

Supplementary Information for

Nanoconfined Membrane Reactors-Mediated Distinct Chemoselectivity in Ring-opening Reaction of Styrene Oxide

Haoran Shi,^{a,b} Xinxin Cui,^{a,b} Shuai Pang,^c Xiang Li,^{a,b} Daoling Peng,^{*d} Yue Long,^{*a} Xiqi Zhang^{*a,c}
and Kai Song^{*a,b}

a. Laboratory of Bio-inspired Smart Interface Science, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China.

b. School of Future Technology, University of Chinese Academy of Sciences, Beijing 100049, P. R. China.

c. Suzhou Institute for Advanced Research, University of Science and Technology of China, Jiangsu 215123, P. R. China.

d. Key Laboratory of Theoretical Chemistry of Environment, Ministry of Education, School of Environment, South China Normal University, Guangzhou 510006, P.R. China.

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1. Materials and methods

1.1 Chemicals and Materials

Single-layer graphene oxide powder (GO, lateral size: 0.5-5 μm , thickness: 0.8-1.2 nm) was purchased from XFNANO (Nanjing, China). Styrene oxide (\pm , 98+%) was purchased from Alfa Aesar. Aniline (AR) was purchased from Aladdin. o-Toluidine (>99.0%) and 2,6-Diethylaniline (>98.0%) and 1-Propanol (>99.5%) were purchased from TCI. 2-Bromoaniline (99%), 2,6-Dimethylaniline (99%), Ethanol (AR, 99.7%), Methyl alcohol (prep, 99.9%), 1-Butanol (99.5%), Ethyl acetate (AR, 99.5%) and n-Hexane (97.5%, extra dry with molecular sieves,) were purchased from Innochem. These chemical reagents were used without further purification. Deionized water (18.2 M Ω -cm, MilliQ) was used in the experiments.

1.2 Assembly of Membrane Reactor and Preparation for Catalysis

First, a GO stock solution was prepared by adding GO powder (8mg) to deionized water (32 mL). The mixture was pre-sonicated for 2 minutes. The resulting stock solution (0.25 mg/mL) was stored at room temperature. To fabricate a GO membrane, 2 mL of the stock solution was further diluted. After 10 minutes of sonication with an ice bath, a homogeneous dispersion of 20 mL was used to fabricate the GO membrane. Second, the fabrication of membrane reactors was performed using a microfiltration device with a cylinder diameter of 15mm (Figure S1). The as-prepared dispersion was filtered through a nylon membrane (d=20 mm, pore size=0.22 μm) overnight. Finally, the membrane was further vacuum-dried for an additional 12 hours after draining the water above completely. The resulting dry membrane was used in the subsequent catalysis performance test.

1.3 Characterizations of the Membrane Reactor and Analysis of Products

The interlayer distance of GOMR was determined using X-ray diffraction (XRD) with a Bruker D8 Focus diffractometer employing Cu K α radiation ($\lambda=1.5406 \text{ \AA}$). The microstructure of the GOMR was characterized using a HITACHI S-4800 scanning electron microscope (SEM) and a Bruker Dimension FastscanBio atomic force microscope (AFM). The chemical composition of GO membranes was analyzed using a Thermo ESCALAB 250Xi X-ray photoelectron spectrometer (XPS). The infrared spectrum of membrane reactors was characterized by a ThermoFisher Nicolet IS20 fourier transform infrared spectroscopy (FTIR). Gas chromatography (GC) was used to analyze product content and calculate conversion by a SHIMADZU GC-2014C gas chromatograph equipped with an AOC-20i PLUS Auto-Injector and a ThermoFisher TG-5SILMS GC COL 30 m \times 0.25 mm column. The micro-syringe was washed with n-hexane 3 times before each injection and twice after each injection. The column oven and injection temperature were set at 50 $^{\circ}\text{C}$ and 250 $^{\circ}\text{C}$, respectively. The column temperature was increased from 50 $^{\circ}\text{C}$ to 320 $^{\circ}\text{C}$ using a ramp rate of 35 $^{\circ}\text{C}/\text{min}$ and held at 320 $^{\circ}\text{C}$ for 4 min. Gas chromatography-mass spectrometry (GCMS) was used to identify each molecule in products by a Thermo Fisher Exactive GC gas chromatograph-mass spectrometer. The reference mass spectrum of reactants were according to the pure chemicals while that of product was according to a previous work.^{1,2} The chromatographic column and method were same to those of GC.

1.4 Measurement of Interlayer Distance in the Wet State of GO Membranes

Due to the interaction of oxygen-containing groups on the surface of GO and solvent, GO membranes swelled in solvent and showed wider interlayer distance than dry state. To measure the interlayer distance in the wet state of GO membrane, the preparation process was the same to that of confined catalysis process. Then 5 mL of solvent was added to the microfiltration device and negative pressure of 0.1 MPa was applied for 3 hours to help the solvent flow into the membrane. The membrane was carefully taken out and put into a 10 mL glass bottle with a diameter of 20 mm, and 2 mL solvent was added into the bottle. The bottle was put in room temperature and the membranes was soaked in the solvent overnight. Then the membrane was taken out and held in air for several seconds. After the solvent on the surface of GO membrane completely volatilized, the membrane was ready for XRD test.

1.5 Confined Catalysis Performance Evaluation of Membrane Reactors

Styrene oxide (SO, 0.1 mmol) and aniline (A, 0.1 mmol) were dissolved in ethanol (1 mL) to prepare a reactant solution with the concentration of 0.1 mol/L. The as-prepared reactant solution was added into the as-prepared GOMR, and a negative pressure of 0.1 MPa was applied to drive the catalytic flow reaction. After vacuum filtration at room temperature ($\sim 25^{\circ}\text{C}$) for 24 hours, the 1 mL of reactant solution was completely transferred into GOMR. Then the GO membrane was taken out, and the filter was thoroughly rinsed with ethyl acetate. The filtrate was collected in the chromatographic bottle and diluted to about 1 mL with ethyl acetate. Then the as-prepared filtrate was analyzed using GC and GC-MS to determine the conversion of styrene oxide and analyze products. Then the aniline was replaced by the other aniline derivatives to prepare reactants solvents and evaluate the catalytic performance and chemoselectivity.

1.6 Bulk Catalysis Performance Evaluation with GO Powder

The bulk reaction was carried out in a 10 mL glass bottle with a diameter of 20 mm. The reactant solution was prepared using the same method as that of confined catalysis. The reactant solution (1 mL) was then added to the 10 mL glass bottle, followed by the careful addition of GO powder (2 mg). The bottle was then kept at room temperature ($\sim 25^{\circ}\text{C}$) for 24 hours. Reactant solution (50 μL) was extracted and filtered to remove the GO powder. The filtrate was then diluted to 1 mL with ethyl acetate and analyzed by GC and GC-MS to determine the conversion of styrene oxide and analyze products.

2. Detailed Information for the Theoretical Simulation

Density functional theory (DFT) calculations were performed using the Gaussian 16 program. The M06-2X exchange–correlation functional was employed for all calculations. The 6-31G(d) basis set was used for geometry optimizations, and the 6-311+G(d,p) basis set was used for single-point free energy calculations. Solvation effects were considered using the SMD implicit solvent model. The Gibbs free energy changes were calculated relative to the corresponding reactants. In the bulk model, the catalytic role of GO was represented by proton catalysis without explicitly including GO in the cluster, whereas the confined model additionally introduces a frozen bilayer graphene framework to impose spatial restriction.



Figure S1. Photograph of the microfiltration device.

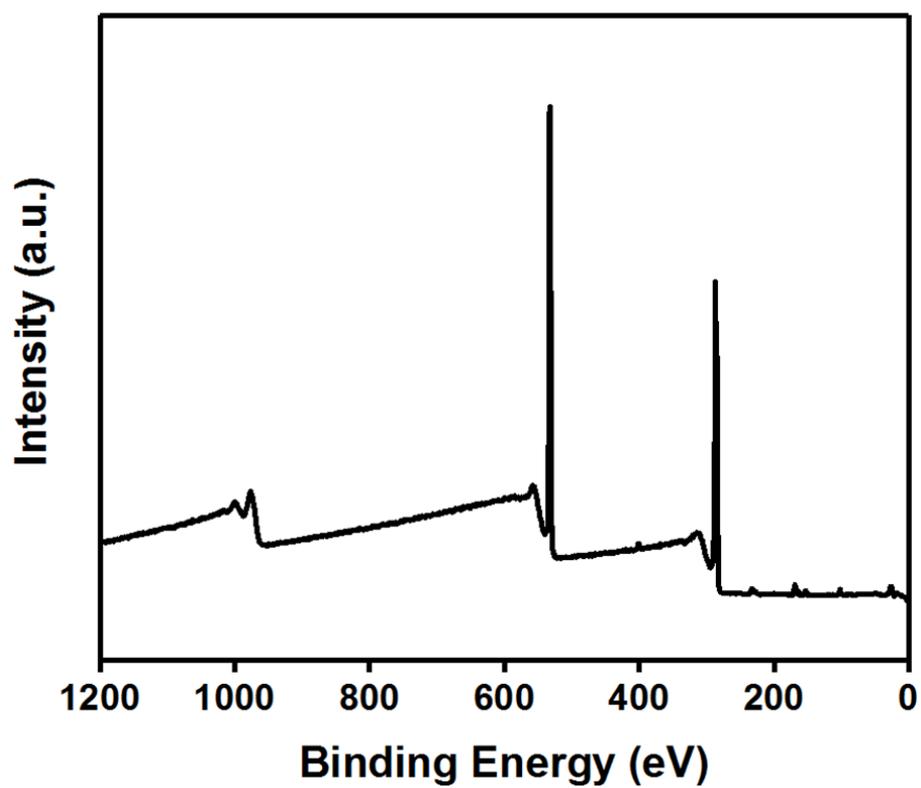


Figure S2. XPS analysis of GO used for constructing GOMR, full spectrum.

