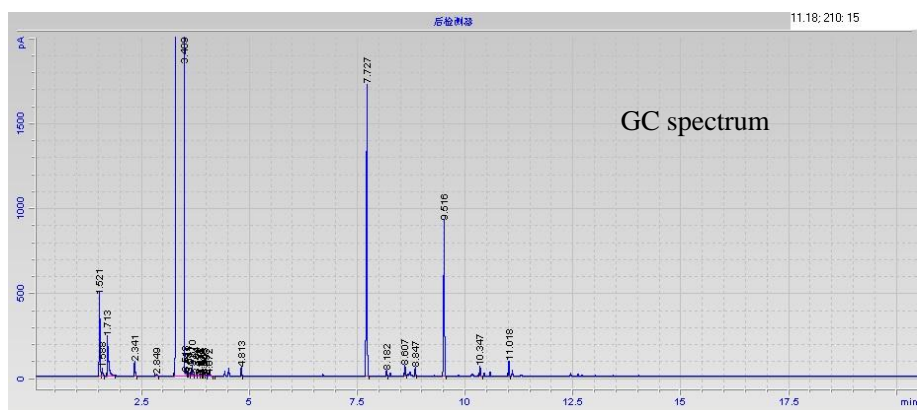


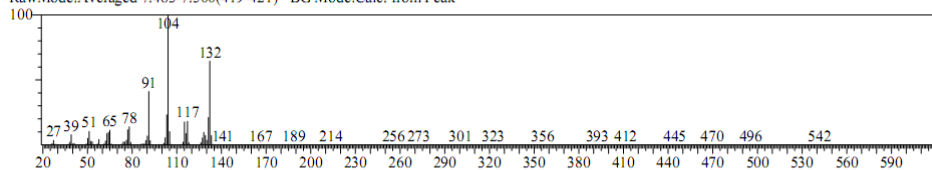
Figure S24. GC and GC/MS spectra of the reaction solution of 4-tert-butylanisole reduction.



<< Target >>

Line#:1 R.Time:7.492(Scan#:420) MassPeaks:156 BasePeak:104.10(1984975)

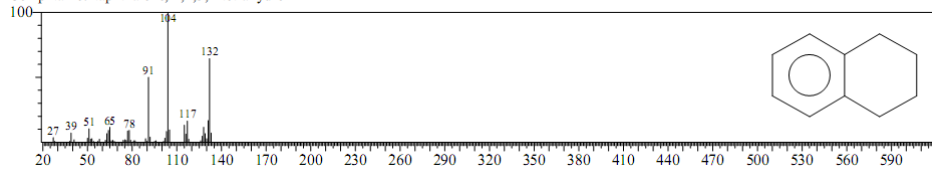
RawMode:Averaged 7.483-7.500(419-421) BG Mode:Calc. from Peak



Hit#:1 Entry:4855 Library:NIST1.LIB

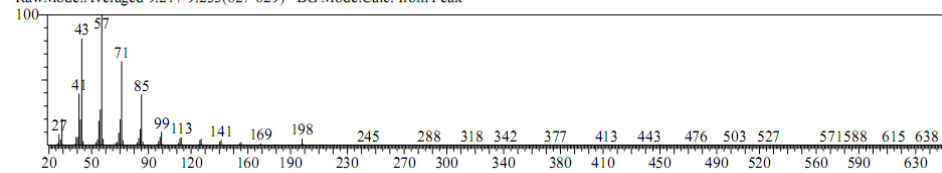
SI:94 Formula:C10H12 CAS:119-64-2 MolWeight:132 RetIndex:0

CompName:Naphthalene, 1,2,3,4-tetrahydro-



Line#:2 R.Time:9.225(Scan#:628) MassPeaks:157 BasePeak:57.15(1744054)

RawMode:Averaged 9.217-9.233(627-629) BG Mode:Calc. from Peak



Hit#:1 Entry:16432 Library:NIST08s.LIB

SI:96 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1413

CompName:Tetradecane SS n-Tetradecane SS

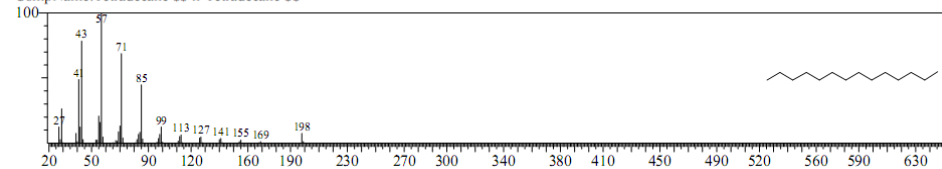
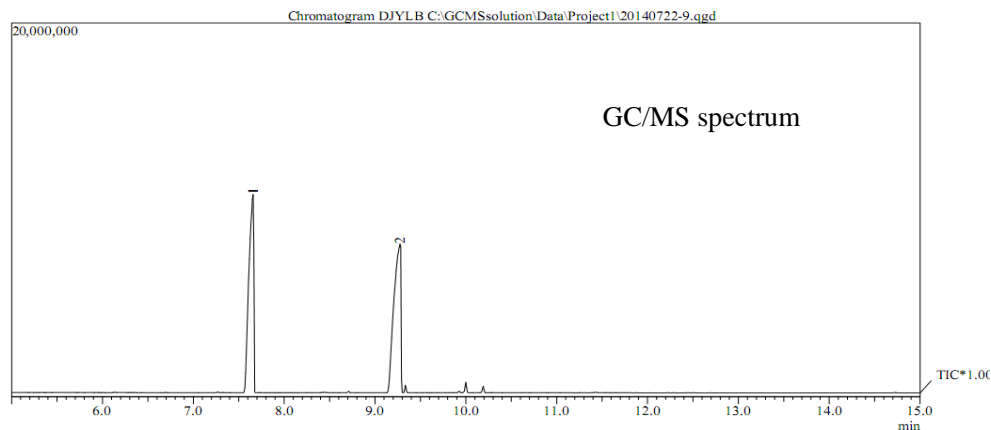
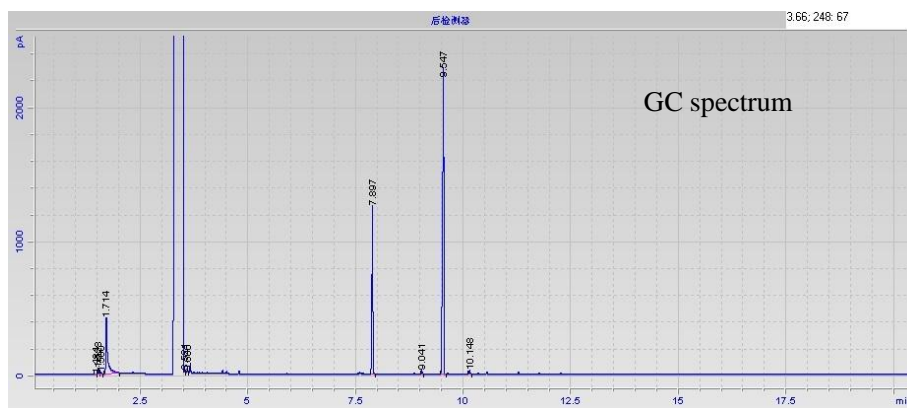
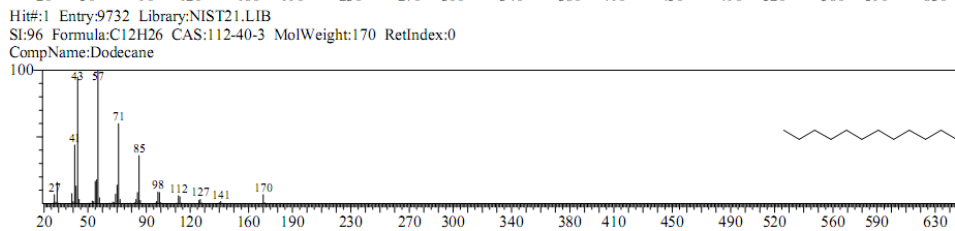
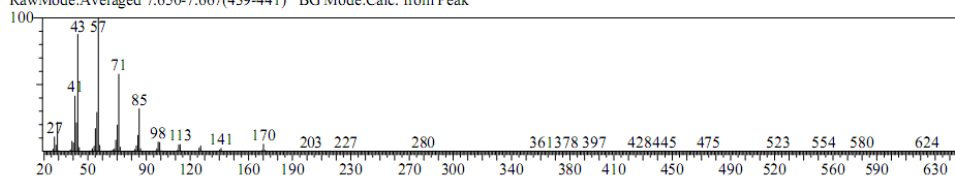


Figure S25. GC and GC/MS spectra of the reaction solution of 2-methoxynaphthalene reduction.



Line#:1 R.Time:7.658(Scan#:440) MassPeaks:140 BasePeak:57.15(1724467)
RawMode:Averaged 7.650-7.667(439-441) BG Mode:Calc. from Peak



Line#:2 R.Time:9.275(Scan#:634) MassPeaks:164 BasePeak:154.15(2232066)
RawMode:Averaged 9.267-9.283(633-635) BG Mode:Calc. from Peak

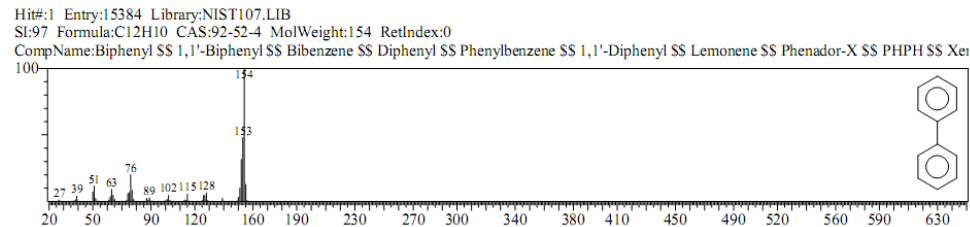
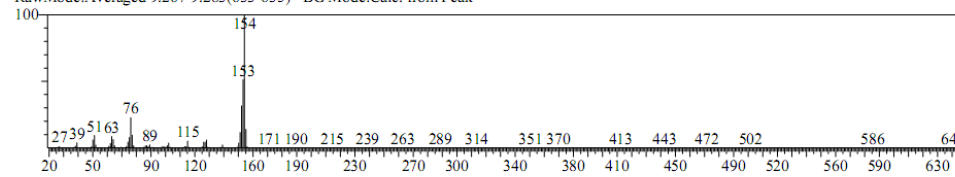


Figure S26. GC and GC/MS spectra of the reaction solution of 4-methoxybiphenyl reduction.

