Supporting Information

Atomically Dispersed Cobalt Catalyst for Tandem Synthesis of Primary Benzylamines from Oxidized β-O-4 Segments

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Experimental Procedures

Materials

2-Methylimidazole (99%) were purchased from J&K Scientific Ltd. Zinc nitrate hexahydrate ($Zn(NO_3)_2·6H_2O$, 98%), cobalt nitrate hexahydrate ($Co(NO_3)_2·6H2O$, 99%), 2-bromoacetophenone (98%), phenol (99%), n-dodecane (99%), bis(1-phenylethyl)amine(98%), 2,6-dimethoxyphenol (99%), acetophenone (99%), guaiacol(99%), 2-phenoxy-1-phenylethanol (98%), p-xylene (99%), hydroxylamine hydrochloride (98%), sodium acetate anhydrous (99%) and palladium on carbon (10%) were purchased from Innochem Technology Co., Ltd. Sodium borohydride (98%) and 4A molecular sieve were purchased from Sinopharm Chemical Reagent Co., Ltd. Methanol, ethanol and toluene (Guaranteed reagent) was supplied by Concord Technology Co., Ltd. 7.0 M solution in methanol was purchased from Adamas Reagent, Ltd. 2-phenoxy-1-phenylethanone (>98%), 1-phenylethylamine (98%), 2-bromo-4'-methoxyacetophenone (98%), 1-(4-methoxyphenyl)ethylamine (98%) and Cobalt phthalocyanine (CoPc, 97%) were obtainbed from Aladdin Chemical Reagent Co., Ltd. 1-(3,4-dimethoxyphenyl)ethanamine (95%) was purchased from Bide Pharmatech Ltd. 2-(2-methoxyphenoxy)-4'-methoxyacetophenone (≥95%) was purchased from Macklin Reagent Co., Ltd. H_2 and Ar (>99.999%) was supplied by Beijing Tailong Electronic Technology Co., Ltd. The synthesis steps of other compounds and the corresponding NMR analysis were shown in the supporting information.

Catalyst Preparation

Synthesis of bimetallic Co/Zn ZIFs, ZIF-67 and ZIF-8. $Co(NO_3)_2·6H_2O$ (1.64 g) and $Zn(NO_3)_2·6H_2O$ (3.35 g) were dissolved in 120 mL of methanol as solution A. Additionally, 2-methylimidazole (3.70 g) were dissolved in 120 mL of methanol as solution B. Solution A and solution B were vigorously mixed and stirred at 25°C for 6 hours. The resulting precipitates were collected after centrifugation, washed 3 times with methanol and subsequently dried under vacuum at 70°C for 12 hours, yielding bimetallic Co/Zn ZIFs. ZIF-67 was prepared using only $Co(NO_3)_2·6H_2O$ without adding $Zn(NO_3)_2·6H_2O$, while ZIF-67 was also prepared using only $Zn(NO_3)_2·6H_2O$ without adding $Co(NO_3)_2·6H_2O$.

Synthesis of CoN4, CoN3, CoN2, CoNP and NC. The bimetallic Co/Zn ZIFs were subjected to different heating procedures under flowing argon gas in a tube furnace to obtain atomically dispersed cobalt catalysts (CoN4, CoN3, and CoN2). For CoN4 and CoN3, the Co/Zn ZIFs were heated to 800°C and 900°C at a rate of 5°C/min, respectively, and held for 3 hours. Regarding CoN2, the Co/Zn ZIFs were heated to 800°C at 5°C/min and maintained for 1 hour, then heated to 900°C at 5°C/min and held for 1 hour, followed by heating to 1000°C at 5°C/min and held for 1 hour. For CoNP, the ZIF-67 was heated to 900°C at 5°C/min and held for 3 hours. Additionally, for NC (nitrogen-containing carbon), the ZIF-8 was heated to 900°C at 5°C/min and kept at that temperature for 3 hours. After the completion of the heating process, the sample was naturally cooled to room temperature. The catalyst preparation process is outlined in Scheme S1.

Synthesis of CoNP-HCl. 0.50 g of CoNP was mixed with 20 mL of a 2M hydrochloric acid aqueous solution and stirred for 12 hours. The resulting CoNP-HCl was obtained through filtration, washed with deionized water, and subsequently dried under vacuum at 70°C for 12 hours.

General procedures to conduct the reaction. In a typical procedure, oxidized lignin β-O-4 model compounds, catalyst, solvent and n-dodecane (internal standard) were charged into a stainless-steel reactor with a quartz coating (20 mL inner volume). The reactor was sealed, purged with H_2 to eliminate residual air, and then pressurized with H2 up to 1MPa. Subsequently, the autoclave was immersed in a constant-temperature air bath, heated to the desired temperature, and reactions were carried out with a stirring speed of 700 rpm for the specified reaction period. Following the reaction, the reactor was cooled to room temperature, and the gas was released. The catalyst was separated via centrifugation, and the liquid supernatant was quantitatively analyzed using a GC (Agilent 7890B) equipped with a flame ionization detector (FID) and an Agilent HP-INNOWax capillary column (0.32 mm in diameter, 30 m in length). For 2-phenoxy-1-phenylethanimine and 1-phenylethanimine, their correction factors are set to the same as those of the corresponding ketones. The products and reactants were identified by a GC-MS (Agilent 7890B 5977A, HP-5MS capillary column (0.25 mm in diameter, 30 m in length)).