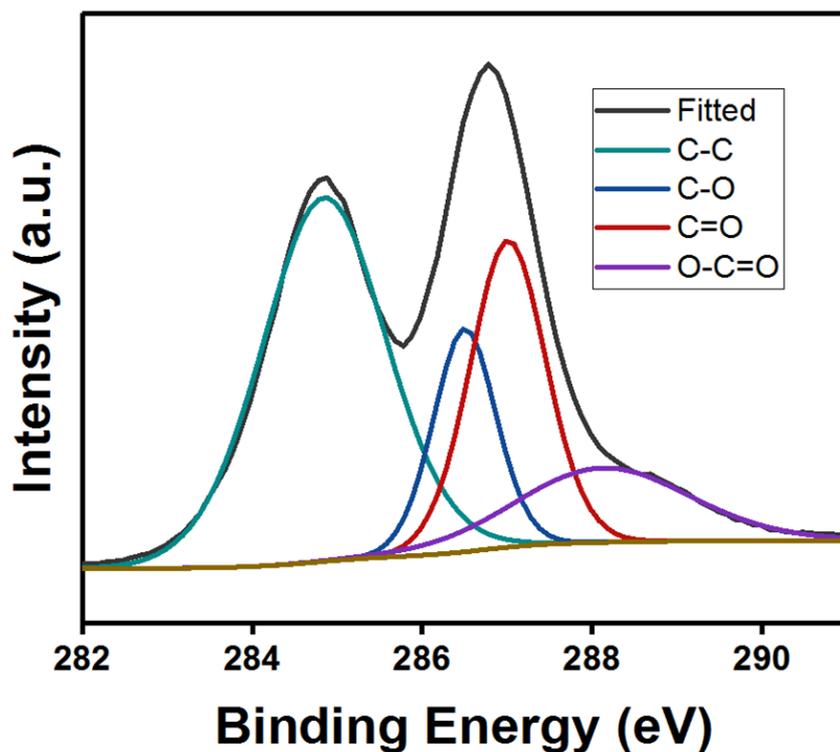


Figure S3. XPS analysis of GO used for constructing GOMR, C 1s.

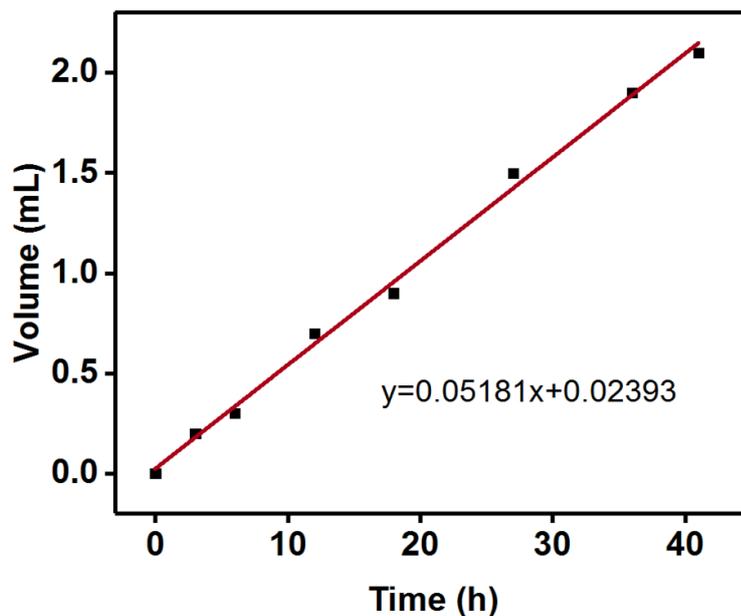


Figure S4. Flow curves of reaction solution. The ethanol solution of styrene oxide (SO) and aniline (A) was taken as the representative example, and concentrations were consistent with that in confined reaction.

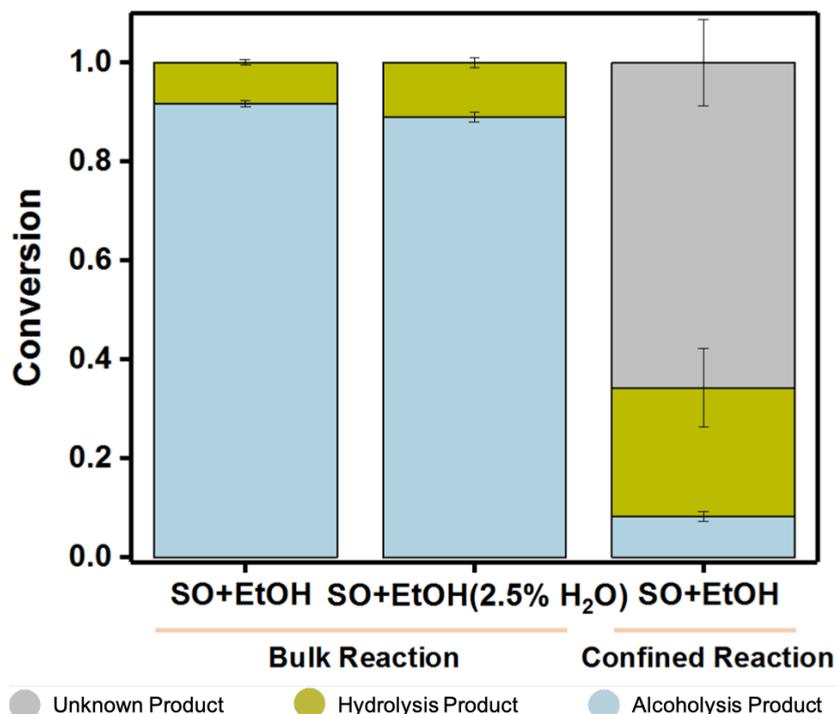


Figure S5. The conversion and product distribution of the ring opening reaction between styrene oxide and ethanol for both confined reactions and bulk reactions. The reactant solution was prepared without amines, and the unknown products were not further pursued.

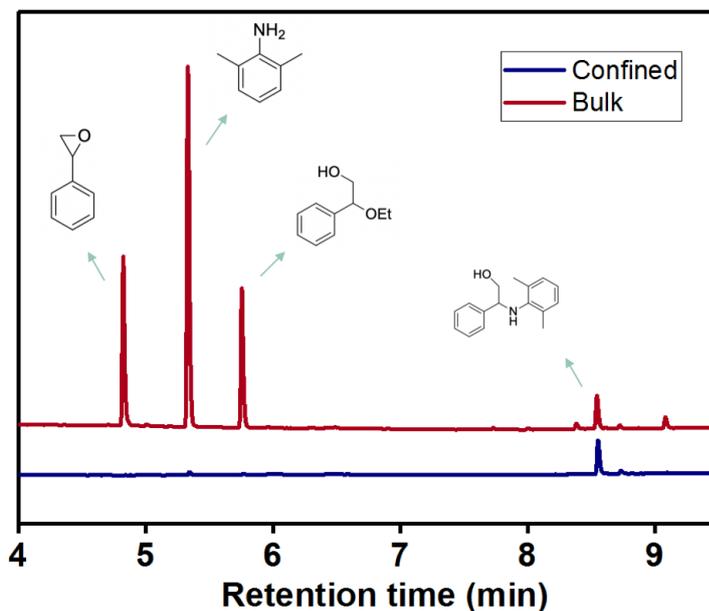


Figure S6. The comparison of the gas chromatograms of bulk reaction and confined reaction. The ring-opening reaction of styrene oxide with 2,6-Dimethylaniline (DMeA) is taken as a representative example.

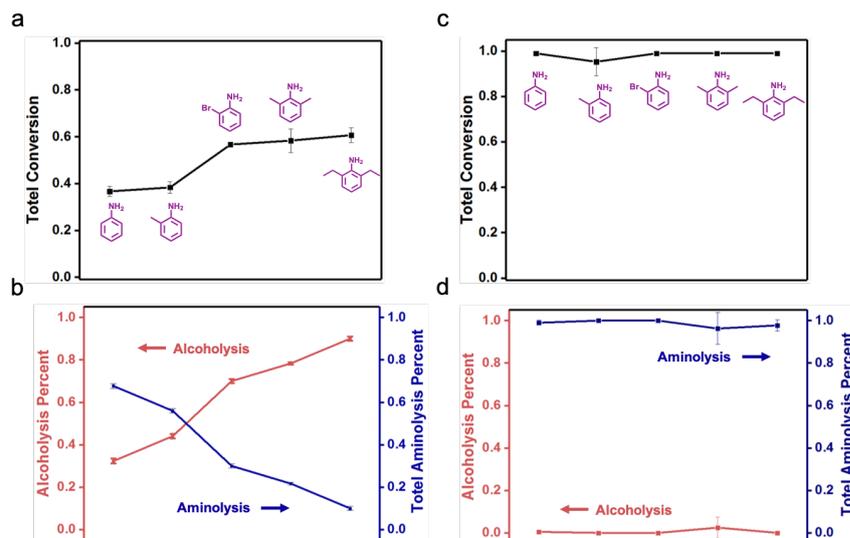


Figure S7. The catalytic performance and product distribution in bulk reaction and confined reaction. (a) The total conversion of styrene oxide with each aniline derivative in bulk reaction. (b) The rate of alcoholysis product and total aminolysis product in bulk reaction (c) The total conversion of styrene oxide with each aniline derivative in confined reaction. (d) The rate of alcoholysis product and total aminolysis product in confined reaction. Total aminolysis product is defined as the summation of aminolysis product-1 and aminolysis product-2