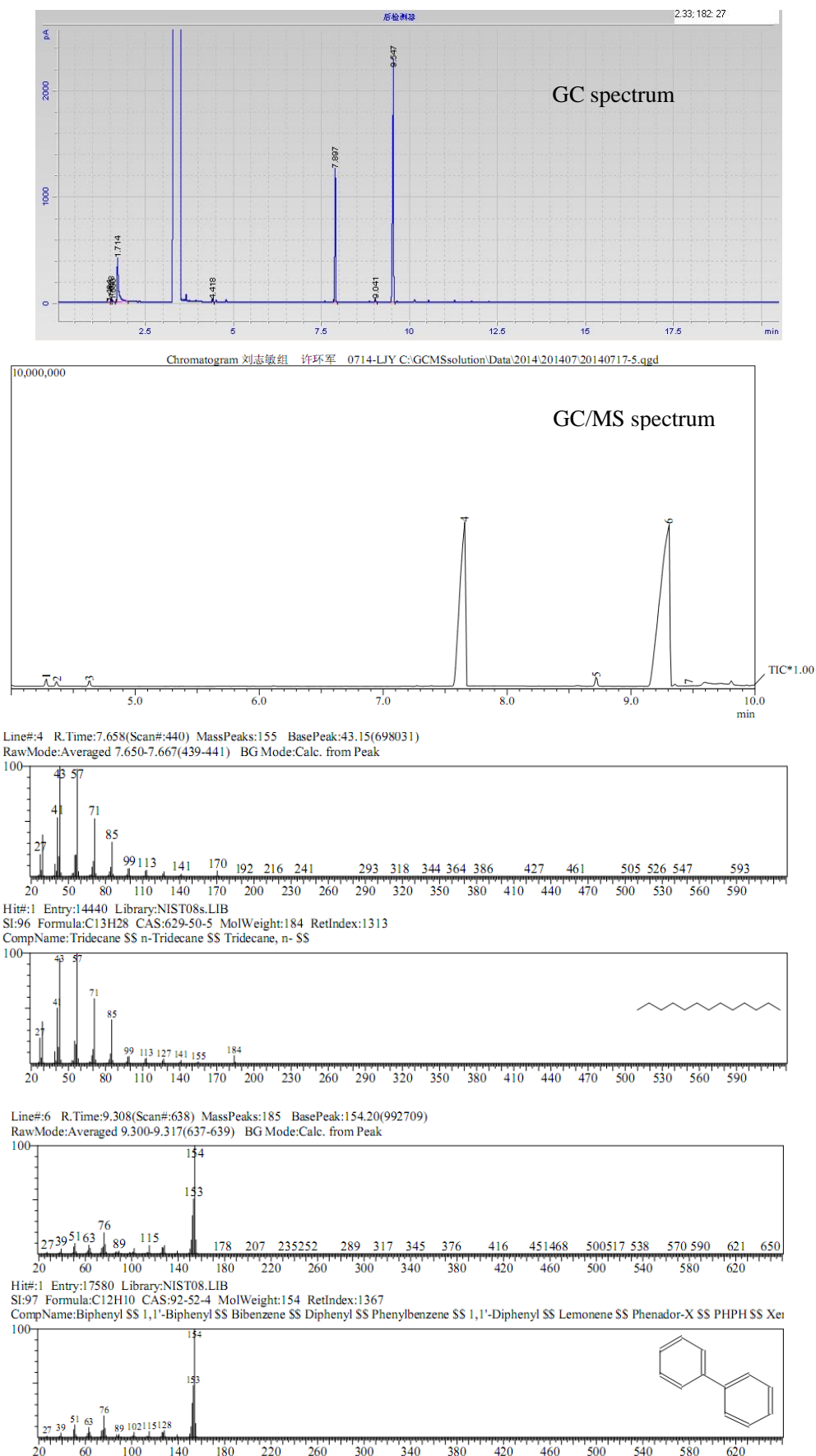
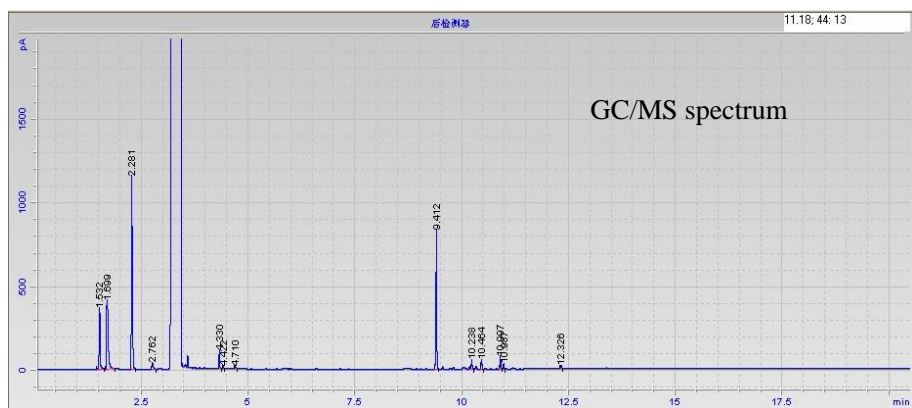
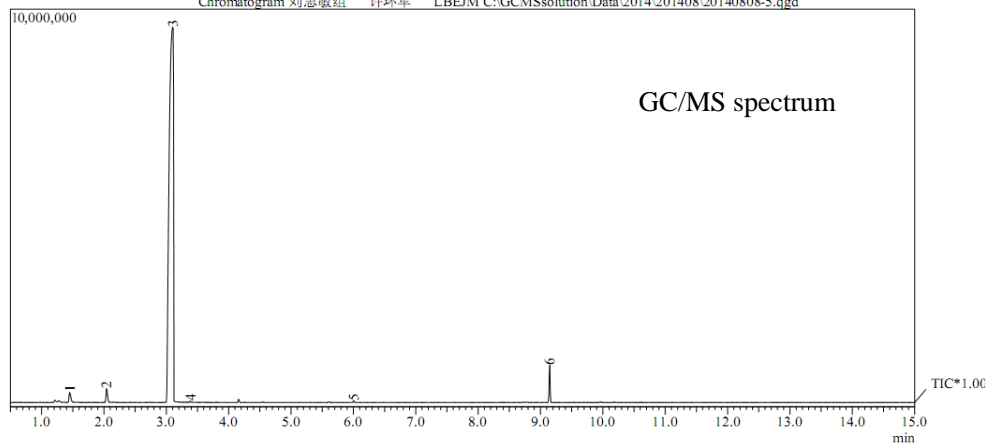


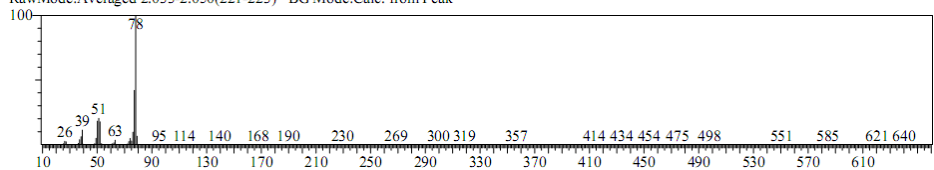
Figure S27. GC and GC/MS spectra of the reaction solution of 2-Methoxybiphenyl reduction.



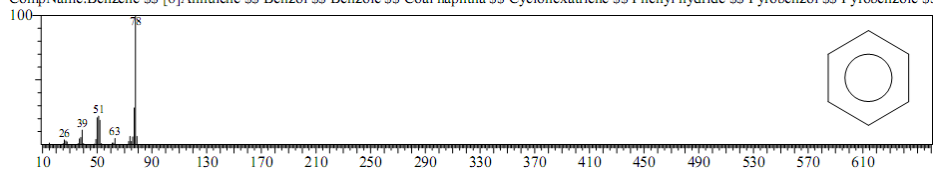
Chromatogram 刘志敏组 许环军 LBEJM C:\GCMSsolution\Data\2014\201408\20140808-5.qgd



Line#:2 R.Time:2.042(Scan#:222) MassPeaks:81 BasePeak:78.15(106217)
RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak

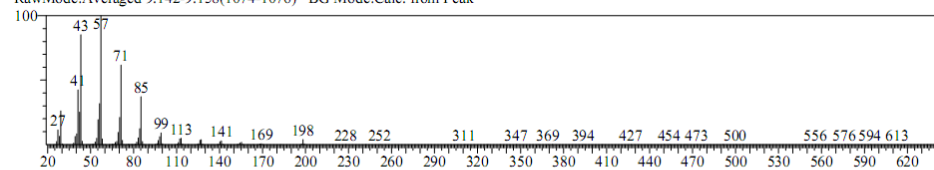


Hit#:1 Entry:467 Library:NIST147.LIB
SI:96 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S:



<< Target >>

Line#:6 R.Time:9.150(Scan#:1075) MassPeaks:118 BasePeak:57.15(105881)
RawMode:Averaged 9.142-9.158(1074-1076) BG Mode:Calc. from Peak



Hit#:1 Entry:16431 Library:NIST08s.LIB
SI:95 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1413
CompName:Tetradecane SS n-Tetradecane SS

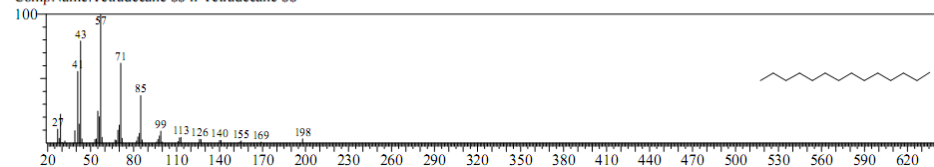


Figure S28. GC and GC/MS spectra of the reaction solution of 1,2-Dimethoxybenzene reduction.

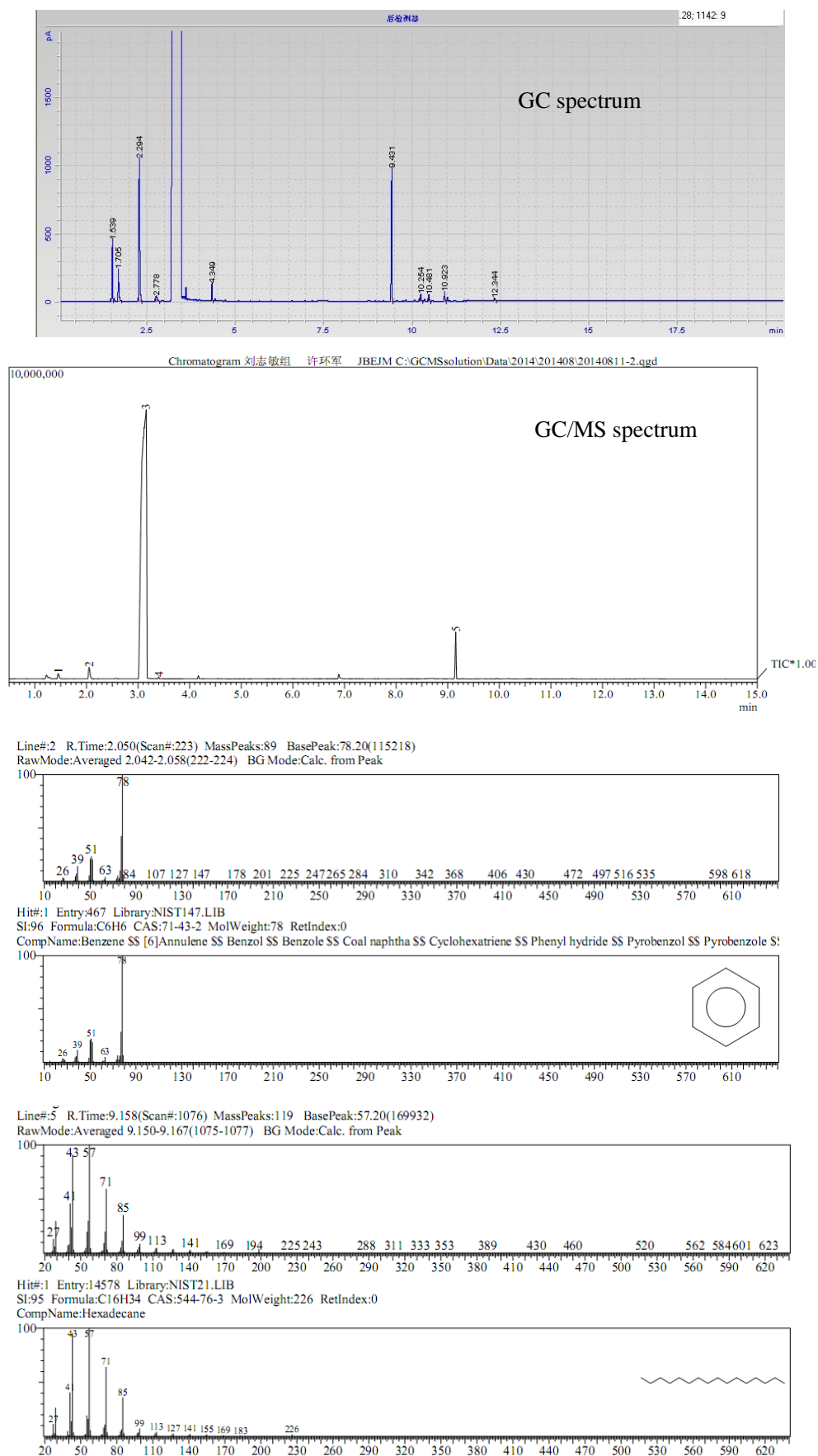
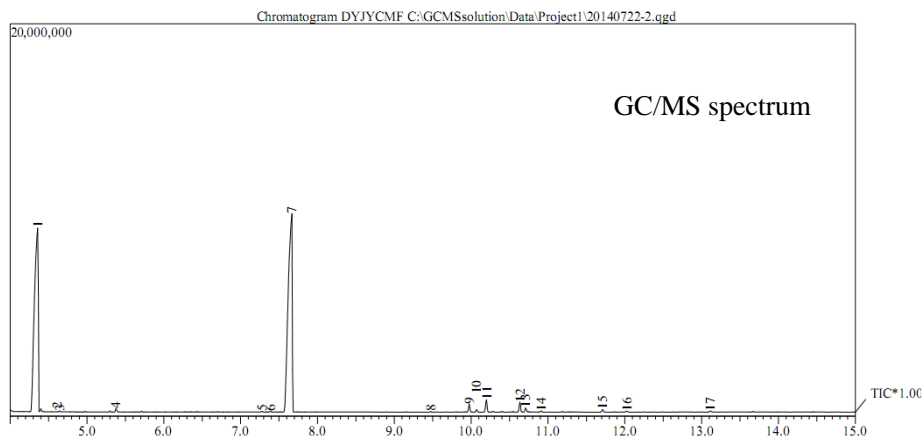
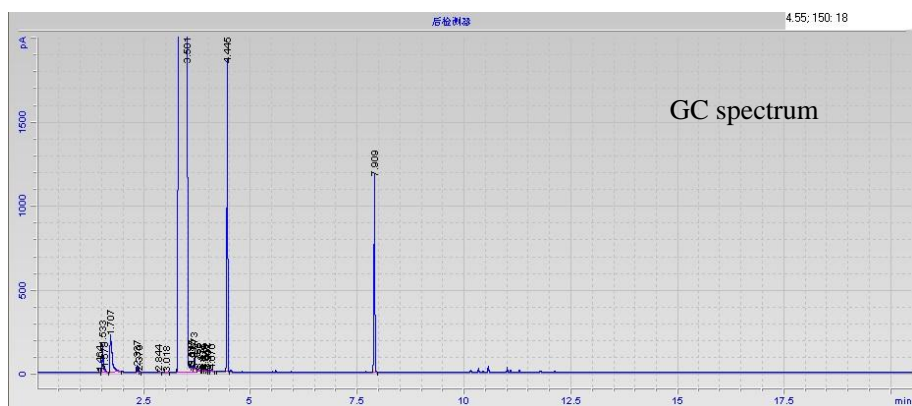
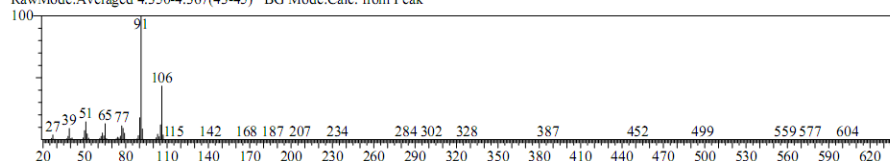