Recycling of catalyst. The spent CoN3 catalyst was gathered via centrifugation, followed by a wash with methanol. Subsequently, the methanol was removed by vacuum drying at room temperature.

Characterizations. The Co content was determined by inductively coupled plasma atomic emission spectrometry (ICP-OES) on Agilent ICPOES730. Inductively coupled plasma atomic emission spectrometry (ICP-AES) was adopted to measure the actual Co content. The X-ray powder diffraction (XRD) patterns were collected on a Rigaku D/max 2500 and operated at 40 kV applying a potential current of 20 mA in a scan rate of 5 °/min. from 8 to 60° with Cu- K_{α} radiation (λ = 0.154 nm). High resolution transmission electron microscopy (HRTEM) images, annular dark-field scanning transmission electron microscopy (ADF-STEM) and element energy dispersive spectroscopy (EDS) mapping images were obtained on JEM-2100F electron microscope operated at 200 kV. JEM ARM300F equipped with an EDX detector (JEOL) and an energy filter (GATAN) operated at 300 kV was used for aberration-corrected resolution high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images of atomically dispersed catalysts. Extended X-ray absorption fine structure (XAFS) spectroscopies of Co K edge (7709 eV) were performed at beamline 1W2B of the Beijing Synchrotron Radiation Facility (BSRF) at room temperature. The incident X-ray beam was tuned by a Si (111) double-crystal monochromators. The samples were measured in the fluorescence excitation mode using a silicon drift detector. The corresponding Co foil, CoO, and CoPc were used as reference samples and the spectrums collected in the transmission mode. X-ray absorption near-edge structures (XANES) and extended x-ray absorption fine structure (EXAFS) analyses were provided using Athena and Artemis program within the IFEFFIT software package. The experimental absorption coefficients as the function of energies were processed by background subtraction and normalization procedure. For the EXAFS analyses, Fourier transformed data in R space were analyzed by applying Co and CoPc model for the Co-Co and Co-N shell. Other details were described in Table S2. ^{1}H and ^{13}C NMR analysis was performed on a Bruker Avance II 400 MHz. Co K-edge XANES simulations were performed using the FDMNES code within the real-space full multiple scattering scheme using the muffin-tin approximation for the potential.[1] The energy-dependent exchange-correlation potential was computed using the real Hedin–Lundqvist scheme. The spectra were convoluted using a Lorentzian function with an energy-dependent width to account for the broadening caused by the core-hole width and the final state width.