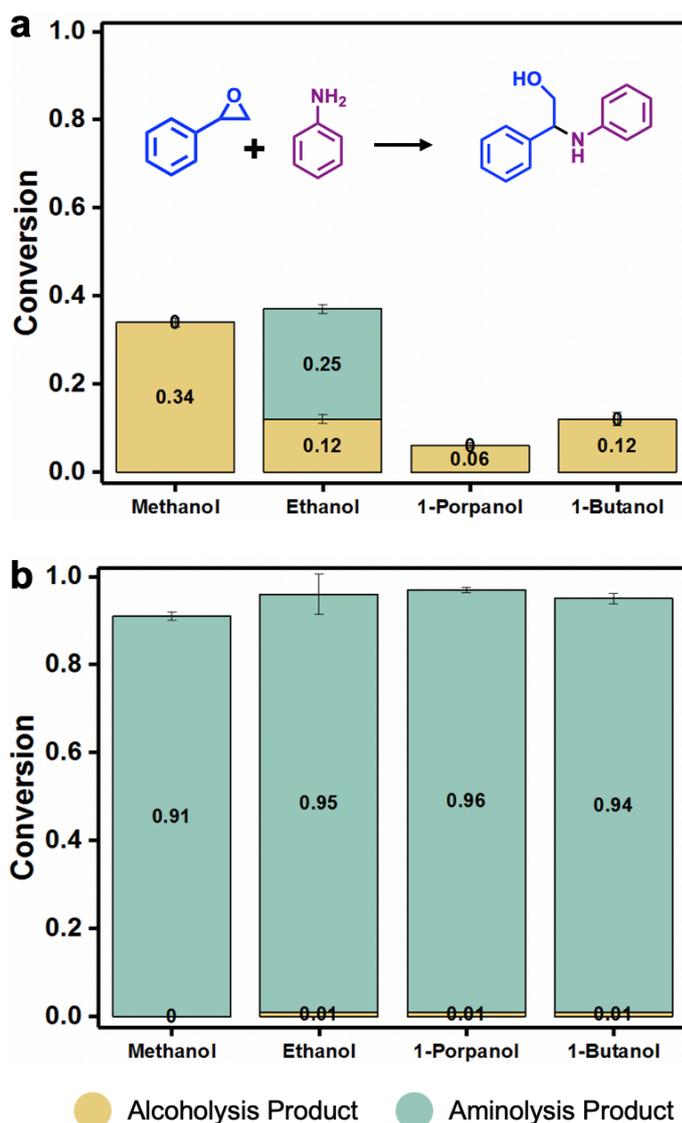


Figure S8. Additional catalytic performance tests with other alcohols, in (a) bulk reaction and (b) confined reaction. The ring-opening reaction of styrene oxide and aniline in alcohols was taken as the example. Methanol, ethanol, 1-propanol and 1-butanol were respectively taken as the solvent, and the catalytic performance and product distribution in bulk reaction and confined reaction were evaluated. In bulk reactions, the total conversion of styrene oxide in methanol and ethanol were obviously higher than that in 1-propanol and 1-butanol. The alcoholysis products took the main part in product in methanol, 1-propanol and 1-butanol, but in ethanol, rate of aminolysis product was about half of that of alcoholysis product. With the group near hydroxyl group changes from methyl to butyl group, the nucleophilic capacity and ability to support the ring-opening reaction decreased. The increase in volume implies greater steric hindrance, which leads to a decrease in the nucleophilicity of the alcohol and consequently a reduction in alcoholysis products. Meanwhile, the elongation of the carbon chain leads to a decline in the alcohol's proton transfer capability^{3,4}, while the bulk reaction relies on the solvent to transport protons for activating styrene oxide⁵. In confined reactions, the total conversion of styrene oxide was all near 100%, and the aminolysis products took the main part in product in all of the four alcohols. The nanoconfined effect assisted the GOMR to provide stable and active microenvironment, which induced efficient activation of reaction and stable chemoselectivity.

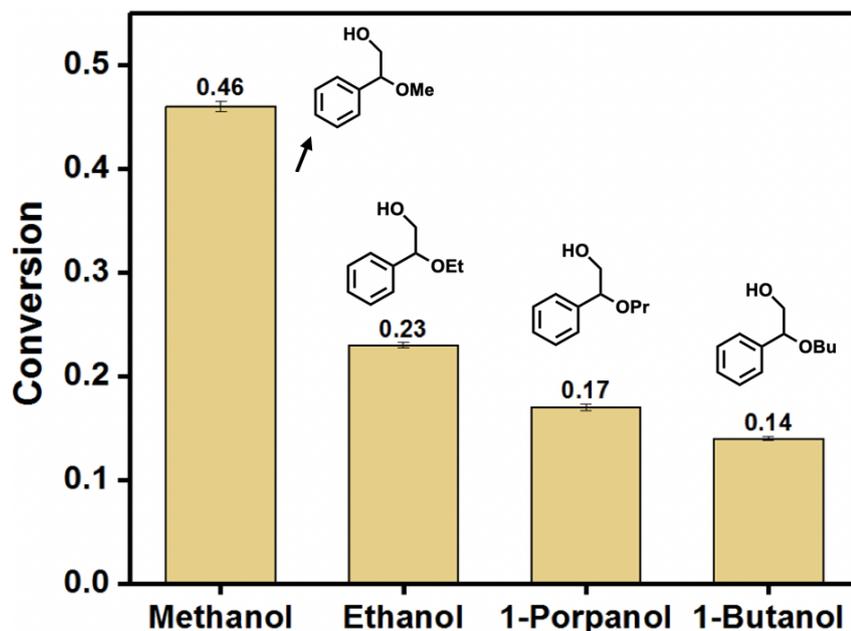


Figure S9. The product distribution of ring-opening reaction between styrene oxide and mixed alcohol in bulk reaction. The mixed alcohol was prepared by mixing the four alcohols in equal proportions, and the volume ratio of methanol, ethanol, 1-propanol and 1-butanol was 1:1:1:1. Without addition of aniline derivative, styrene oxide reacted with alcohols only in bulk reaction. After 24 hours, the total conversion of styrene oxide was near 100%, and the proportion of alcoholysis products of styrene oxide with methanol, ethanol, 1-propanol and 1-butanol was 0.46, 0.23, 0.17 and 0.14, which further confirmed the fact that with the group near hydroxyl group changes from methyl to butyl group, the nucleophilic capacity and ability to support the ring-opening reaction decreased.

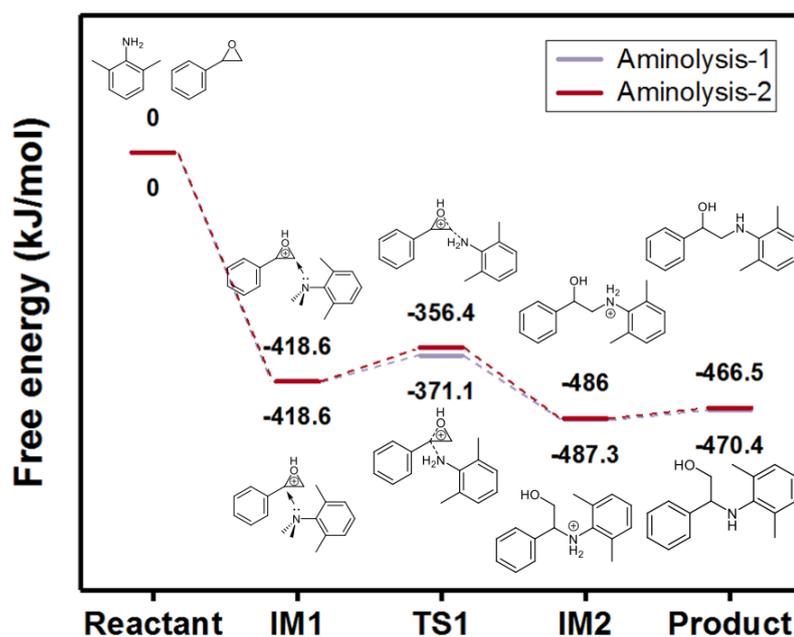


Figure S10. Reaction pathways of regioselectivity of ring-opening reaction in bulk reaction calculated by DFT. The labels TS and IM indicate the transition state and intermediate of the reaction, respectively. The Gibbs free energy of IM1 for aminolysis product-1 and aminolysis product-2 are both -418.6 kJ/mol. The formation of the oxonium ion weakens the C–O bond in the epoxide ring, making it susceptible to nucleophilic attack by amine. Then amine attacks either carbon atoms of the epoxide group would form the IM2. This step proceeds through TS1, and the Gibbs free energy of TS1 are -371.1 kJ/mol for aminolysis product-1 and -356.4 kJ/mol for aminolysis product-2. The transition from IM1 to TS1 is the rate-determining step of the ring opening reaction. The energy barriers for this step is 47.5 kJ/mol for aminolysis product-1 and 62.2 kJ/mol for aminolysis product-2. The energy barrier for aminolysis product-1 is 14.7 kJ/mol lower than that for aminolysis product-2, explaining why aminolysis product-1 dominate in aminolysis reaction.

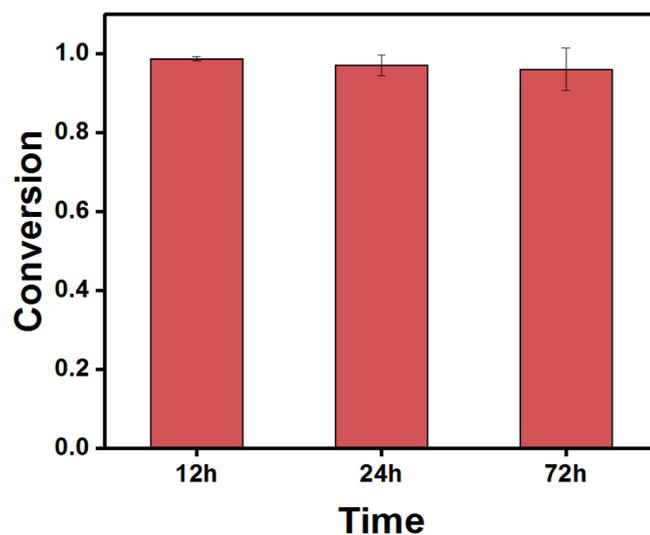


Figure S11. The time-dependent catalytic performance of GOMR. The catalytic duration time of the GOMR was varied by adjusting the volume of the reactant solution. The ring opening reaction between SO and A was taken as the representative case. Catalytic performance of the GOMR was tested at 12h, 24h and 72h using ethanol as the solvent. The results showed no significant degradation, indicating that the catalytic activity of the GOMR could be remained over a period of 72 hours.