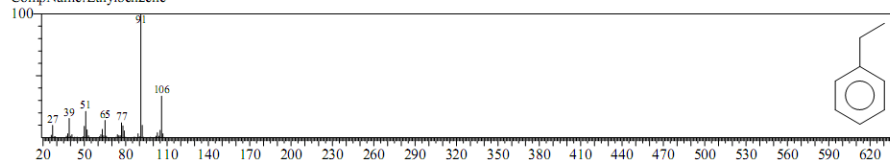
Figure S29. GC and GC/MS spectra of the reaction solution of 1, 3-dimethoxybenzene reduction.



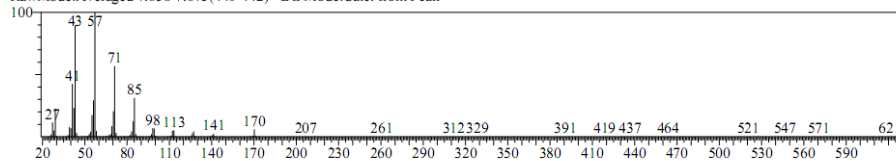
Line#:1 R.Time:4.358(Scan#:44) MassPeaks:142 BasePeak:91.15(2698170)
RawMode:Averaged 4.350-4.367(43-45) BG Mode:Calc. from Peak



Hit#:9 Entry:2122 Library:NIST21.LIB
SI:94 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
CompName:Ethylbenzene



Line#:7 R.Time:7.667(Scan#:441) MassPeaks:139 BasePeak:57.15(1316430)
RawMode:Averaged 7.658-7.675(440-442) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodecane

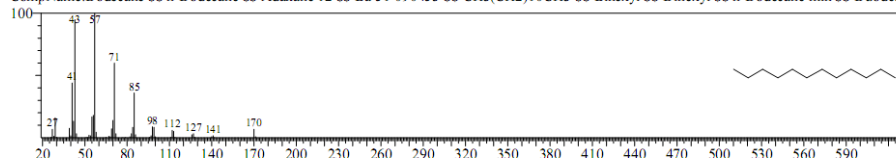
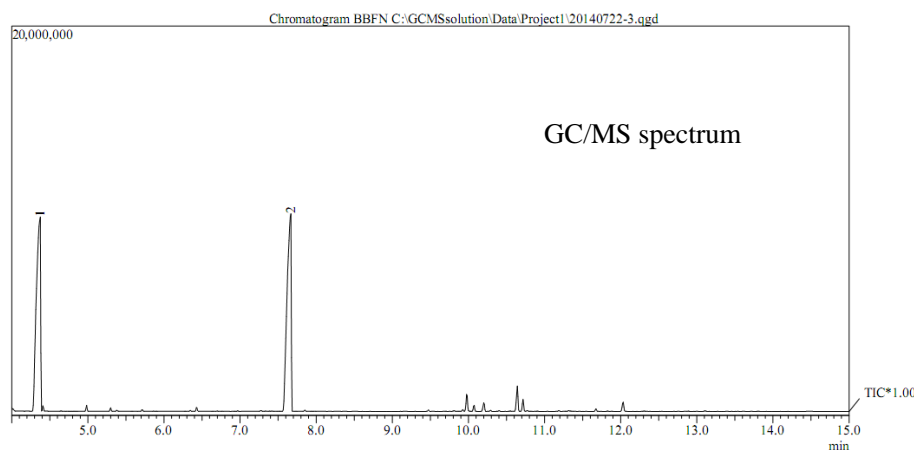
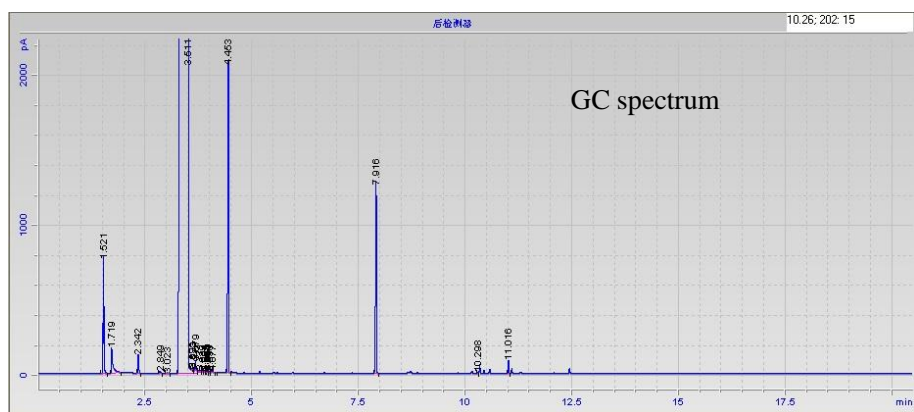
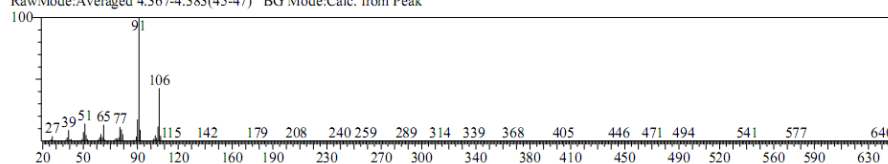


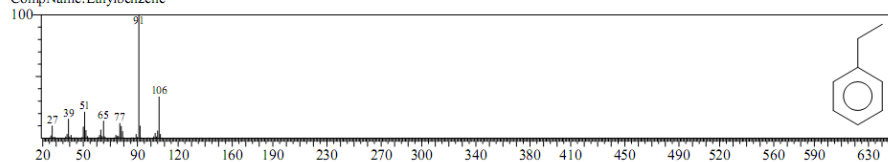
Figure S30. GC and GC/MS spectra of the reaction solution of 4-ethylguaiacol reduction.



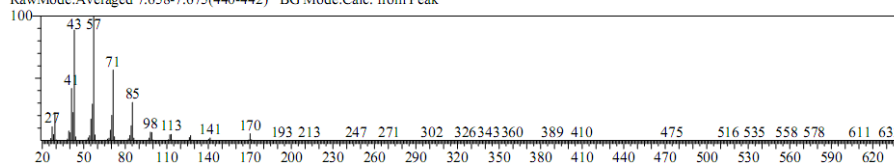
Line#:1 R.Time:4.375(Scan#:46) MassPeaks:135 BasePeak:91.10(2503628)
RawMode:Averaged 4.367-4.383(45-47) BG Mode:Calc. from Peak



Hit#:9 Entry:2122 Library:NIST21.LIB
SI:94 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
CompName:Ethylbenzene



Line#:2 R.Time:7.667(Scan#:441) MassPeaks:152 BasePeak:57.15(1374662)
RawMode:Averaged 7.658-7.675(440-442) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane

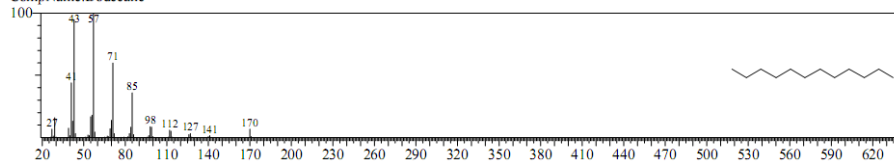
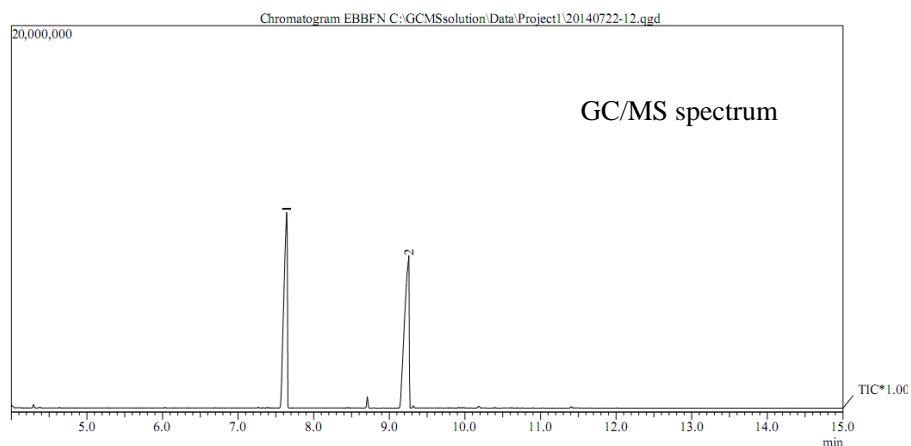
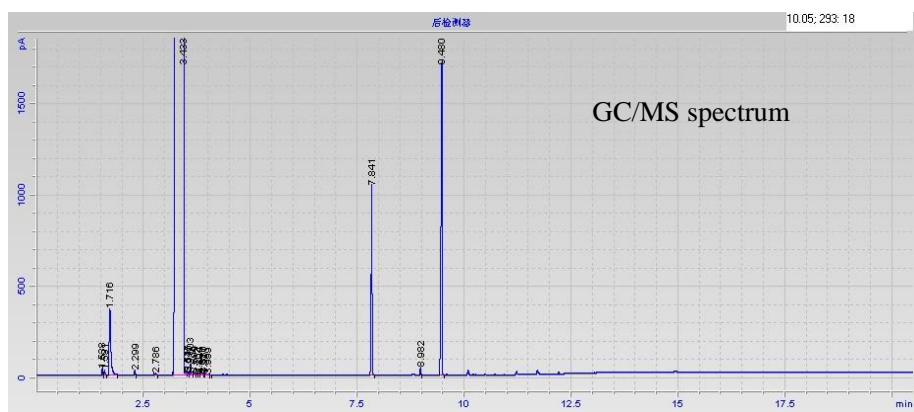
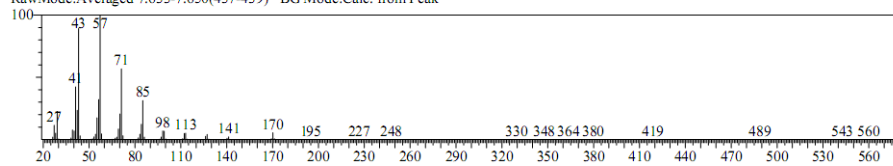


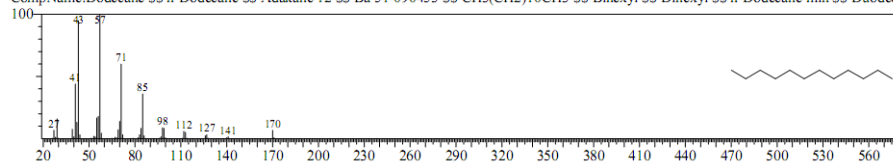
Figure S31. GC and GC/MS spectra of the reaction solution of benzofuran reduction.