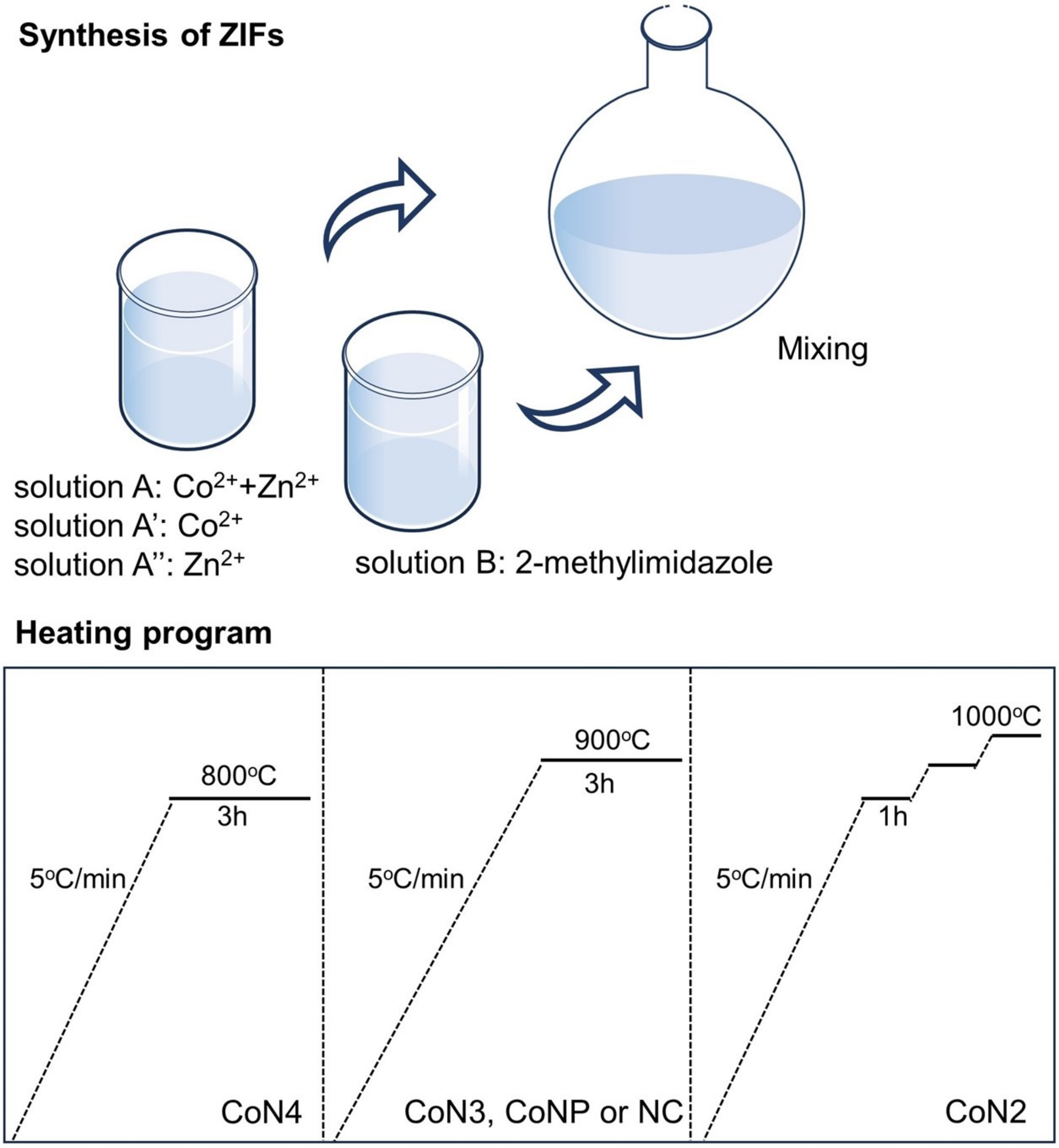
DFT calculations. We utilized the Vienna Ab initio Simulation Package (VASP) for all density functional theory (DFT) computations using the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). The projected augmented wave (PAW) method was employed to represent ionic cores and valence electrons, using a plane wave basis set with a kinetic energy cutoff of 450 eV. Geometry optimizations were conducted with forces converging to less than 0.05 eV/Å and an energy convergence of 1×10-5 eV. A Gamma Scheme k-point grid of 1×1×1 was applied, relaxing all atoms in the calculation. Additionally, spin-polarization effects were considered, with initial magnetic moments of Co atoms set at +2μB. The lattice parameters were defined as follows: a = b = c = 25.000 Å, α =90°, β = 90°, γ = 90°.

The adsorption energy (Ea) is calculated by the equation:

$$Ea = E(slab + C8H9N) - E(slab) - E(C8H9N).$$

where E(slab + C8H9N)and E(slab) are the total energy of the surface slab with and without C8H9N-adsorption, respectively, and E(C8H9N)is the total energy of the PMS molecule in the gas phase.

Results and Discussion



Scheme S1. Schematic illustrations of the synthesis process of ZIFs precursors and the heating program of CoN4, CoN3, CoN2, CoNP and NC (nitrogen-containing carbon).