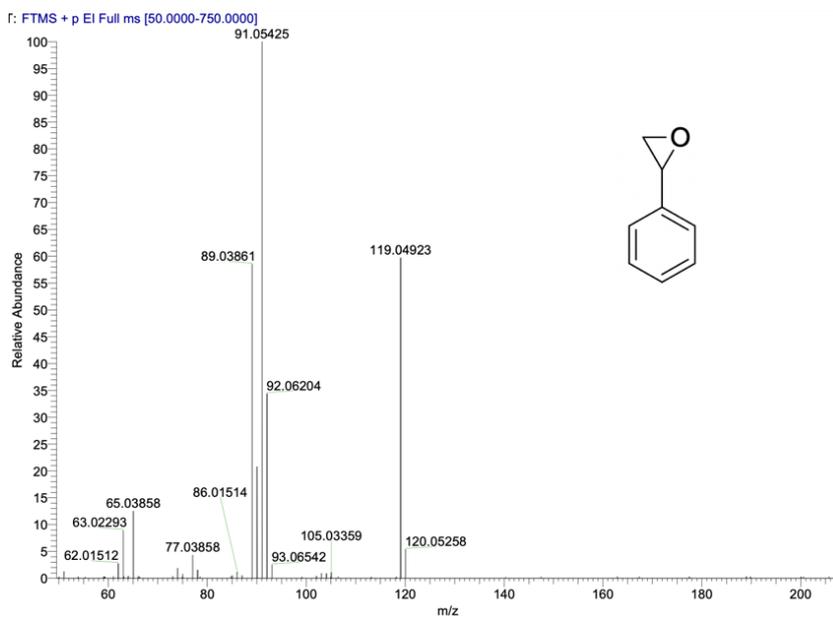


Figure S12. Mass spectrum of styrene oxide.

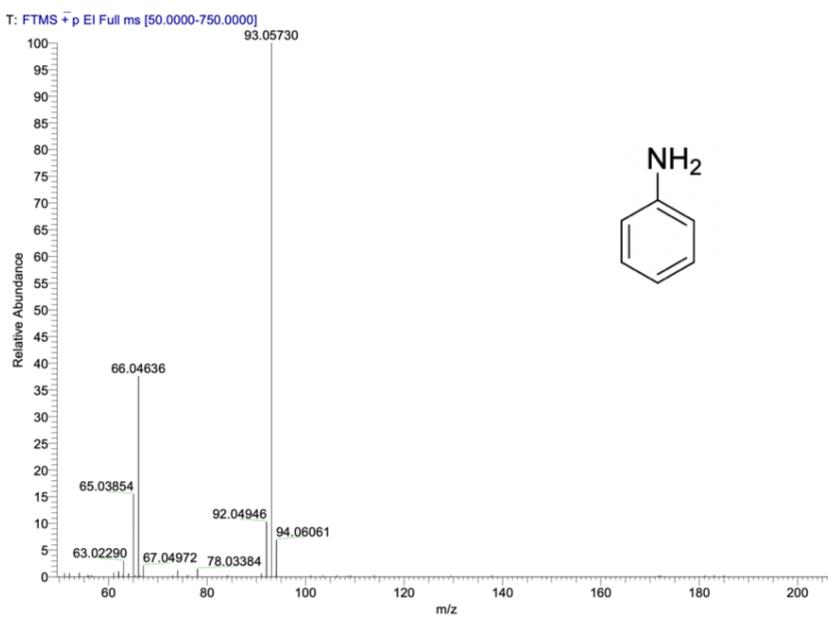


Figure S13. Mass spectrum of aniline.

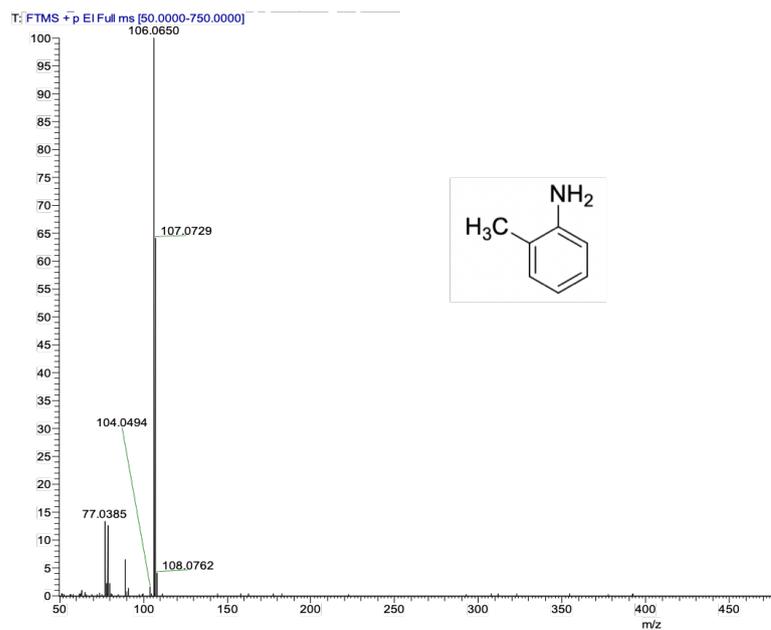


Figure S14. Mass spectrum of o-toluidine.

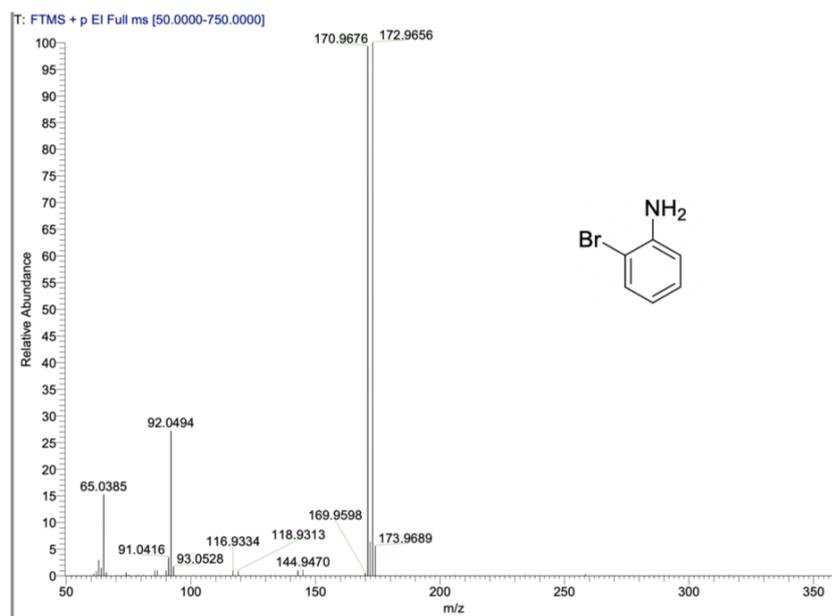


Figure S15. Mass spectrum of 2-Bromoaniline.

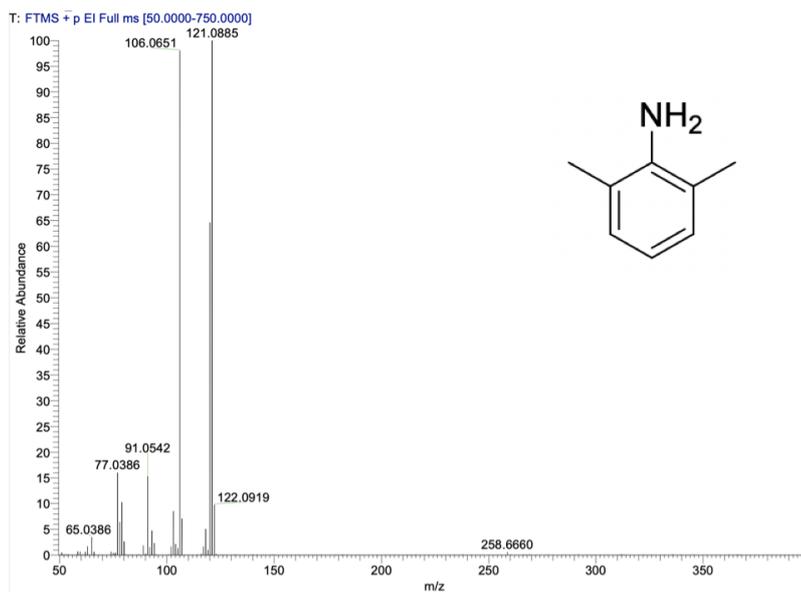


Figure S16. Mass spectrum of 2,6-Dimethylaniline.

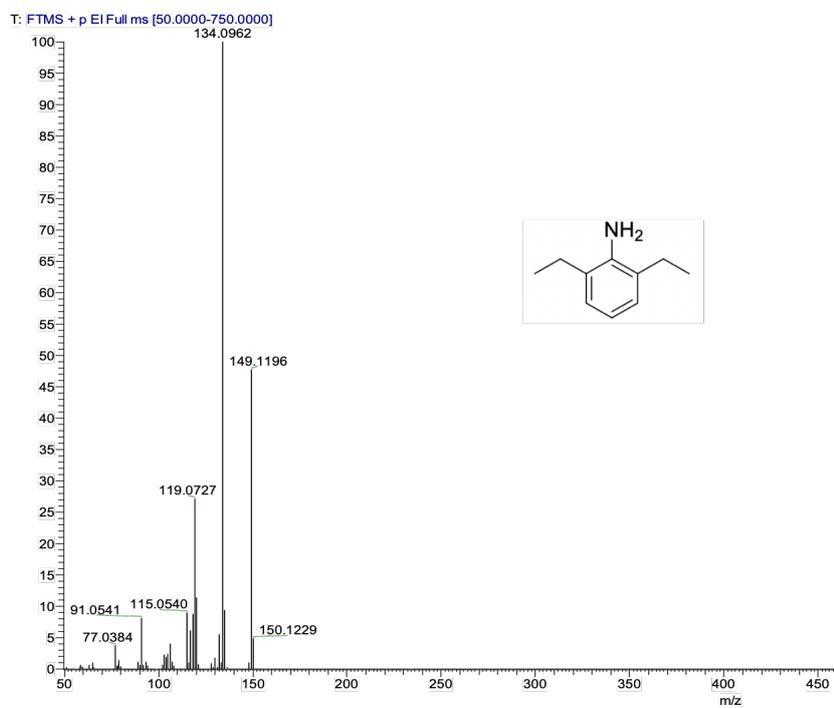


Figure S17. Mass spectrum of 2,6-Diethylaniline.