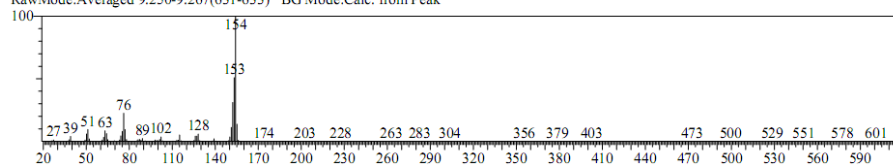
Line#:1 R.Time:7.642(Scan#:438) MassPeaks:132 BasePeak:57.15(1678452)
RawMode:Averaged 7.633-7.650(437-439) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodecane



Line#:2 R.Time:9.258(Scan#:632) MassPeaks:163 BasePeak:154.15(1627183)
RawMode:Averaged 9.250-9.267(631-633) BG Mode:Calc. from Peak



Hit#:1 Entry:15384 Library:NIST107.LIB
SI:97 Formula:C12H10 CAS:92-52-4 MolWeight:154 RetIndex:0
CompName:Biphenyl SS 1,1'-Biphenyl SS Bibenzene SS Diphenyl SS Phenylbenzene SS 1,1'-Diphenyl SS Lemonene SS Phenador-X SS PPHP SS Xei

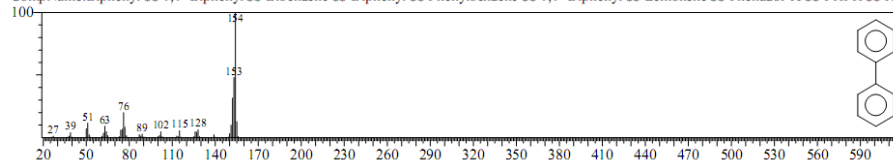
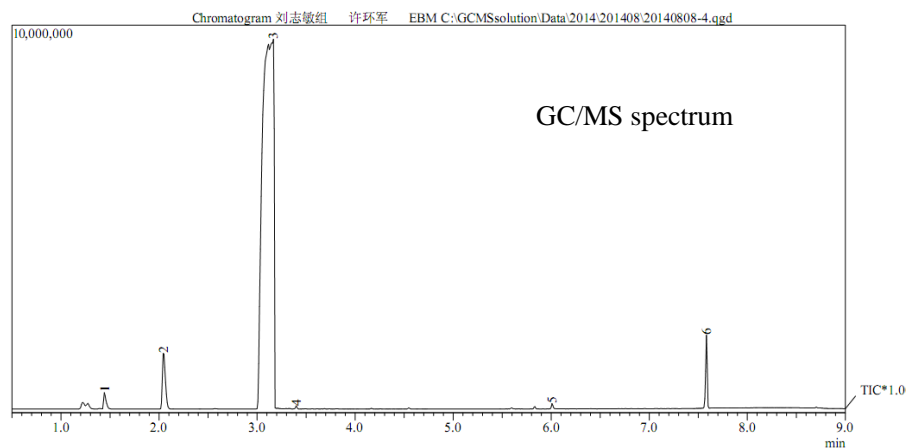
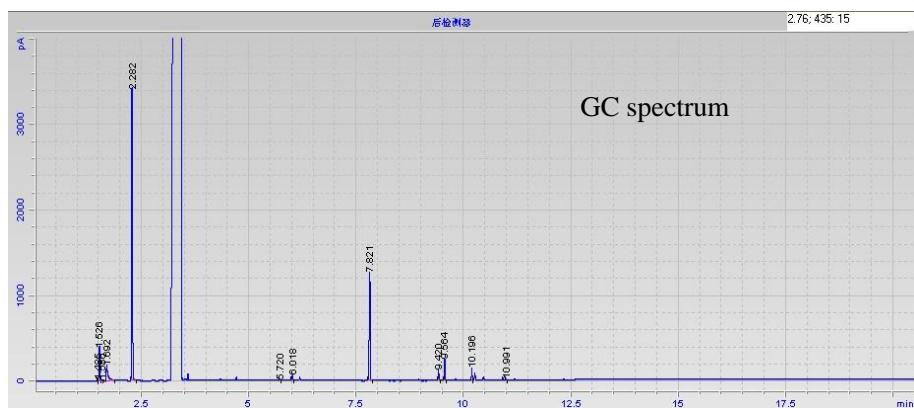
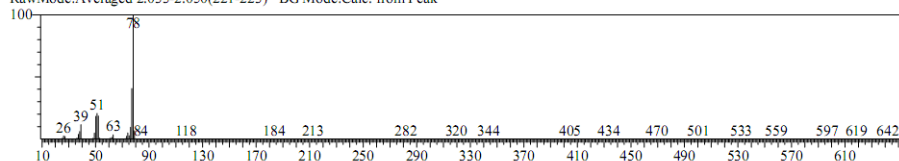


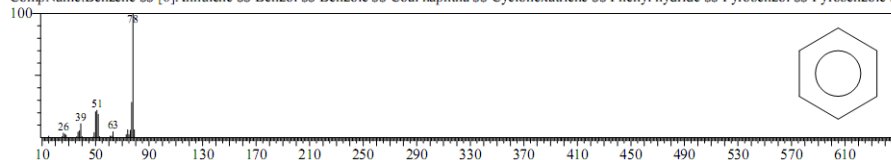
Figure S32. GC and GC/MS spectra of the reaction solution of Dibenzofuran reduction.



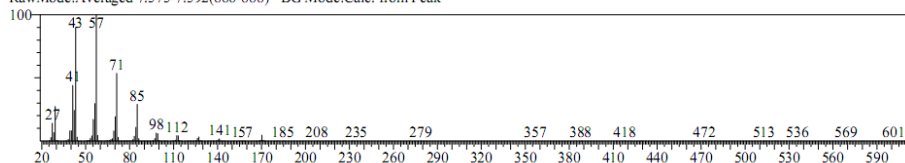
Line#:2 R.Time:2.042(Scan#:222) MassPeaks:73 BasePeak:78.15(463439)
RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak



Hit#:1 Entry:467 Library:NIST147.LIB
SI:97 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



Line#:6 R.Time:7.583(Scan#:887) MassPeaks:130 BasePeak:57.20(237885)
RawMode:Averaged 7.575-7.592(886-888) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodec

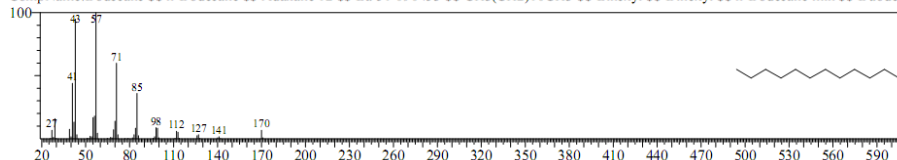
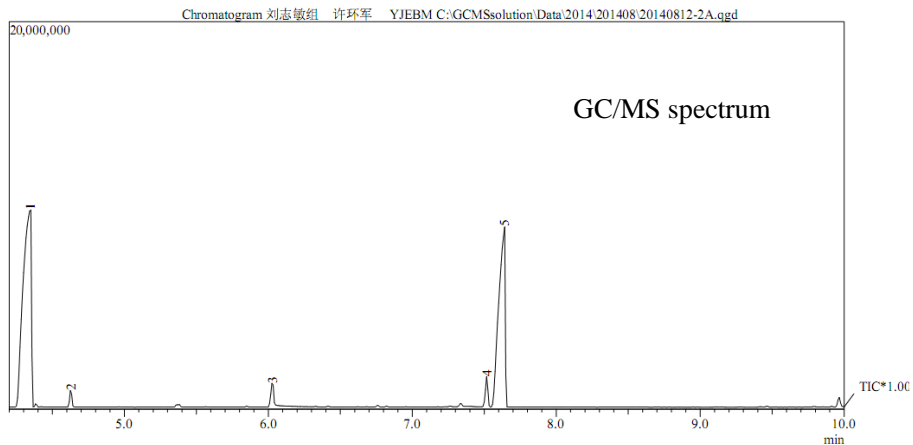
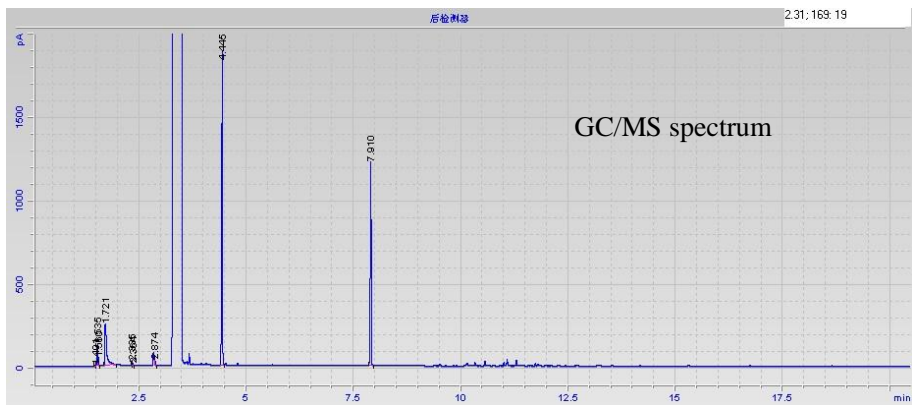
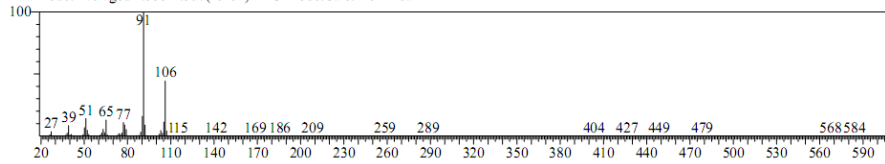


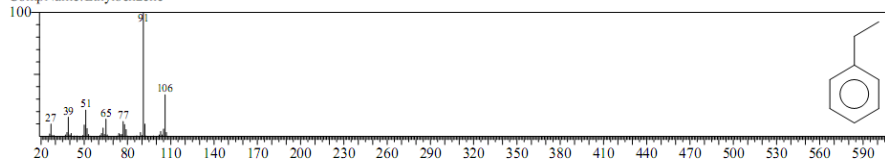
Figure S33. GC and GC/MS spectra of the reaction solution of Diphenyl ether reduction.