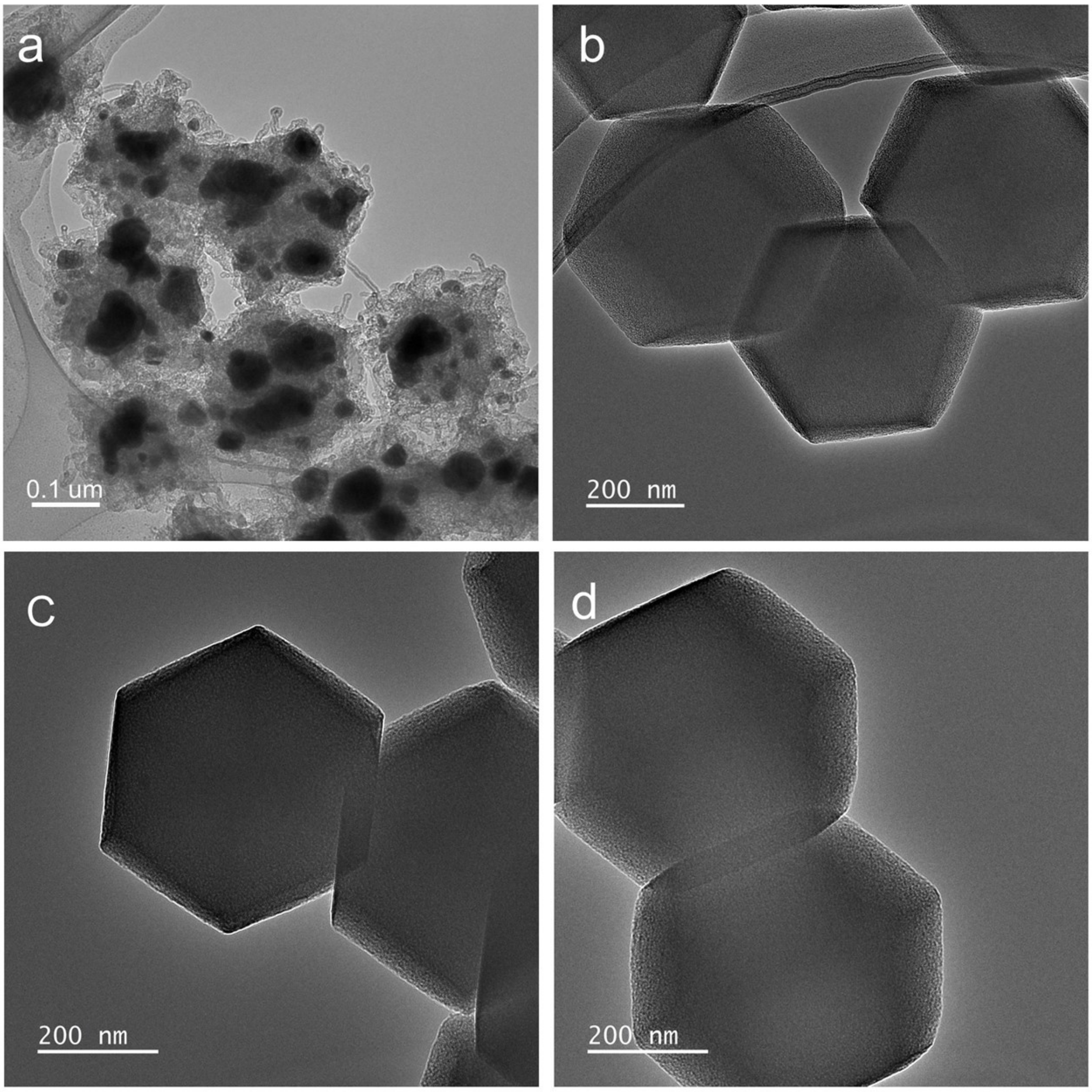


Figure S1. Transmission electron microscopy (TEM) images of (a) CoNP, (b) CoN4, (c) CoN3 and (d) CoN2. Obvious cobalt nanoparticles were observed in CoNP catalyst. Aggregation of cobalt species not found in zinc-cobalt bimetallic ZIFs after calcination at 800 °C to 1000 °C.