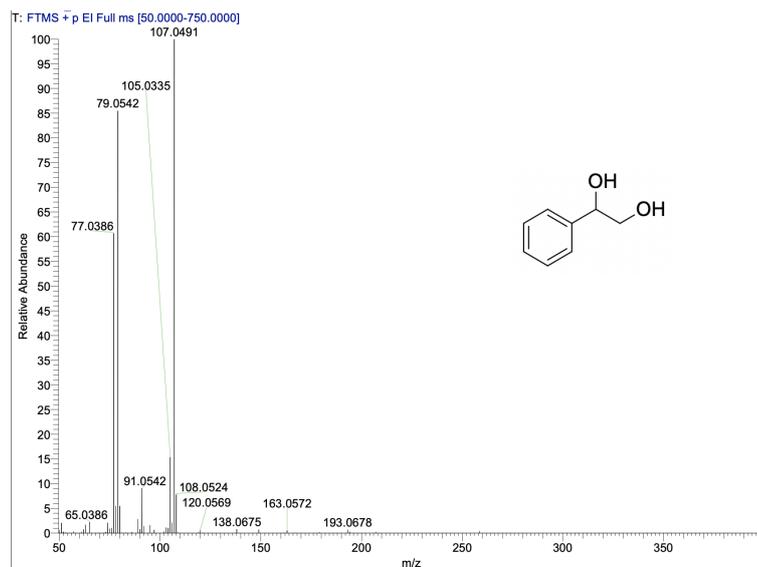


Figure S18. Mass spectrum of 1-phenylethane-1,2-diol

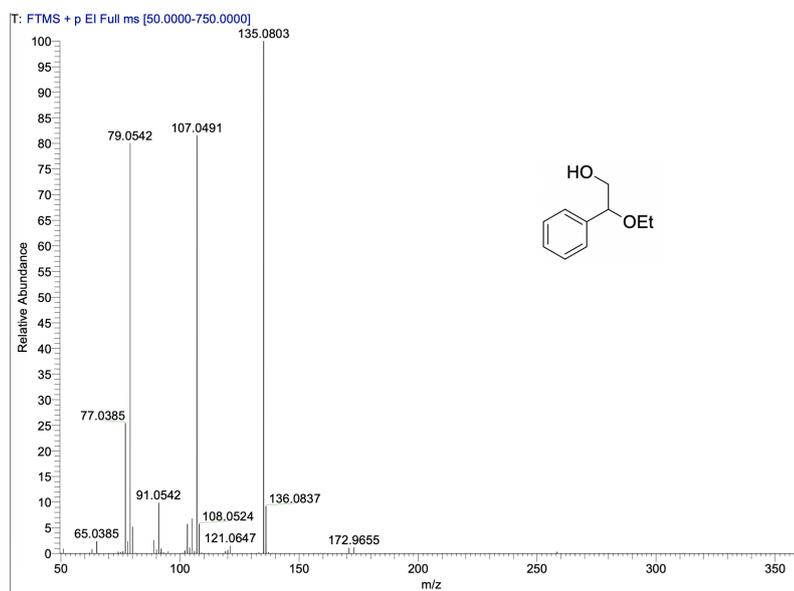


Figure S19. Mass spectrum of 2-ethoxy-2-phenylethan-1-ol

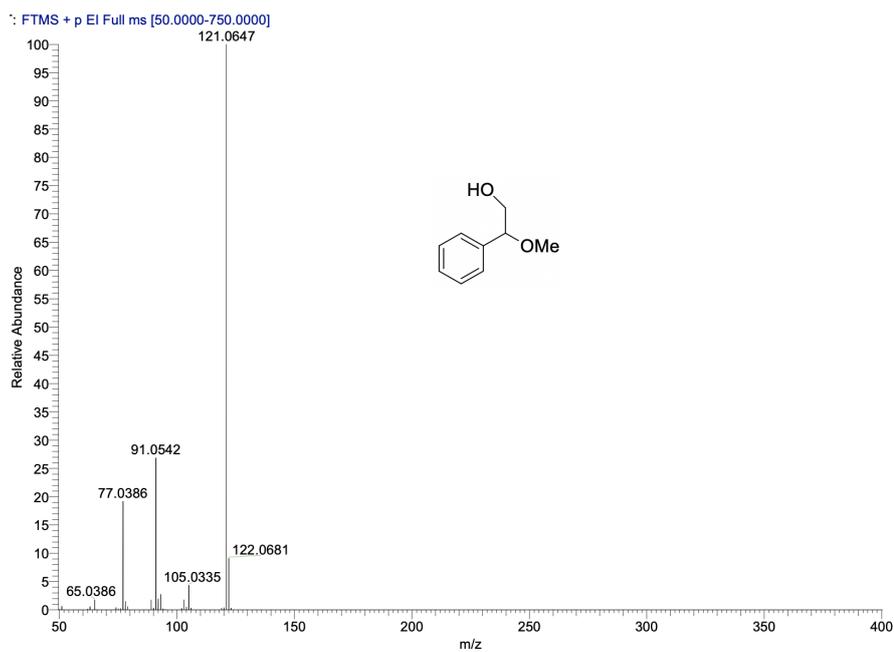


Figure S20. Mass spectrum of 2-methoxy-2-phenylethan-1-ol

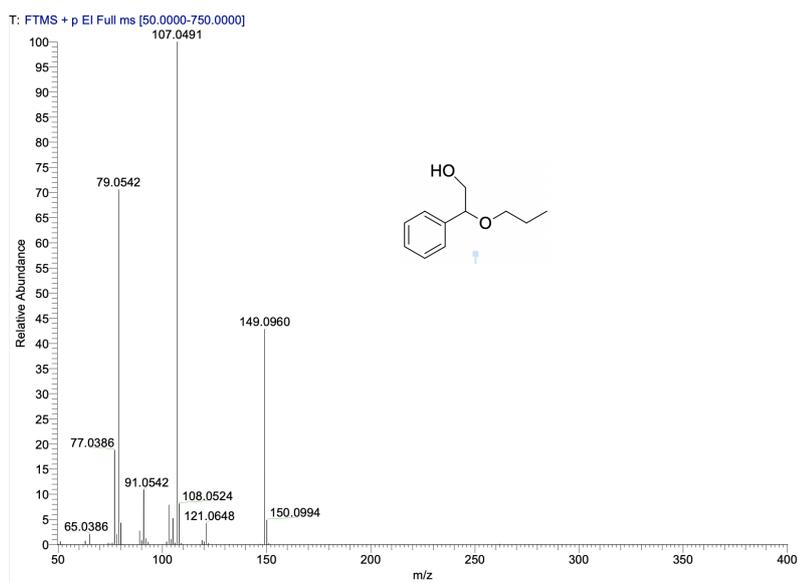


Figure S21. Mass spectrum of 2-phenyl-2-propoxyethan-1-ol

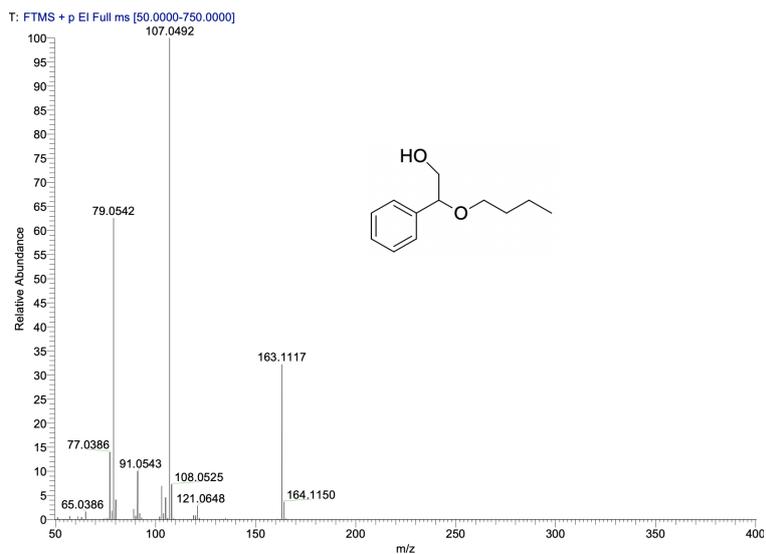


Figure S22. Mass spectrum of 2-butoxy-2-phenylethan-1-ol

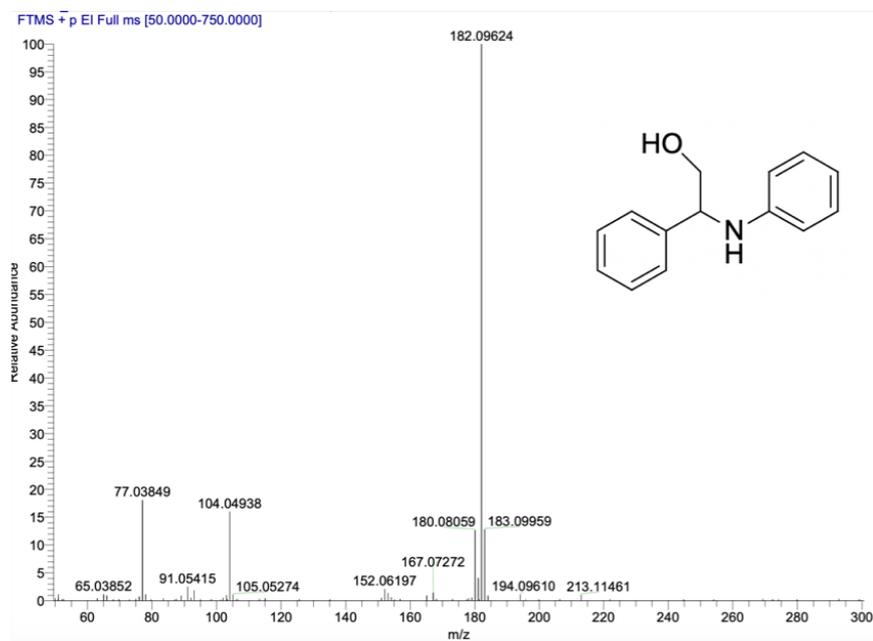


Figure S23. Mass spectrum of 2-phenyl-2-(phenylamino)ethan-1-ol.