<< Target >>
 Line#:1 R.Time:4.342(Scan#:30) MassPeaks:120 BasePeak:91.15(3309574)
 RawMode:Averaged 4.333-4.350(29-31) BG Mode:Calc. from Peak

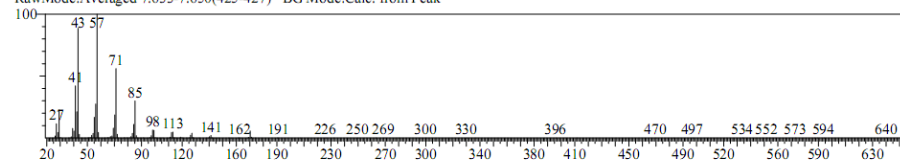


Hit#:9 Entry:2122 Library:NIST21.LIB
 SI:94 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
 CompName:Ethylbenzene



<< Target >>

Line#:5 R.Time:7.642(Scan#:426) MassPeaks:147 BasePeak:57.15(1199994)
 RawMode:Averaged 7.633-7.650(425-427) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
 SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
 CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodec

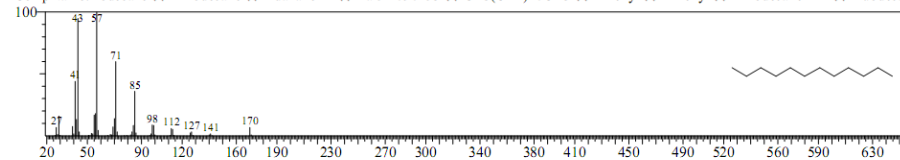
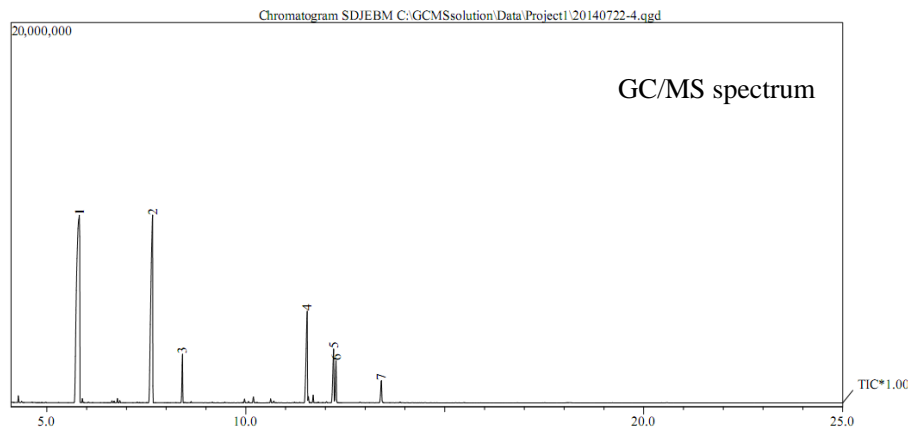
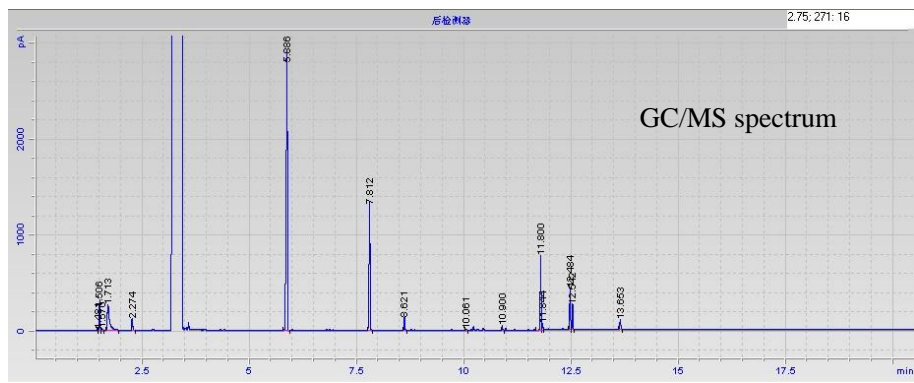
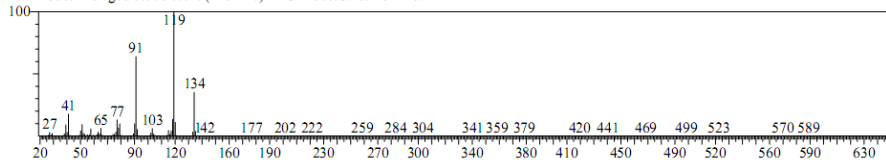


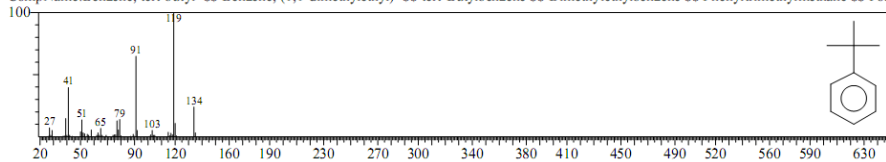
Figure S34. GC and GC/MS spectra of the reaction solution of Di-4-ethylphenyl ether reduction.



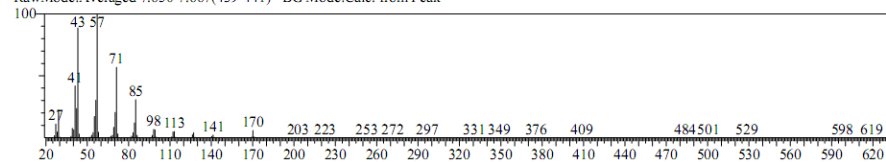
Line#:1 R.Time:5.817(Scan#:219) MassPeaks:141 BasePeak:119.15(2420064)
RawMode:Averaged 5.808-5.825(218-220) BG Mode:Calc. from Peak



Hit#:1 Entry:8101 Library:NIST07.LIB
SI:93 Formula:C10H14 CAS:98-06-6 MolWeight:134 RetIndex:0
CompName:Benzene, tert-butyl- SS Benzene, (1,1-dimethylethyl)- SS tert-Butylbenzene SS Dimethylethylbenzene SS Phenyltrimethylmethane SS Pse



Line#:2 R.Time:7.658(Scan#:440) MassPeaks:144 BasePeak:57.15(1206759)
RawMode:Averaged 7.650-7.667(439-441) BG Mode:Calc. from Peak



Hit#:1 Entry:12263 Library:NIST08s.LIB
SI:96 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodec

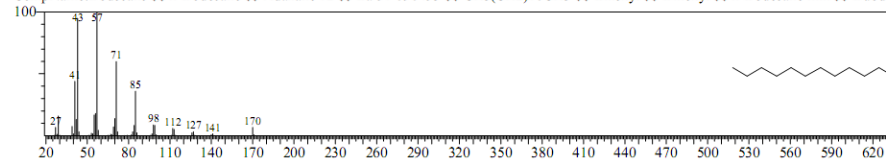
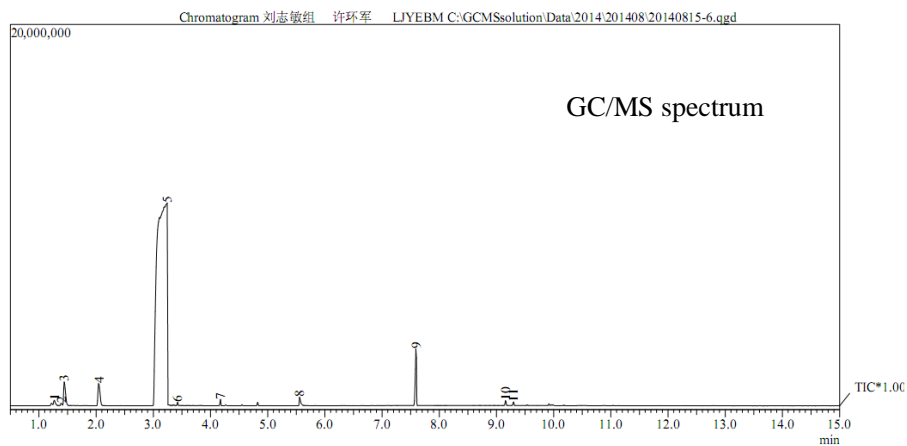
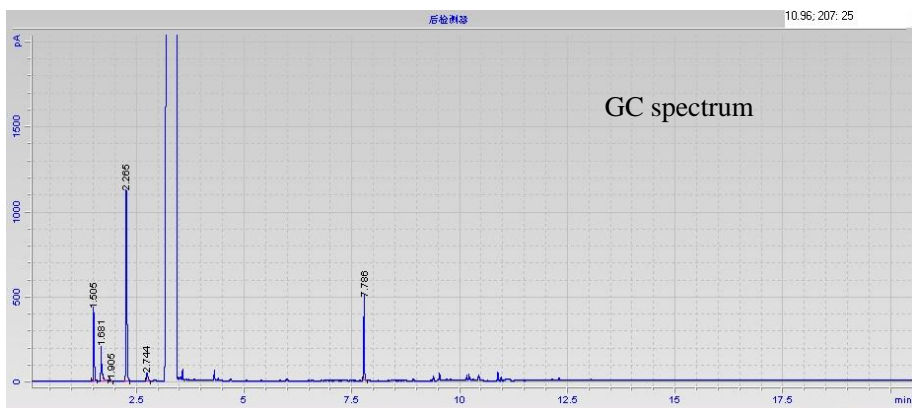
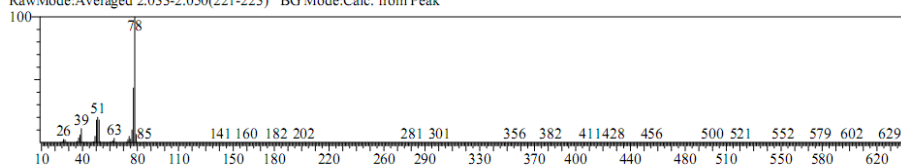


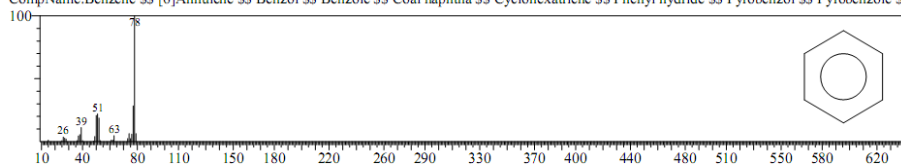
Figure S35. GC and GC/MS spectra of the reaction solution of Di-4-tert-butylphenyl ether reduction.



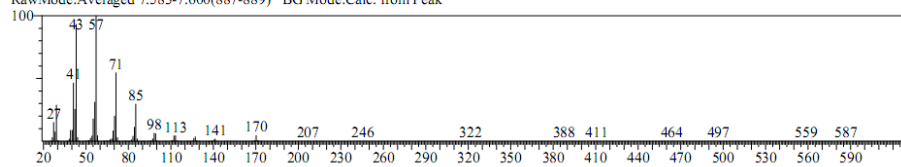
Line#:4 R.Time:2.042(Scan#:222) MassPeaks:80 BasePeak:78.15(388339)
RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak



Hit#:1 Entry:467 Library:NIST147.LIB
SI:96 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



Line#:9 R.Time:7.592(Scan#:888) MassPeaks:119 BasePeak:57.20(422147)
RawMode:Averaged 7.583-7.600(887-889) BG Mode:Calc. from Peak



Hit#:1 Entry:9732 Library:NIST21.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:0
CompName:Dodecane

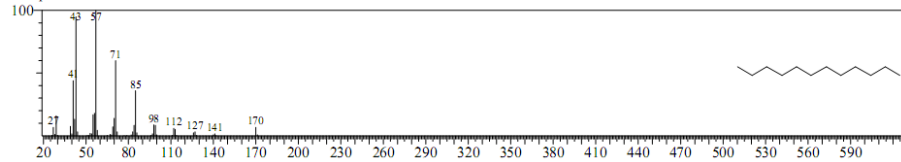
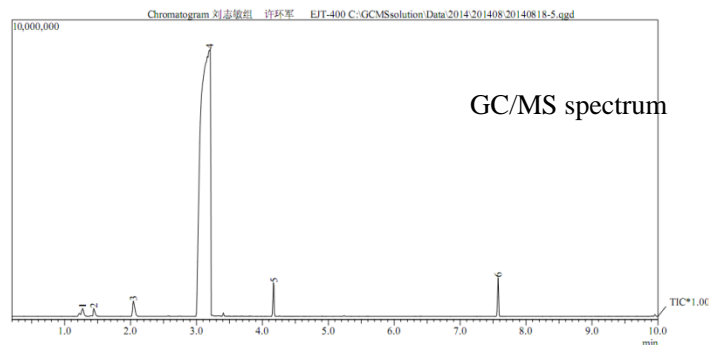
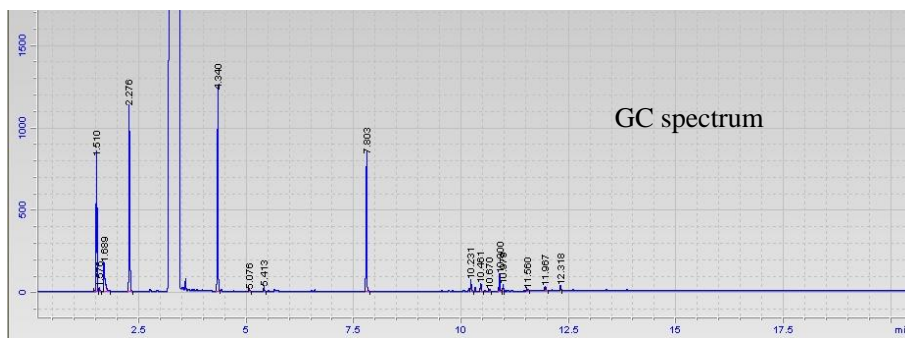
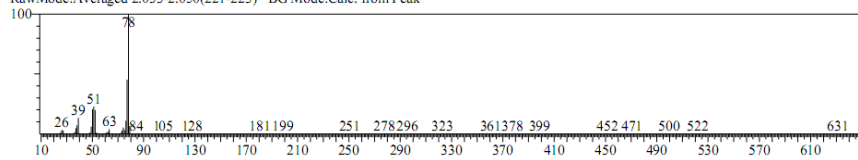


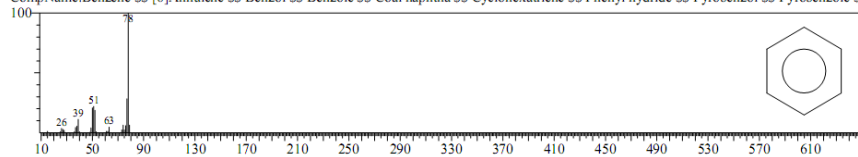
Figure S36. GC and GC/MS spectra of the reaction solution of Di-2-methoxyphenyl ether reduction.