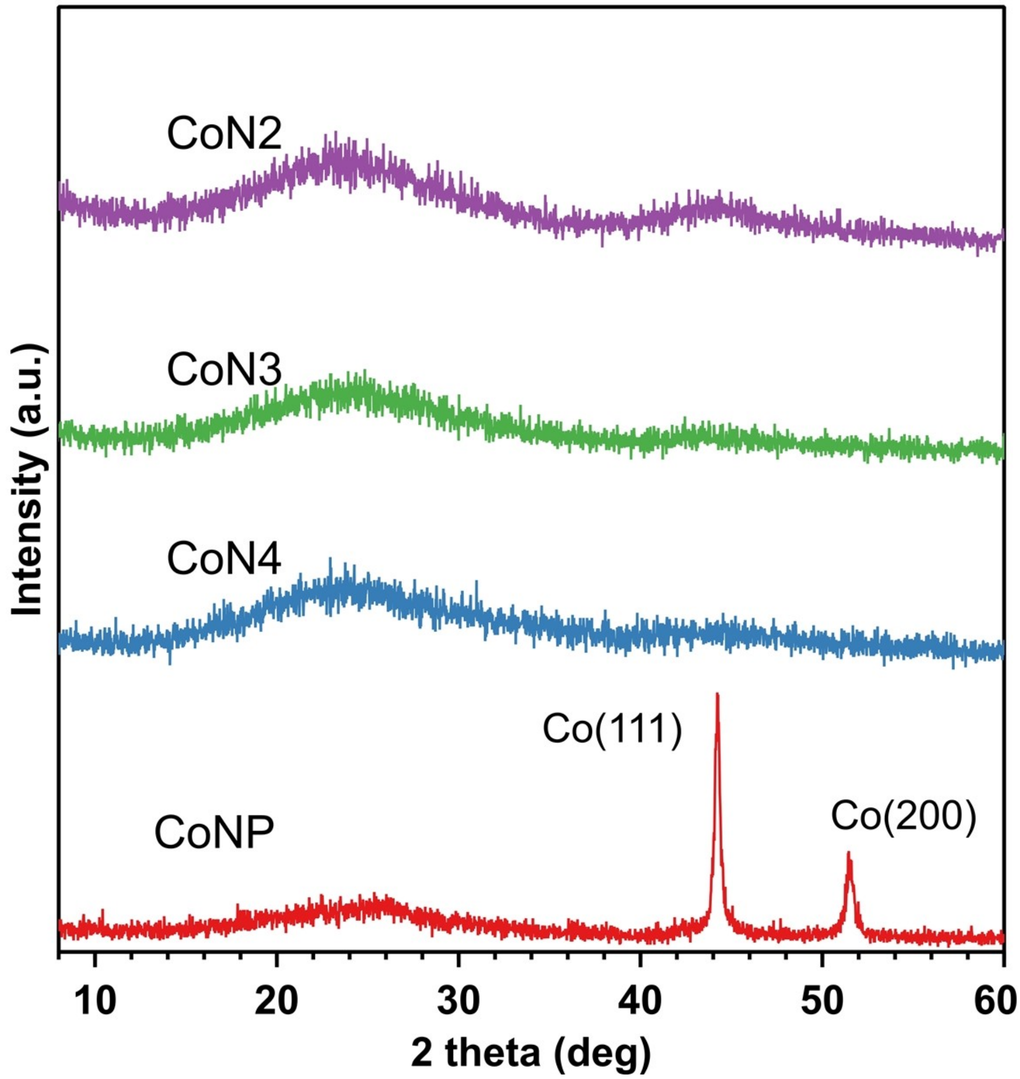


Figure S2. XRD patterns of CoNP, CoN4, CoN3 and CoN2. Two main diffraction peaks of CoNP located at 44.2 and 51.4^{o}, which can be assigned to the (111) and (200) crystal planes of metallic Co. There are no obvious diffraction peaks in zinc-cobalt bimetallic ZIFs after calcination at 800 °C to 1000 °C, except for the weak diffraction peaks from the carbon matrix.

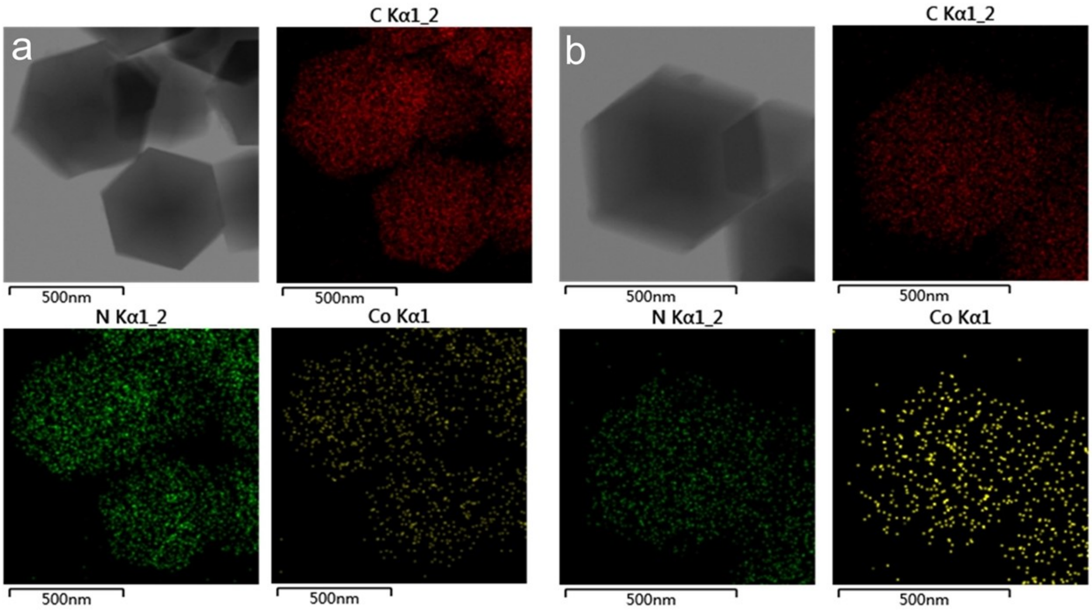


Figure S3. Scanning transmission electron microscopy (STEM) and EDS mapping images of (a) CoN4 and (b) CoN2.

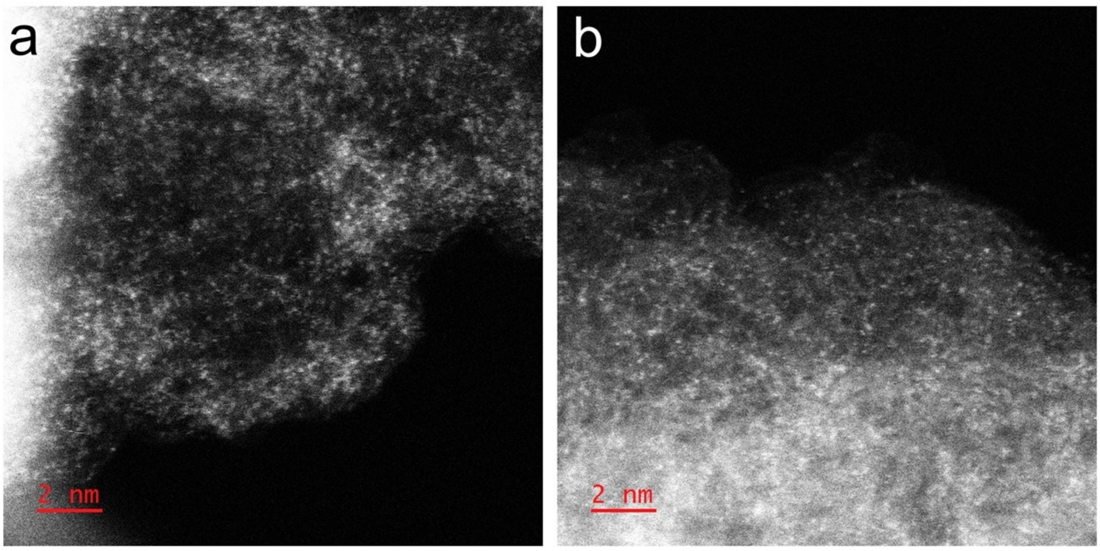


Figure S4. Aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images of (a) CoN4 and (b) CoN2.