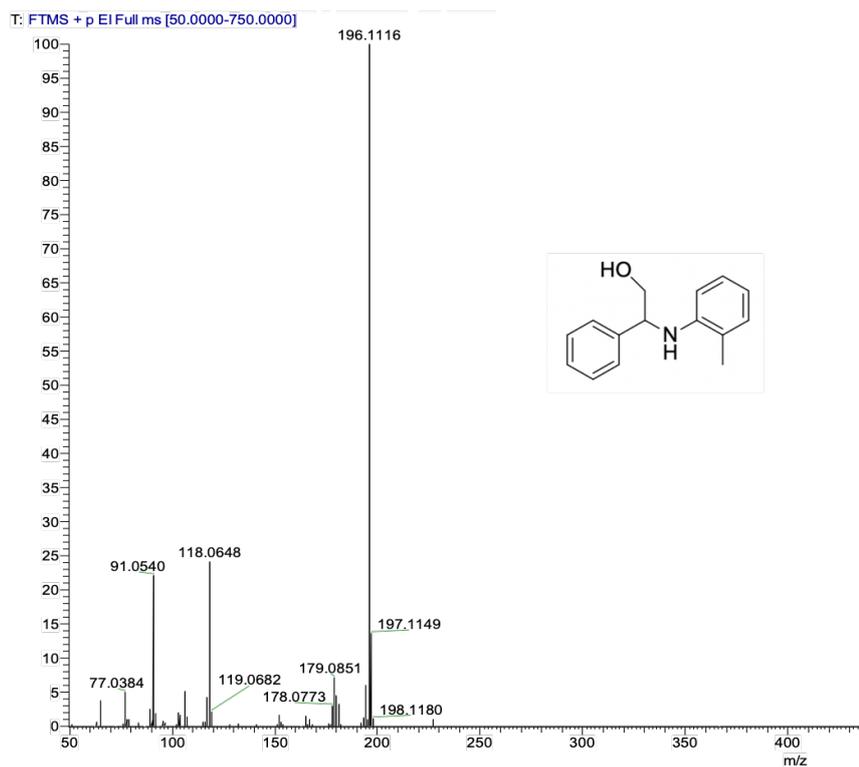


Figure S24. Mass spectrum of 2-phenyl-2-(o-tolylamino) ethan-1-ol.

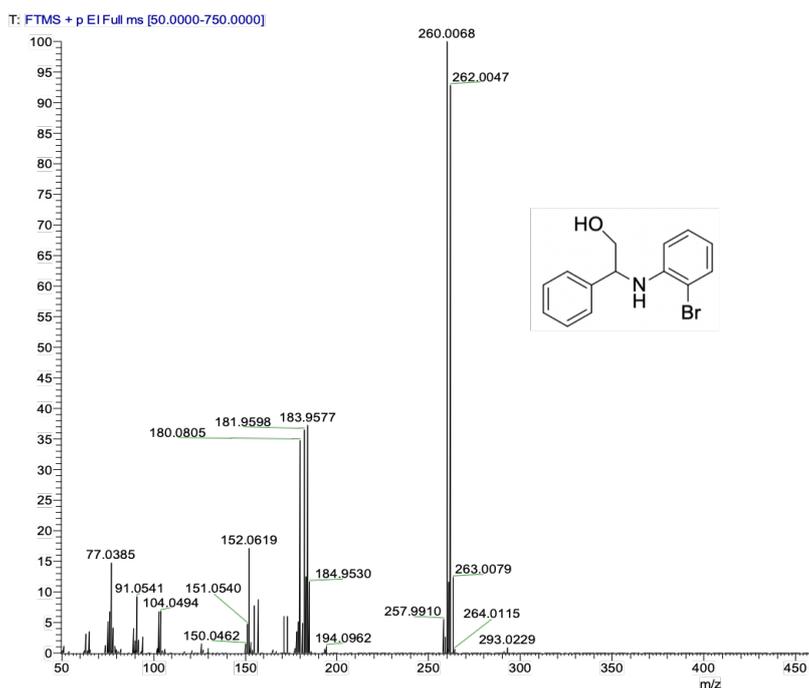


Figure S25. Mass spectrum of 2-((2-bromophenyl) amino)-2-phenylethan-1-ol.

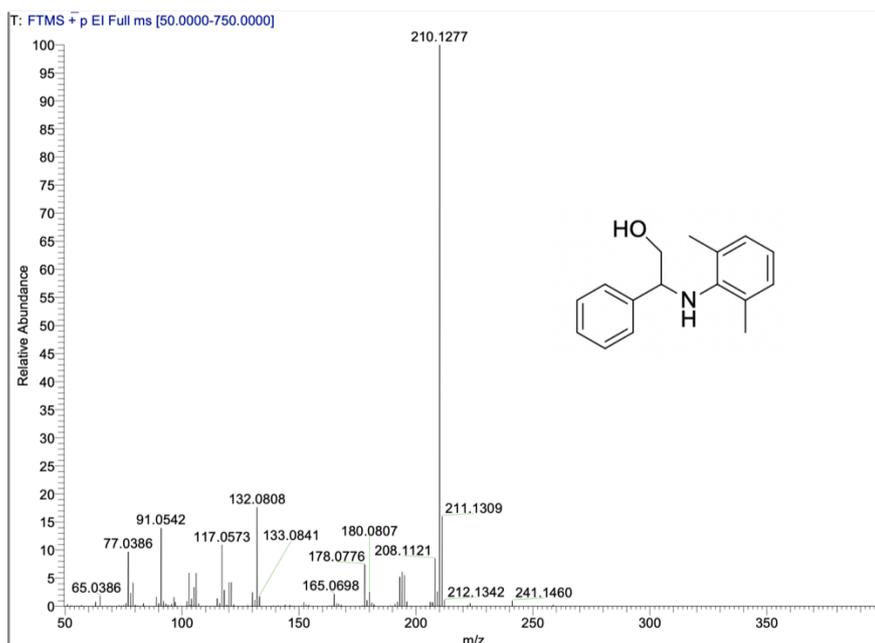


Figure S26. Mass spectrum of 2-((2,6-dimethylphenyl) amino)-2-phenylethan-1-ol

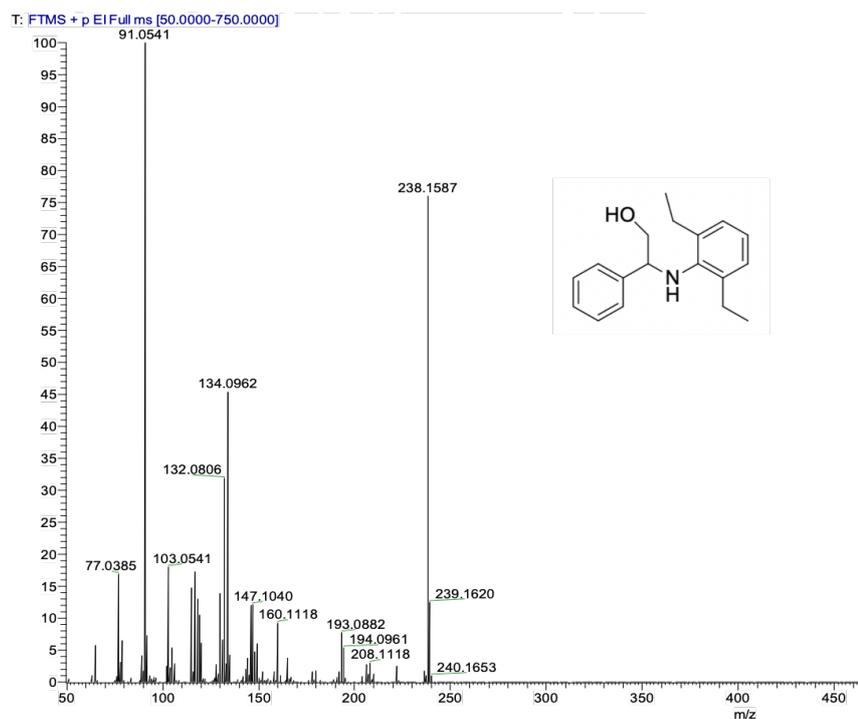


Figure S27. Mass spectrum of 2-((2,6-diethylphenyl) amino)-2-phenylethan-1-ol.

Cartesian coordinates of all optimized geometries in DFT calculations

styrene oxide

C	-1.63743700	-1.34664700	0.00956400
C	-0.27997400	-1.04915500	-0.06359500
C	0.14718600	0.28145000	-0.07715100
C	-0.79739400	1.30768200	-0.02662100
C	-2.15622600	1.00878900	0.05112900
C	-2.57886600	-0.31868400	0.07000200
H	-1.96255100	-2.38248900	0.01707700
H	0.45472700	-1.84778200	-0.12049000
H	-0.46508600	2.34234700	-0.04885500
H	-2.88382500	1.81359400	0.09135700
H	-3.63742400	-0.55265700	0.12660500
C	1.59735700	0.61651900	-0.12533800
H	1.83606200	1.63436700	-0.42888500
C	2.57403200	-0.08986700	0.71968800
H	3.48962800	0.41461900	1.01824900
H	2.21706100	-0.87924700	1.37812500
O	2.46741900	-0.37541000	-0.67240800

2,6-Dimethylaniline

C	1.22022700	0.03900400	0.00050800
C	0.00002100	-0.65956800	0.00497700
C	-1.22023100	0.03898700	0.00052200
C	-1.19894400	1.43138100	0.00767800
C	-0.00003400	2.13635500	0.01513200
C	1.19887100	1.43141300	0.00767900
H	-2.14506200	1.96710300	0.00493300
H	-0.00000900	3.22126400	0.01971600
H	2.14496700	1.96718000	0.00496800
C	-2.51763700	-0.72493900	-0.02460700
H	-3.36936700	-0.04415300	-0.08929900
H	-2.56140300	-1.40608500	-0.88285400
H	-2.65339600	-1.33188300	0.88108000