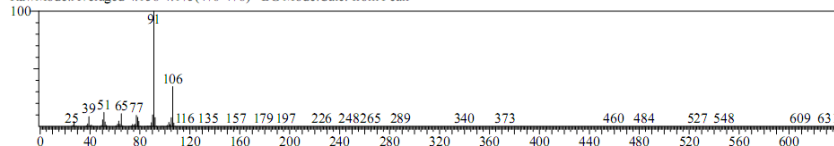
Line#:3 R.Time:2.042(Scan#:222) MassPeaks:78 BasePeak:78.15(163015)
RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak



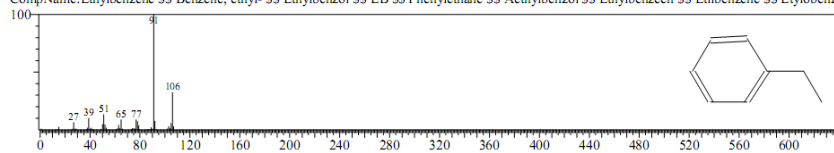
Hit#:1 Entry:467 Library:NIST147.LIB
SI:96 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



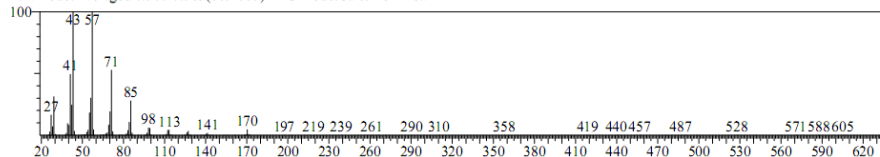
Line#:5 R.Time:4.167(Scan#:477) MassPeaks:101 BasePeak:91.15(325644)
RawMode:Averaged 4.158-4.175(476-478) BG Mode:Calc. from Peak



Hit#:1 Entry:2359 Library:NIST08s.LIB
SI:96 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:893
CompName:Ethylbenzene SS Benzene, ethyl- SS Ethylbenzol SS EB SS Phenylethane SS Aethylbenzol SS Ethylbenzene SS Etibenzene SS Etylbenze



Line#:6 R.Time:7.575(Scan#:886) MassPeaks:111 BasePeak:43.20(160773)
RawMode:Averaged 7.567-7.583(885-887) BG Mode:Calc. from Peak



Hit#:1 Entry:12254 Library:NIST08s.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodec

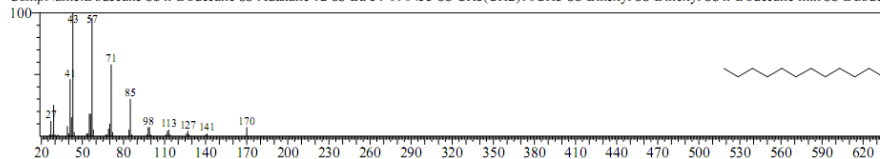
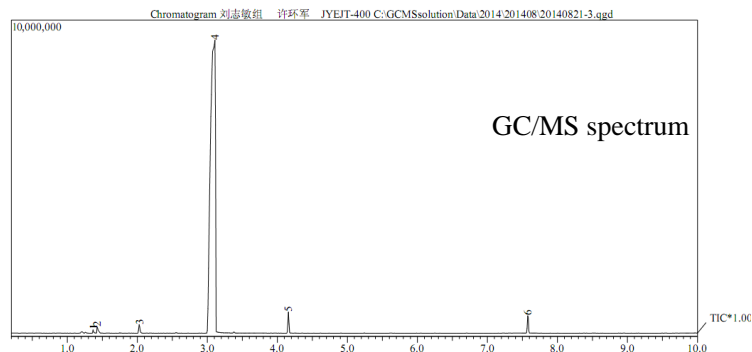
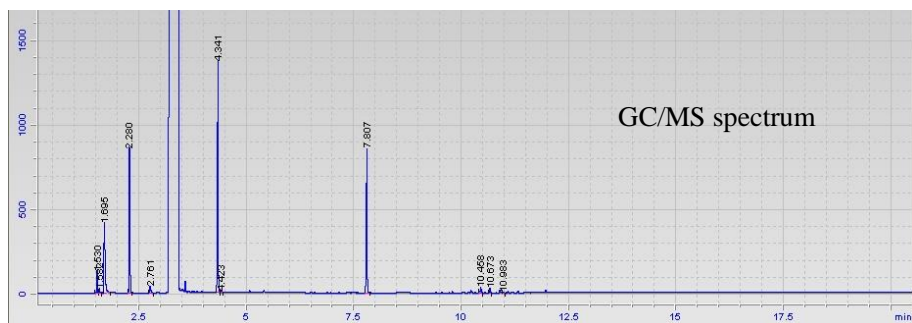
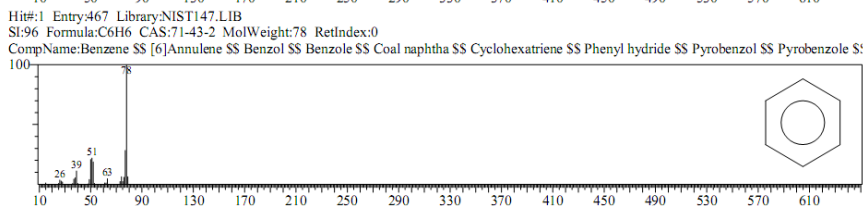
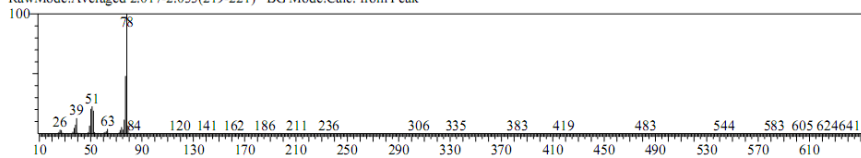


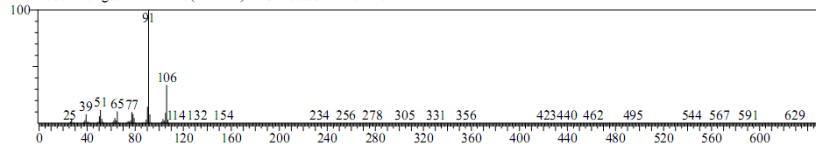
Figure S37. GC and GC/MS spectra of the reaction solution of 2-phenoxy-1-phenethanol reduction.



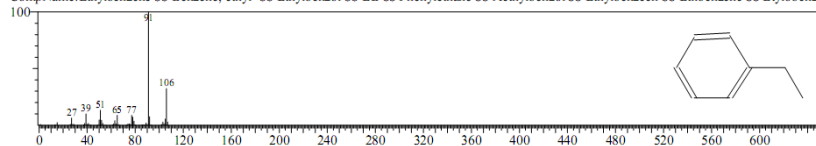
Line#:5 R.Time:2.025(Scan#:220) MassPeaks:74 BasePeak:78.15(66569)
RawMode:Averaged 2.017-2.033(219-221) BG Mode:Calc. from Peak



Line#:5 R.Time:4.158(Scan#:476) MassPeaks:109 BasePeak:91.15(160324)
RawMode:Averaged 4.150-4.167(475-477) BG Mode:Calc. from Peak



Line#:6 R.Time:7.575(Scan#:886) MassPeaks:120 BasePeak:57.20(65378)
RawMode:Averaged 7.567-7.583(885-887) BG Mode:Calc. from Peak



Line#:6 R.Time:7.575(Scan#:886) MassPeaks:120 BasePeak:57.20(65378)
RawMode:Averaged 7.567-7.583(885-887) BG Mode:Calc. from Peak

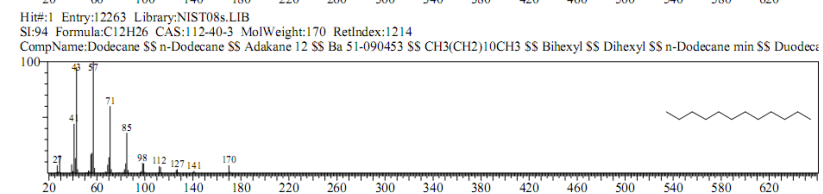
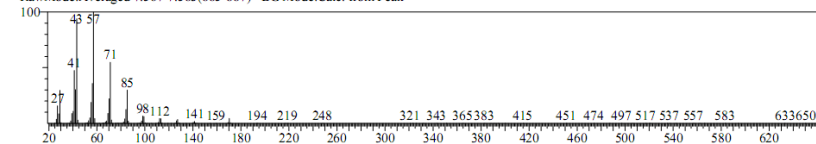
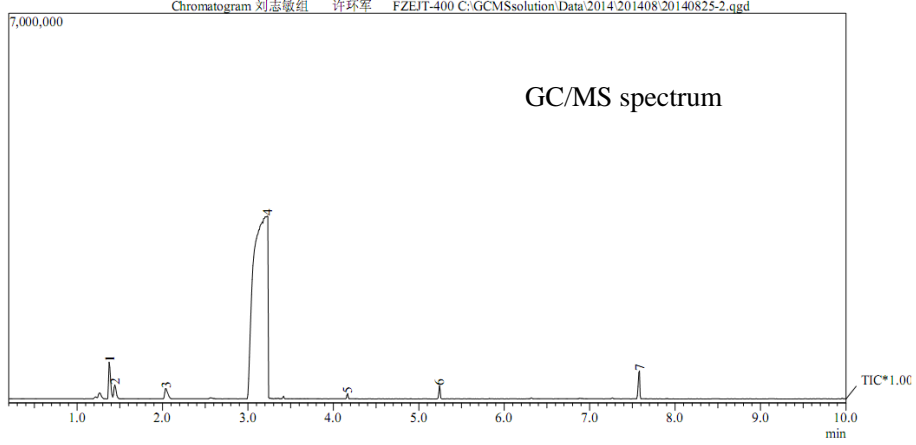
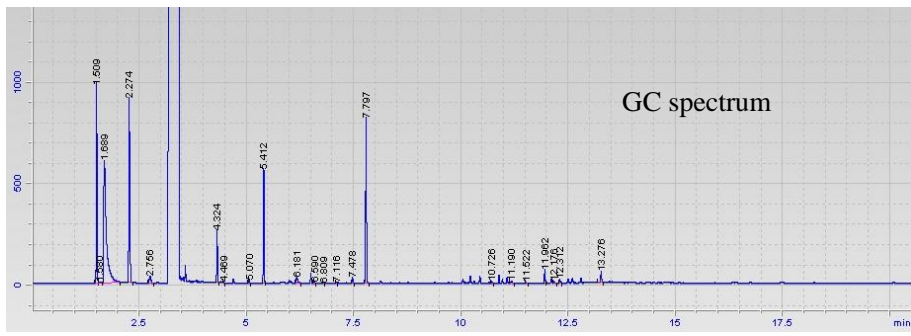
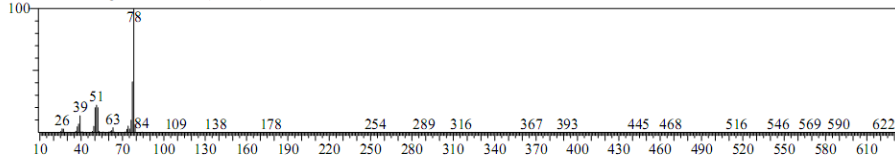


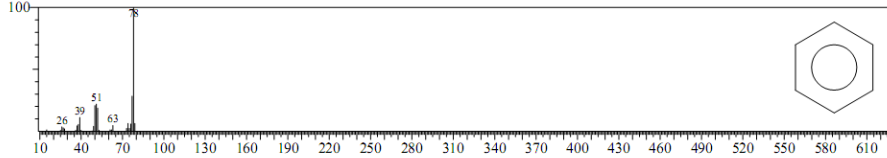
Figure S38. GC and GC/MS spectra of the reaction solution of 2-(2-methoxyphenoxy)-1-phenylethanol reduction.