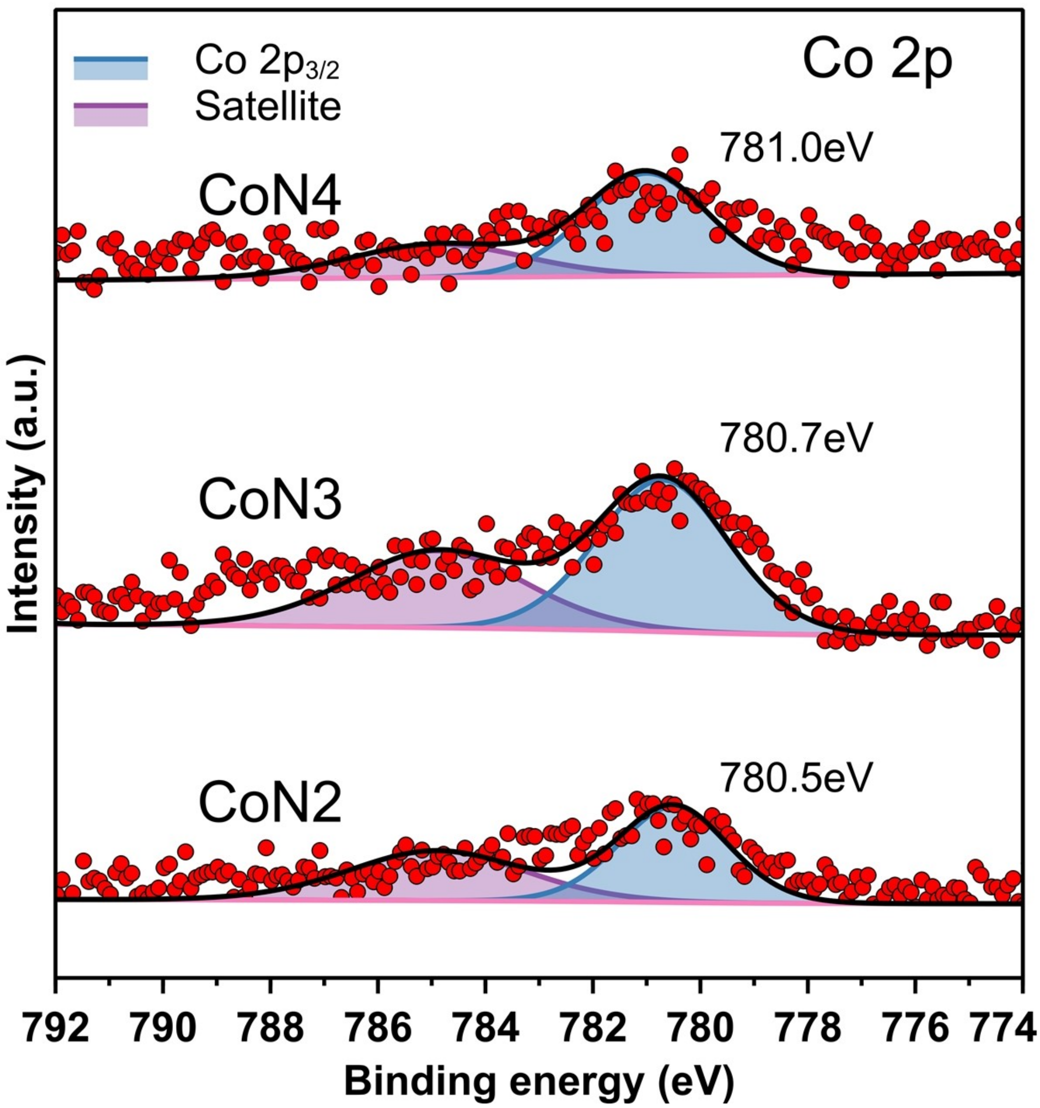


Figure S5. Co 2p XPS spectra of CoN4, CoN3 and CoN2. The binding energies of the Co 2p XPS measurements for CoN4, CoN3, and CoN2 samples exhibit a decreasing trend, consistent with the findings of XAFS (X-ray absorption fine structure) spectroscopy.