C	2.51766300	-0.72486500	-0.02459700
H	2.65326700	-1.33211100	0.88090500
H	2.56164400	-1.40572000	-0.88306800
H	3.36938900	-0.04402800	-0.08891500
N	0.00003200	-2.05855800	-0.05785200
H	0.83303700	-2.49412400	0.31682200
H	-0.83291500	-2.49415100	0.31692600

ethanol

C	-0.08383200	0.54607100	-0.00005000
H	-0.14448700	1.19108900	0.88614900
H	-0.14468700	1.19150500	-0.88582500
O	-1.15081900	-0.39907300	0.00001100
H	-1.98149000	0.10017800	-0.00003300
C	1.22141100	-0.22072300	-0.00004000
H	1.29187600	-0.85558200	-0.88829800
H	2.06888200	0.47006400	0.00098900
H	1.29098000	-0.85675700	0.88746900

aminolysis product-1

C	-2.18772300	0.62632100	0.75088800
C	-1.40442200	0.35784300	-0.39189500
C	-1.62063200	-0.82059300	-1.12932800
C	-2.57047000	-1.73504600	-0.67402500
C	-3.32505400	-1.49564600	0.46690900
C	-3.13733800	-0.30576800	1.16088800
H	-2.72938800	-2.64503300	-1.24745000
H	-4.06265600	-2.21792300	0.80125900
H	-3.73226000	-0.09160100	2.04531600
C	-0.89951800	-1.07981000	-2.42646200
H	-1.41494300	-1.85753800	-2.99591000
H	-0.86770100	-0.17150800	-3.03774000
H	0.13180000	-1.41650800	-2.26736200
C	-2.01499400	1.91714700	1.51325300
H	-0.97921700	2.07660600	1.84050000

H	-2.29391300	2.78665400	0.90450000
H	-2.64904000	1.92430500	2.40274400
N	-0.45934100	1.31521600	-0.80840200
H	-0.46449300	2.12421300	-0.19783900
C	0.93129400	0.95718600	-1.08959000
H	1.02656700	0.60869900	-2.12521200
C	1.73531000	2.25605000	-1.01459300
H	2.79358200	2.03074900	-1.19848800
H	1.37258600	2.94147000	-1.79371700
C	1.54213000	-0.10616600	-0.18987800
C	2.44048300	-1.02609700	-0.73264600
C	1.26871700	-0.15809800	1.17761500
C	3.06066700	-1.97946900	0.07082100
H	2.65372300	-0.99664000	-1.80019000
C	1.88232400	-1.11184900	1.98306900
H	0.57007700	0.55136200	1.60899500
C	2.78016100	-2.02447800	1.43314700
H	3.75473100	-2.68961600	-0.36849000
H	1.65671900	-1.14469200	3.04461800
H	3.25448200	-2.77035100	2.06354300
O	1.53646900	2.80954700	0.27486000
H	2.01736900	3.64531400	0.33181000

aminolysis product-2

C	-2.96592500	1.05750000	0.17429300
C	-2.22181800	-0.04091700	-0.29517400
C	-2.67752900	-1.35273300	-0.08286000
C	-3.87398100	-1.54569300	0.60865300
C	-4.61822100	-0.46877000	1.07460700
C	-4.16328600	0.82603600	0.84861400
H	-4.22999900	-2.56091800	0.76637000
H	-5.55031000	-0.63593100	1.60526100
H	-4.73815700	1.67541000	1.20911300
C	-1.90880700	-2.53201000	-0.61945100

H	-2.58140500	-3.36991600	-0.82215900
H	-1.39099600	-2.25931300	-1.54357100
H	-1.15493700	-2.88644500	0.09395700
C	-2.47170700	2.46517100	-0.05343800
H	-1.42623300	2.58405100	0.25369900
H	-2.53077000	2.75154600	-1.11110800
H	-3.07488400	3.18036100	0.51076400
N	-1.00990200	0.16630200	-1.00598600
H	-0.94639800	1.12718600	-1.33022600
C	0.20700300	-0.11555900	-0.24753900
H	0.32589100	-1.19504900	-0.11059700
C	1.40692700	0.42084700	-1.01643300
H	1.40989600	-0.05182100	-2.01062100
O	1.17949200	1.81842300	-1.14127400
H	1.90580500	2.19763000	-1.65662400
H	0.20254100	0.35018400	0.75251600
C	2.70312800	0.10881800	-0.30097600
C	3.39219400	-1.07254600	-0.57776600
C	3.19882700	0.97668600	0.67301200
C	4.56016000	-1.38643300	0.11059800
H	3.01113700	-1.74805200	-1.34079400
C	4.37012900	0.66640600	1.35887200
H	2.65927400	1.89593300	0.88176100
C	5.05227300	-0.51539300	1.08009600
H	5.09027300	-2.30680700	-0.11442000
H	4.75040400	1.34810400	2.11364700
H	5.96605000	-0.75611300	1.61447800

alcoholysis product-1

C	2.42192000	-1.09414200	-1.06778300
C	1.10079300	-0.74494500	-0.79423600
C	0.79352900	0.02324400	0.33093800
C	1.82677500	0.44125100	1.17244900
C	3.14826900	0.09749500	0.89714500

C	3.44892000	-0.67349100	-0.22467500
H	2.64933100	-1.69448700	-1.94362800
H	0.30320200	-1.07272700	-1.45286000
H	1.59124100	1.03744400	2.05109300
H	3.94151600	0.42604700	1.56177600
H	4.47756300	-0.94661900	-0.43915100
C	-0.62620400	0.46048200	0.61961000
H	-0.75080300	0.59193600	1.70620300
C	-0.92506400	1.81239000	-0.02693000
H	-1.90067700	2.18321200	0.31156000
H	-0.16112900	2.52754100	0.30500600
O	-0.90818400	1.64235600	-1.43482900
H	-1.07347800	2.50886700	-1.83661900
O	-1.50071000	-0.55586900	0.15888000
C	-2.88017500	-0.28061900	0.36544000
H	-3.03168300	0.10561100	1.38358100
H	-3.22122000	0.48657300	-0.34182400
C	-3.64689100	-1.56955500	0.15888800
H	-4.71831500	-1.39541400	0.28947600
H	-3.47980900	-1.95516200	-0.85109200
H	-3.32580900	-2.32738300	0.87900400
alcoholysis product-2			
C	3.13818500	-1.36104400	0.35432900
C	1.83923200	-1.05791300	0.75365900
C	1.22344800	0.12068900	0.32546300
C	1.92446800	0.99390700	-0.50772400
C	3.22667000	0.69387000	-0.90461800
C	3.83572200	-0.48373200	-0.47586800
H	3.60885900	-2.27791600	0.69598200
H	1.29630200	-1.73704800	1.40724300
H	1.44920500	1.91264500	-0.83792600
H	3.76547600	1.38138100	-1.54969700
H	4.85050800	-0.71626000	-0.78378400

C	-0.20862700	0.41453700	0.72548100
C	-1.16373800	-0.23702600	-0.25974800
H	-1.01691900	0.21306400	-1.25453900
H	-0.39970000	-0.01195600	1.72042500
O	-2.48809100	-0.03355500	0.18579100
C	-3.43711500	-0.60261600	-0.70400400
H	-3.31922400	-0.15555300	-1.70184400
H	-3.24998800	-1.68212700	-0.80054900
C	-4.82371500	-0.34197700	-0.15669100
H	-5.00516900	0.73308100	-0.06939900
H	-5.57788100	-0.76810000	-0.82364500
H	-4.93765400	-0.79649000	0.83160000
H	-0.94016600	-1.31143000	-0.33239400
O	-0.50566400	1.80235200	0.72067200
H	0.09921500	2.23417300	1.34515000

IM1 aminolysis

C	1.91063800	1.34345500	0.00000600
C	0.55442500	1.11893700	0.00006100
C	0.06538500	-0.22164900	0.00007100
C	0.98107400	-1.31372700	-0.00000100
C	2.33892700	-1.07224200	-0.00006100
C	2.79504400	0.25044400	-0.00005900
H	2.30219100	2.35391900	0.00000400
H	-0.14520400	1.94899600	0.00010700
H	0.58925400	-2.32639600	-0.00000500
H	3.04666200	-1.89288600	-0.00011400
H	3.86406800	0.44062100	-0.00011300
C	-1.29036200	-0.51457200	0.00009000
H	-1.58081600	-1.56553800	0.00003700
C	-2.39392600	0.45837300	0.00010800
H	-2.28029900	1.11014100	0.88248700
H	-2.28021700	1.11036500	-0.88208000
O	-3.61905800	-0.23694700	-0.00004200

H	-4.33040100	0.42225300	-0.00127700
IM1 alcoholysis			
C	1.92942900	1.34096200	0.00002300
C	0.56858800	1.12552300	0.00006600
C	0.06355700	-0.21437500	0.00005500
C	0.98048900	-1.31336000	-0.00000800
C	2.34226800	-1.07974400	-0.00005800
C	2.81143600	0.24214400	-0.00004200
H	2.32642700	2.35016100	0.00003300
H	-0.12234000	1.96177300	0.00011100
H	0.58605800	-2.32464500	-0.00002000
H	3.04394100	-1.90664200	-0.00011000
H	3.88195600	0.42554300	-0.00008400
C	-1.29573600	-0.50429600	0.00005000
H	-1.58188500	-1.55565400	0.00001800
C	-2.41084700	0.45875700	0.00007200
H	-2.30610000	1.11755800	0.88029100
H	-2.30607900	1.11770400	-0.88001700
O	-3.63868700	-0.24259700	-0.00000100
H	-4.34758900	0.42131300	-0.00115600
TS1 aminolysis			
C	-3.21448000	0.54952500	0.82691600
C	-1.92634000	0.97381200	0.57997300
C	-1.08801400	0.21775200	-0.28487500
C	-1.58176200	-0.97817500	-0.87222800
C	-2.87167600	-1.39802400	-0.61381000
C	-3.68179800	-0.63241700	0.23192200
H	-3.86514400	1.12098000	1.47906600
H	-1.55691800	1.88370800	1.04204800
H	-0.93552300	-1.54986000	-1.53280400
H	-3.25660700	-2.30664700	-1.06239700
H	-4.69697400	-0.96069200	0.43447300
C	0.20700100	0.63440900	-0.61982300