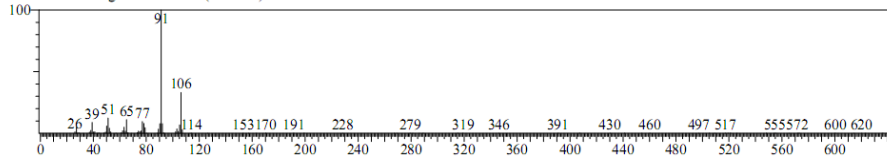
Line#:3 R.Time:2.042(Scan#:222) MassPeaks:82 BasePeak:78.15(61513)
RawMode:Averaged 2.033-2.050(221-223) BG Mode:Calc. from Peak



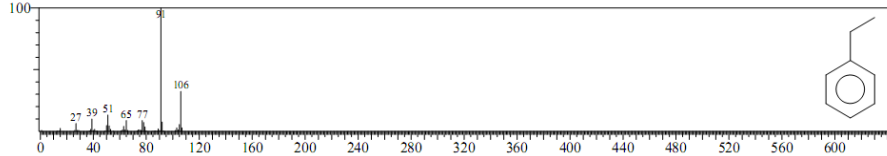
Hit#:1 Entry:467 Library:NIST147.LIB
SI:97 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



Line#:5 R.Time:4.167(Scan#:477) MassPeaks:89 BasePeak:91.20(24422)
RawMode:Averaged 4.158-4.175(476-478) BG Mode:Calc. from Peak



Hit#:1 Entry:2121 Library:NIST21.LIB
SI:96 Formula:C8H10 CAS:100-41-4 MolWeight:106 RetIndex:0
CompName:Ethylbenzene



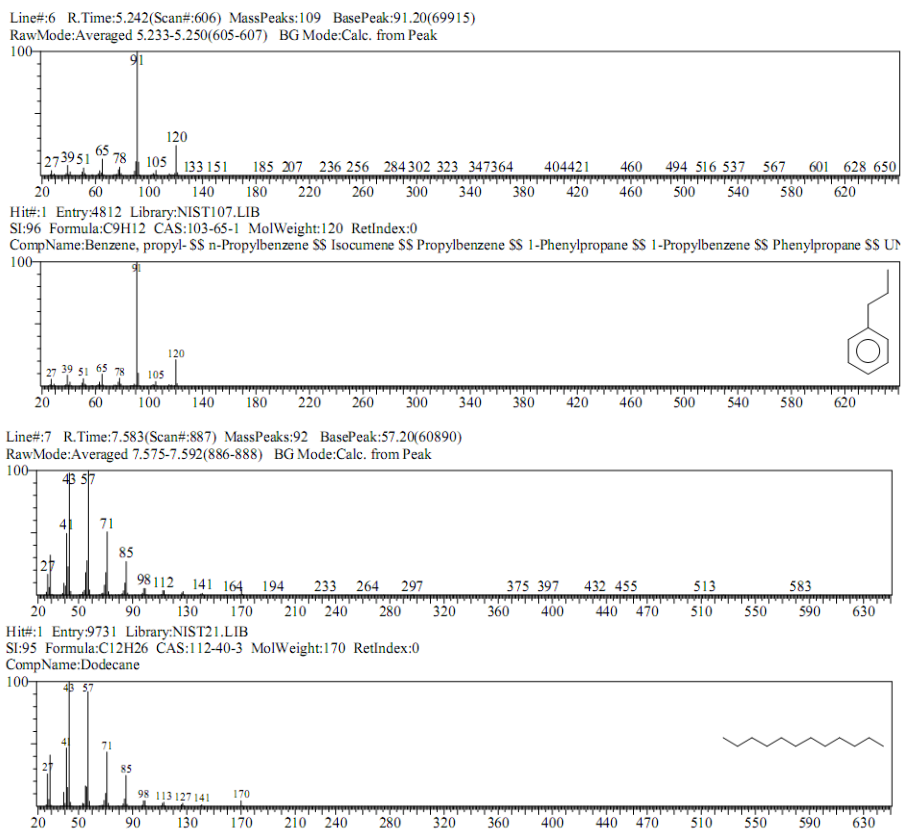
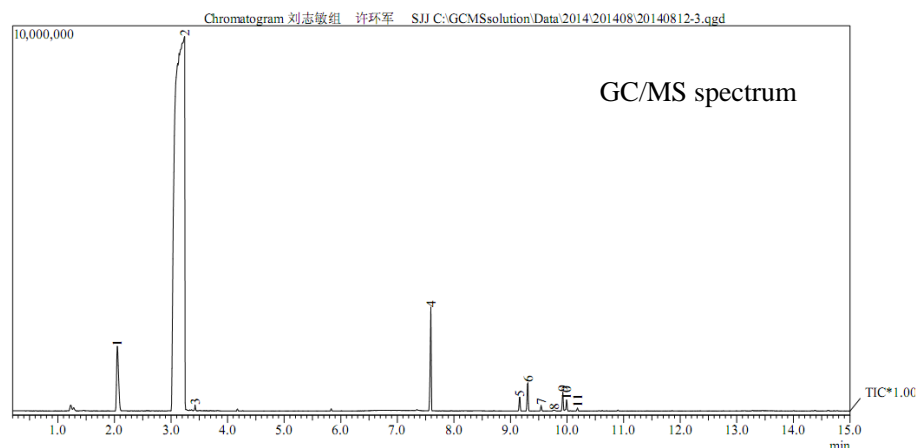
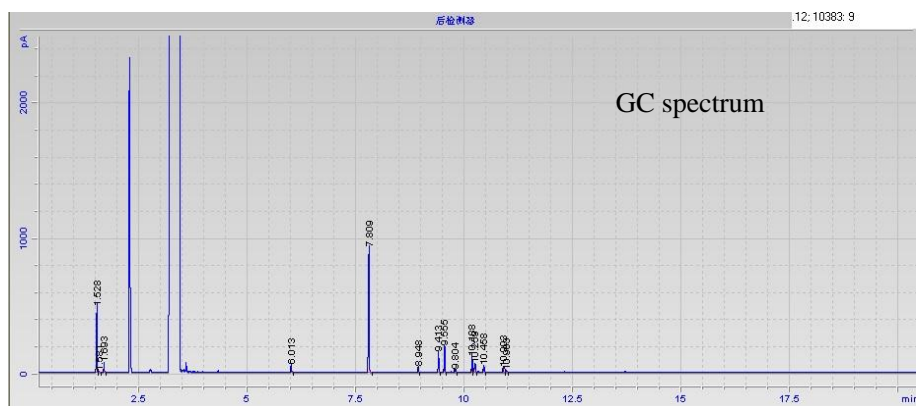
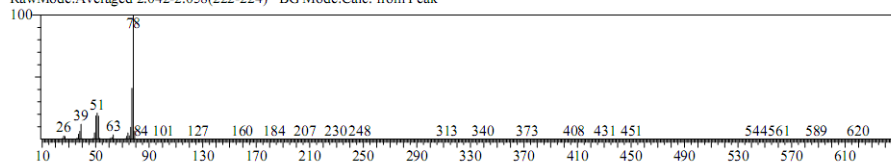


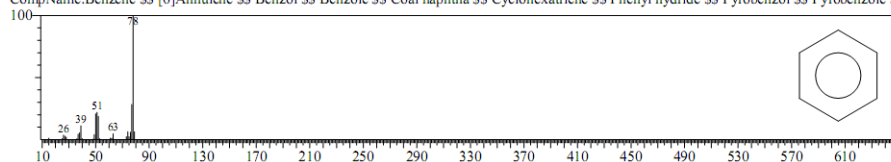
Figure S39. GC and GC/MS spectra of the reaction solution of 2-phenoxy-1-phenylpropane-1, 3-diol reduction.



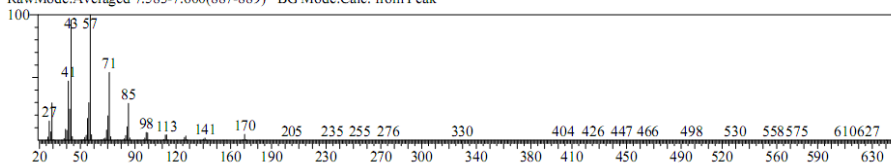
Line#:1 R.Time:2.050(Scan#:223) MassPeaks:99 BasePeak:(8.125/2203)
RawMode:Averaged 2.042-2.058(222-224) BG Mode:Calc. from Peak



Hit#:1 Entry:467 Library:NIST147.LIB
SI:97 Formula:C6H6 CAS:71-43-2 MolWeight:78 RetIndex:0
CompName:Benzene SS [6]Annulene SS Benzol SS Benzole SS Coal naphtha SS Cyclohexatriene SS Phenyl hydride SS Pyrobenzol SS Pyrobenzole S



Line#:4 R.Time:7.592(Scan#:888) MassPeaks:132 BasePeak:57.20(329614)
RawMode:Averaged 7.583-7.600(887-889) BG Mode:Calc. from Peak



Hit#:1 Entry:12254 Library:NIST08s.LIB
SI:95 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1214
CompName:Dodecane SS n-Dodecane SS Adakane 12 SS Ba 51-090453 SS CH3(CH2)10CH3 SS Bihexyl SS Dihexyl SS n-Dodecane min SS Duodece

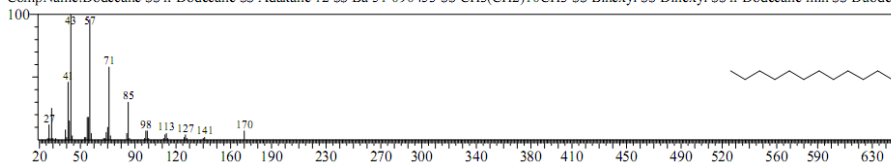


Figure S40. GC and GC/MS spectra of the reaction solution of 1,4-diphenoxybenzene reduction.

10. ^1H NMR and ^{13}C NMR spectra of the isolated products from the reduction of 2-hydroxydiphenyl, 4-hydroxydiphenyl, and 1,2,3,4-tetrahydro-1-naphthol.