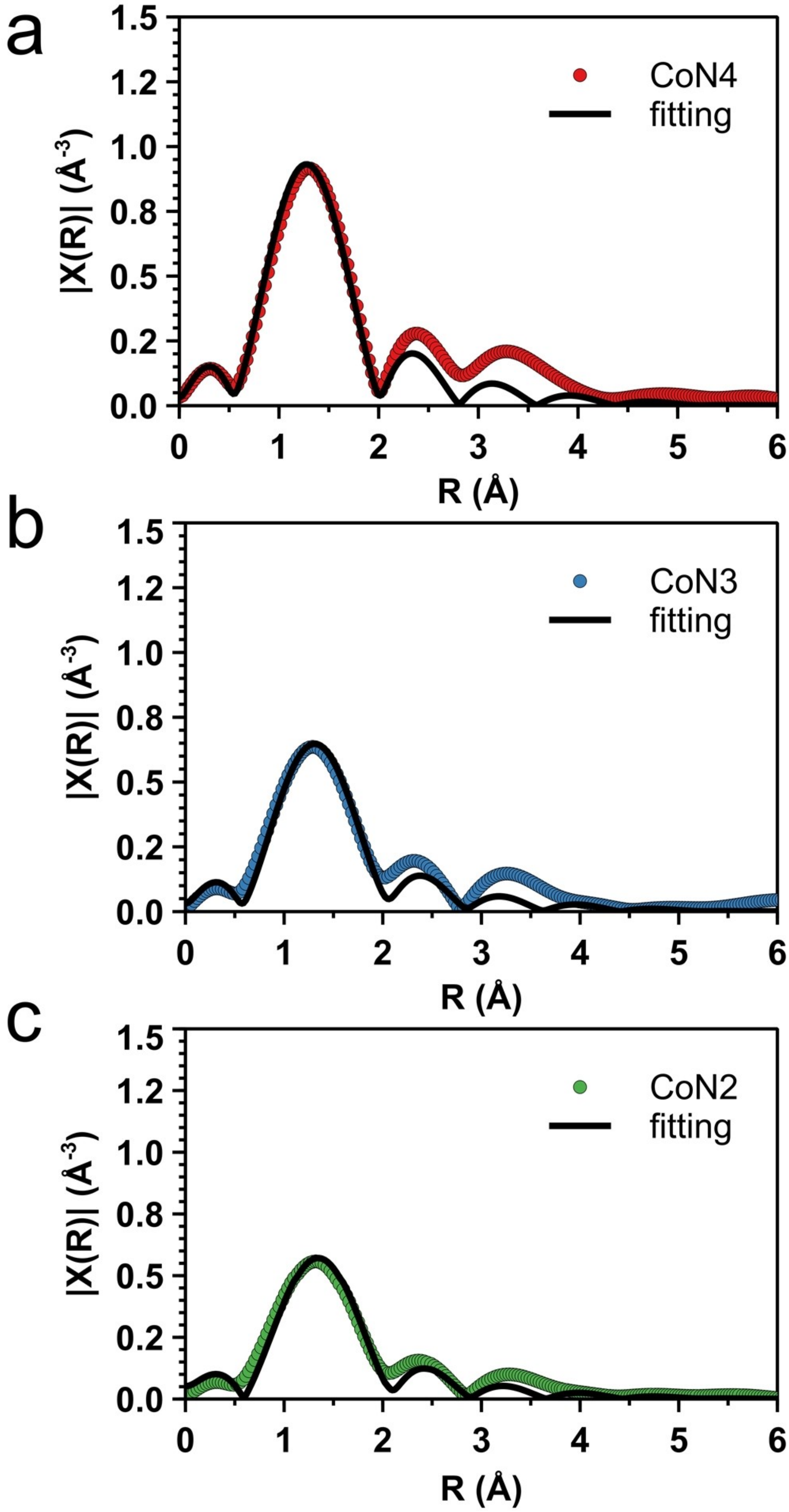


Figure S6. Co K-edge EXAFS spectra and fitting for (a) Co-N4, (b) Co-N3, (c) Co-N2. Structure parameters extracted from the EXAFS fitting are shown in Table S2.