H	0.76566100	0.03387300	-1.33688800
C	0.85435000	1.92992400	-0.28387800
H	0.41184500	2.66796400	-0.97441300
H	0.58604700	2.25654400	0.73110300
O	2.22456700	1.91200400	-0.51296800
H	2.60518100	1.30720500	0.14552100
C	2.89007195	-1.11843688	1.58067960
C	1.68655569	-0.49115297	1.94808809
C	1.61420739	0.27738583	3.12330199
C	2.74833116	0.39288562	3.92310725
C	3.94264390	-0.23131727	3.57898965
C	4.00191043	-0.97855793	2.40745611
H	2.68727650	0.98762597	4.83123781
H	4.81792868	-0.13104334	4.21213281
H	4.93011342	-1.46610500	2.11955278
C	0.32558025	0.96667088	3.48634875
H	0.44791723	1.57180015	4.38743191
H	-0.01420880	1.62557422	2.67835554
H	-0.48205805	0.24829657	3.68317152
C	2.95804177	-1.91330258	0.30355983
H	2.29207565	-2.78676296	0.32858240
H	2.66442199	-1.30437631	-0.55984421
H	3.97086799	-2.28277578	0.12810157
N	0.57337765	-0.57411210	1.10246823
H	0.55506903	-1.39754969	0.51458133
H	-0.31592410	-0.44478498	1.56767509
TS1 alcoholysis			
C	-3.21448000	0.54952500	0.82691600
C	-1.92634000	0.97381200	0.57997300
C	-1.08801400	0.21775200	-0.28487500
C	-1.58176200	-0.97817500	-0.87222800
C	-2.87167600	-1.39802400	-0.61381000
C	-3.68179800	-0.63241700	0.23192200

H	-3.86514400	1.12098000	1.47906600
H	-1.55691800	1.88370800	1.04204800
H	-0.93552300	-1.54986000	-1.53280400
H	-3.25660700	-2.30664700	-1.06239700
H	-4.69697400	-0.96069200	0.43447300
C	0.20700100	0.63440900	-0.61982300
H	0.76566100	0.03387300	-1.33688800
C	0.85435000	1.92992400	-0.28387800
H	0.41184500	2.66796400	-0.97441300
H	0.58604700	2.25654400	0.73110300
O	2.22456700	1.91200400	-0.51296800
H	2.60518100	1.30720500	0.14552100
C	3.96674400	-1.12902900	0.10699500
H	4.54697400	-1.96100500	-0.30078700
H	4.42118400	-0.82917300	1.05520900
H	4.03357200	-0.29563000	-0.59913200
C	2.52335600	-1.54496100	0.30687700
H	2.06307000	-1.82938600	-0.64567900
H	2.43694800	-2.40249400	0.97971700
O	1.74160700	-0.44824400	0.83045000
H	1.58700300	-0.58238000	1.77669400

IM2 aminolysis

C	3.91923700	1.38433900	0.01700800
C	2.60321800	1.03309100	0.29741300
C	2.17573900	-0.28916500	0.12572000
C	3.07795600	-1.25209700	-0.32846600
C	4.39647500	-0.89970600	-0.60454600
C	4.81572300	0.41690300	-0.43423000
H	4.24766400	2.40845300	0.15867400
H	1.91849100	1.79380800	0.67028700
H	2.75384400	-2.28223400	-0.45380100
H	5.09502600	-1.65412300	-0.95028400
H	5.84337000	0.69041400	-0.64882900

C	0.74688100	-0.66672300	0.41180000
H	0.60584400	-1.74663400	0.33248900
C	0.22074500	-0.23922200	1.78491800
H	1.00847500	-0.48740100	2.50252800
H	0.07071100	0.84738400	1.83247800
O	-0.93246400	-0.95918800	2.13750500
H	-1.71861800	-0.41702400	1.98504200
C	-2.37172800	-1.04814300	-0.57085100
C	-1.56713400	0.09354000	-0.53421100
C	-2.05197300	1.38838300	-0.32083500
C	-3.42599000	1.52069200	-0.11143500
C	-4.26116600	0.40884800	-0.13128400
C	-3.73894200	-0.85893600	-0.36661800
H	-3.83975600	2.50987500	0.05674100
H	-5.32677900	0.53205600	0.02979400
H	-4.39563600	-1.72305600	-0.38708400
C	-1.15832600	2.60662900	-0.34489900
H	-1.75064600	3.50851000	-0.18366100
H	-0.39097900	2.58831200	0.43810600
H	-0.65677700	2.73283900	-1.31309100
C	-1.81118100	-2.43418000	-0.75257700
H	-1.00786700	-2.48400300	-1.49771300
H	-1.42105400	-2.80636700	0.20118000
H	-2.59373900	-3.11805100	-1.08529100
N	-0.10984100	-0.06252100	-0.72946300
H	0.07331600	-0.62614400	-1.56911500
H	0.29649900	0.85902200	-0.93369300

IM2 alcoholysis

C	-2.93892700	0.60893500	0.94228000
C	-1.57301700	0.81936700	0.78632800
C	-0.86975300	0.12786900	-0.21071600
C	-1.54373100	-0.77058400	-1.04333400
C	-2.91192700	-0.96819100	-0.89060600

C	-3.60691700	-0.28120000	0.10280000
H	-3.48328700	1.14650400	1.71115300
H	-1.06603200	1.53015100	1.43524400
H	-1.00047700	-1.30190600	-1.82072300
H	-3.43449400	-1.65740300	-1.54504000
H	-4.67394800	-0.43730900	0.22194200
C	0.60434800	0.31018000	-0.36090100
H	1.00905600	-0.24317300	-1.21137800
C	1.13407100	1.72508200	-0.37432500
H	0.63809000	2.23746200	-1.21038500
H	0.85833400	2.24168600	0.55504500
O	2.52332900	1.62590800	-0.53882600
H	2.90984100	2.51161400	-0.59398900
C	3.39420100	-1.24653100	0.00139600
H	3.97118600	-2.16874800	-0.11190200
H	3.93853200	-0.56464700	0.65607600
H	3.29019800	-0.77811300	-0.97848300
C	2.06509400	-1.61390400	0.60375000
H	1.44368400	-2.25043700	-0.03185600
H	2.16307100	-2.05559600	1.59593600
O	1.27158000	-0.36720500	0.85023500
H	0.55633200	-0.54585600	1.49704700

TS2 aminolysis

C	4.01012500	1.36227500	-0.12159500
C	2.69492500	1.07184200	0.23882500
C	2.20940600	-0.24390800	0.14926700
C	3.06296800	-1.25894200	-0.30510900
C	4.37996300	-0.96688500	-0.66078700
C	4.85315900	0.34327100	-0.57176700
H	4.37897200	2.38034500	-0.04267600
H	2.05926100	1.87481300	0.60753000
H	2.70251100	-2.28329000	-0.36686900
H	5.03473700	-1.76196000	-1.00391200

H	5.87832200	0.57047300	-0.84786800
C	0.78555600	-0.57537400	0.52203800
H	0.62571500	-1.65386400	0.50567500
C	0.31684000	-0.06992600	1.89578300
H	1.11740700	-0.32793100	2.59644100
H	0.21721900	1.02327200	1.91488000
O	-0.85356100	-0.72891400	2.33124200
H	-1.62837200	-0.18750400	2.12192300
C	-2.36271000	-1.11438800	-0.53856100
C	-1.60074600	0.06341800	-0.49133100
C	-2.15528000	1.34835500	-0.35706700
C	-3.54722100	1.42747100	-0.22853700
C	-4.33686700	0.27987000	-0.25349200
C	-3.74972500	-0.97310900	-0.41589400
H	-4.01090700	2.40352600	-0.12303400
H	-5.41489600	0.36354200	-0.15769900
H	-4.37103500	-1.86303600	-0.44791100
C	-1.32309200	2.61400100	-0.38737800
H	-1.96820000	3.49041400	-0.29413600
H	-0.59442700	2.67248100	0.43119400
H	-0.77804600	2.73437800	-1.33483300
C	-1.75298500	-2.48887000	-0.67975100
H	-0.94408300	-2.53272100	-1.42162800
H	-1.35219100	-2.83705600	0.27973400
H	-2.50980000	-3.20869000	-1.00002200
N	-0.12327700	-0.03226100	-0.64299600
H	0.10124300	-0.61260700	-1.45988100
H	0.24209000	0.89793700	-0.87373200
TS2 alcoholysis			
C	-3.10238704	0.51154246	1.05453292
C	-1.73704904	0.74037346	0.89518192
C	-1.03235004	0.10142546	-0.14370608
C	-1.71693404	-0.76461654	-1.01334408

C	-3.08434804	-0.97943254	-0.85612208
C	-3.77573004	-0.34446654	0.17873992
H	-3.64212004	1.00759446	1.85508592
H	-1.22952504	1.42131146	1.57389092
H	-1.18189604	-1.25409454	-1.82345208
H	-3.60936604	-1.64016554	-1.53874508
H	-4.84109904	-0.51416954	0.30160592
C	0.43146796	0.30987446	-0.32378508
H	0.82507796	-0.19079354	-1.20909008
C	0.96651296	1.72302846	-0.24354408
H	0.41475396	2.29912646	-1.00273308
H	0.74345796	2.16436146	0.73826992
O	2.35005396	1.66778546	-0.50712808
H	2.65121660	0.74793145	-0.44435052
C	3.54563700	-1.19308100	0.08635700
H	4.14436600	-2.08943100	-0.11234000
H	4.01649300	-0.63373500	0.89809600
H	3.53879700	-0.57167500	-0.81085300
C	2.16380000	-1.65082800	0.47396600
H	1.64003400	-2.20520500	-0.30891100
H	2.15422600	-2.22372200	1.40312100
O	1.73344425	-0.39214856	0.45532274

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