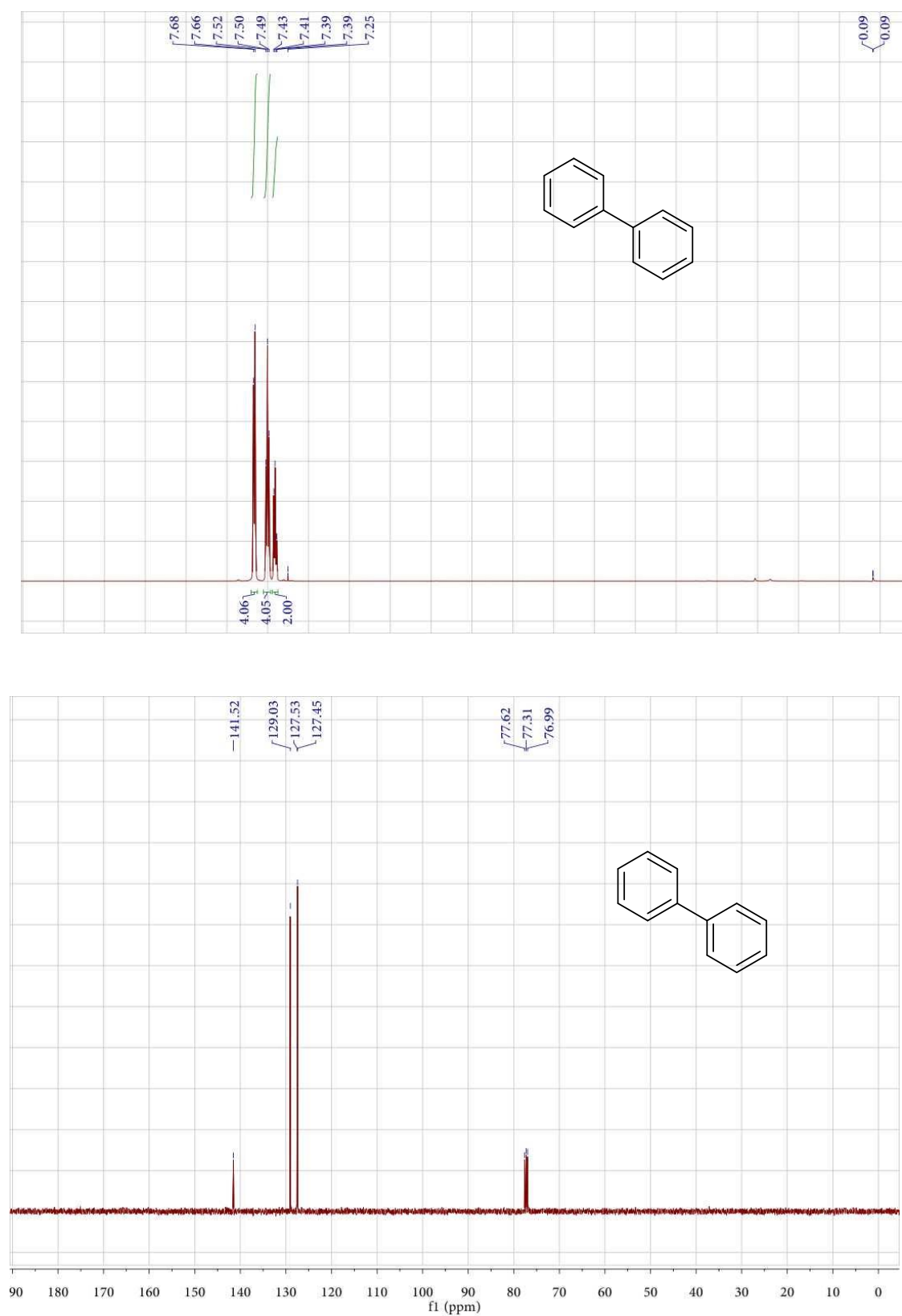


Figure S41 ^1H (top) and ^{13}C (bottom) NMR spectra of the isolated product of 2-hydroxydiphenyl reduction

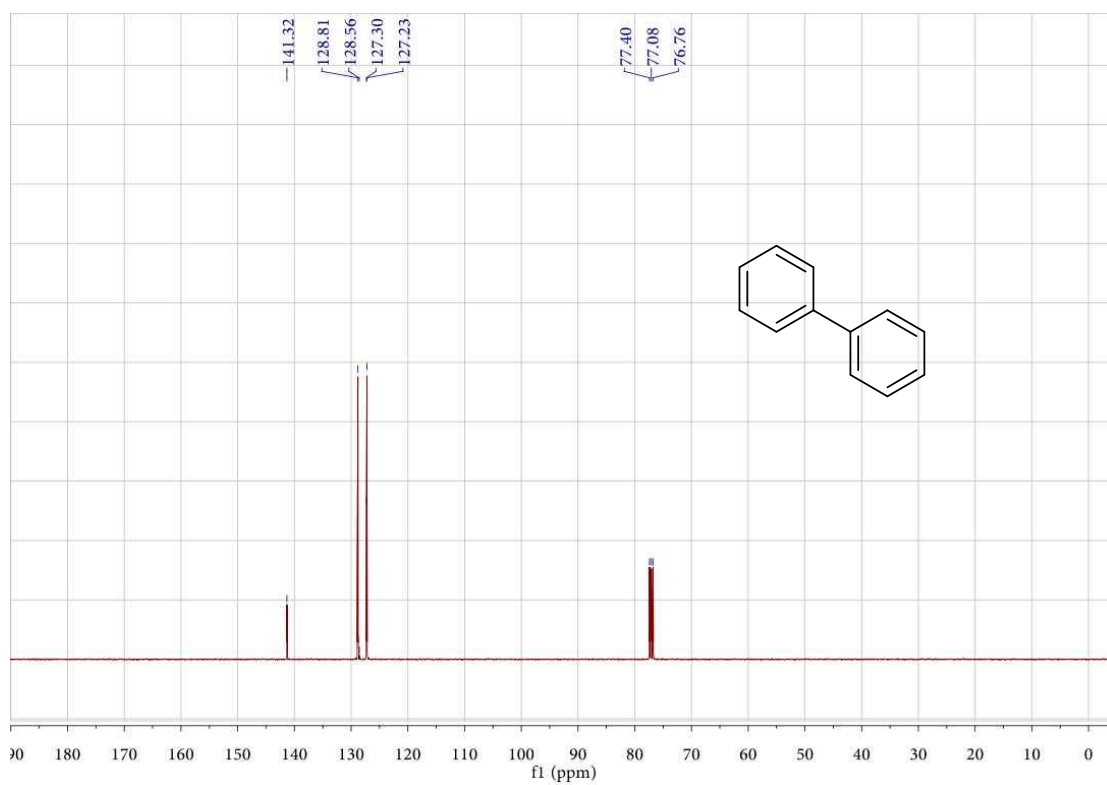
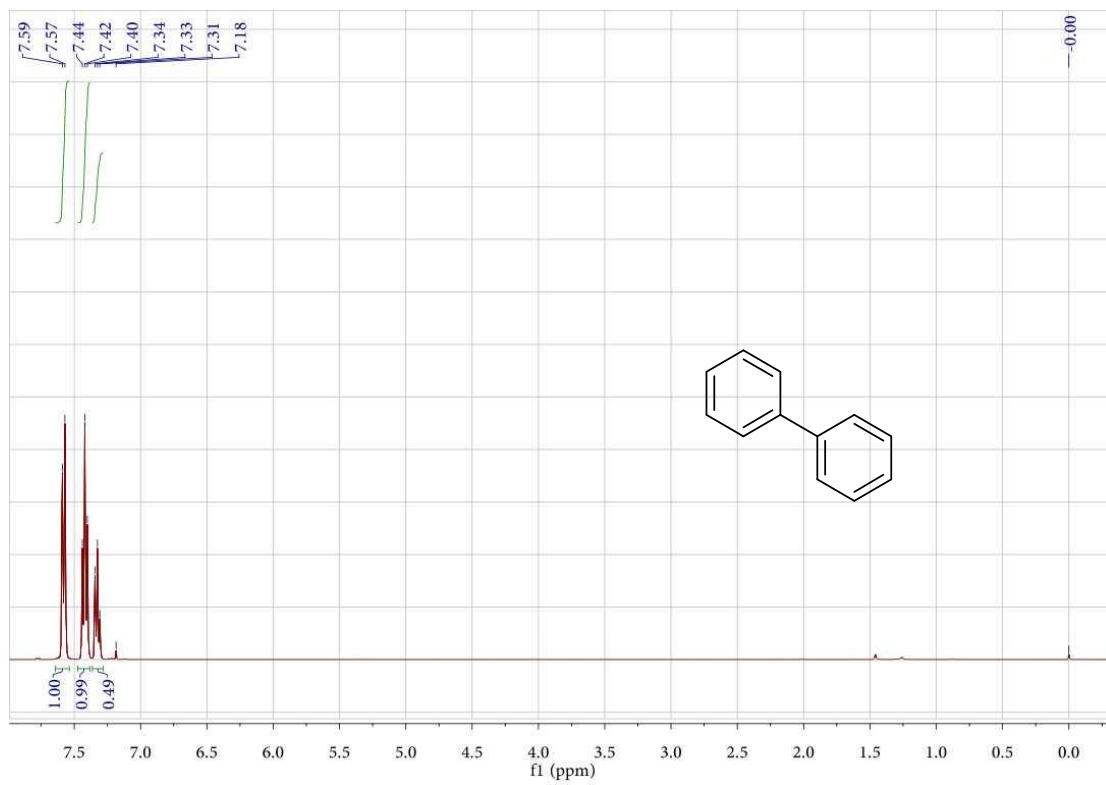


Figure S42 ¹H (top) and ¹³C (bottom) NMR spectra of the isolated product of 4-hydroxydiphenyl reduction

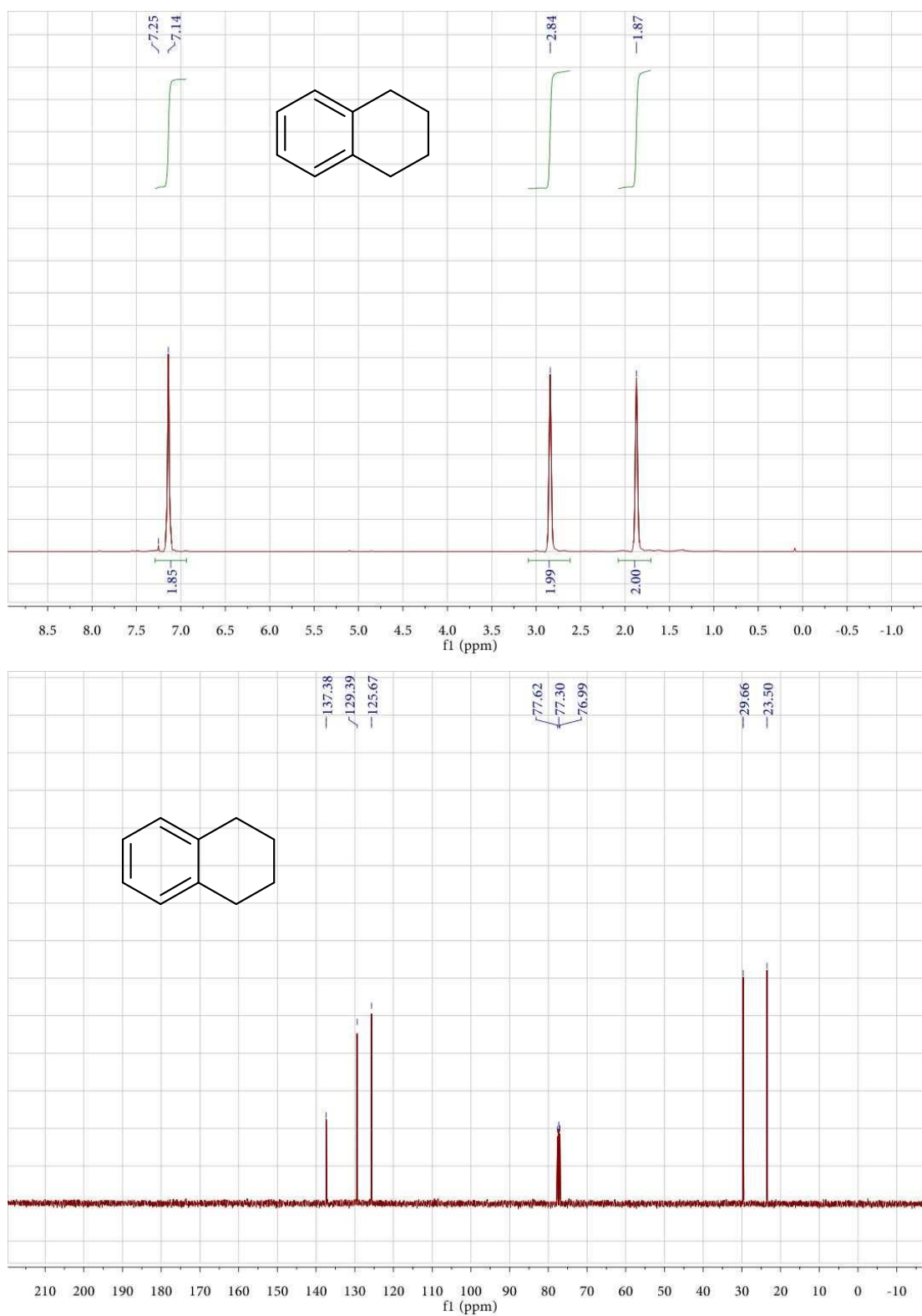


Figure S43 ^1H (top) and ^{13}C (bottom) NMR spectra of the isolated product of 1,2,3,4-tetrahydro-1-naphthol reduction

11. References:

- S1. A. G. Sergeev, J. F. Hartwig, *Science*, 2010, 332, 439.
- S2. Z. Strassberger, A. H. Alberts, M. J. Louwerse, S. Tanase, G. Rothenberg, *Green Chem.*, 2013, 15, 768.
- S3. Q. Song, F. Wang, J. Xu, *Chem. Commun.*, 2012, 48, 7019.