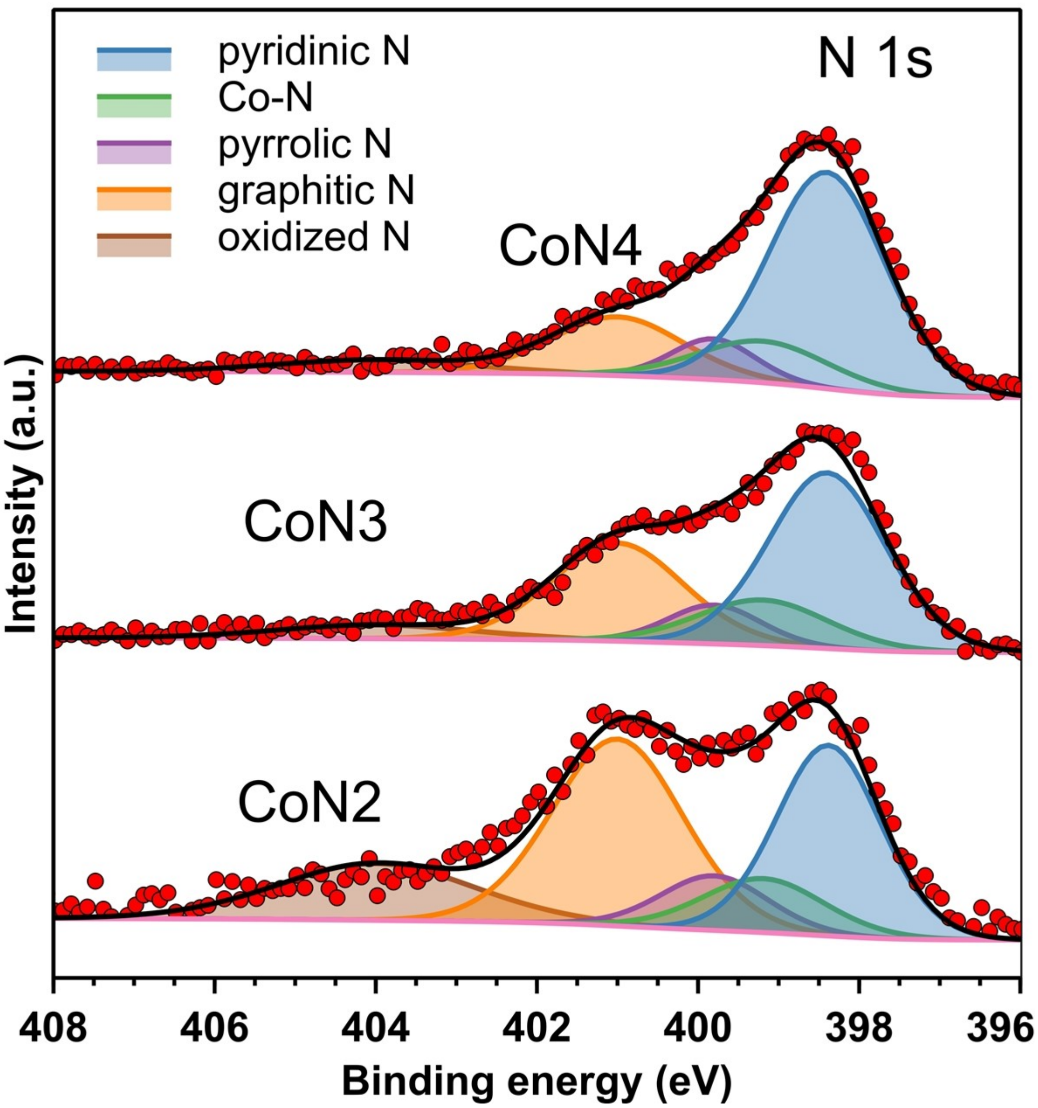


Figure S7. N 1s XPS spectra of CoN4, CoN3 and CoN2. The peaks of 398.4, 399.2, 399.8, 401.0 and 404.1 eV correspond to pyridinic N, Co-N, pyrrolic N, graphitic N and oxidized N, respectively.

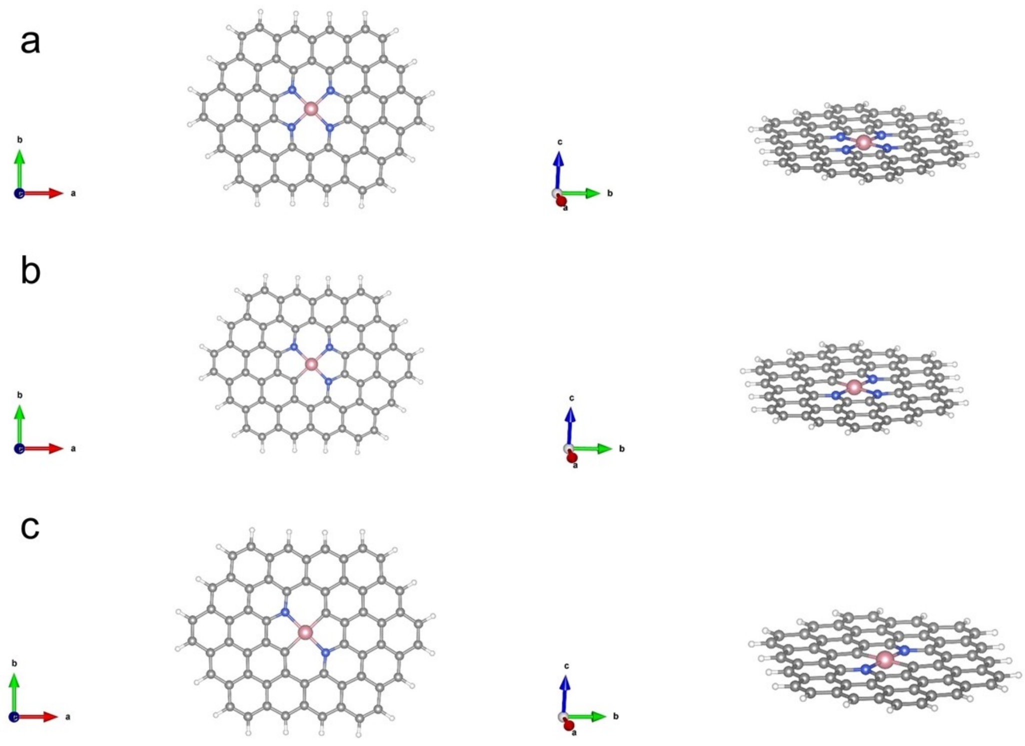


Figure S8. The top and side views of (a) CoN4, (b) CoN3 and (c) CoN2 structure.

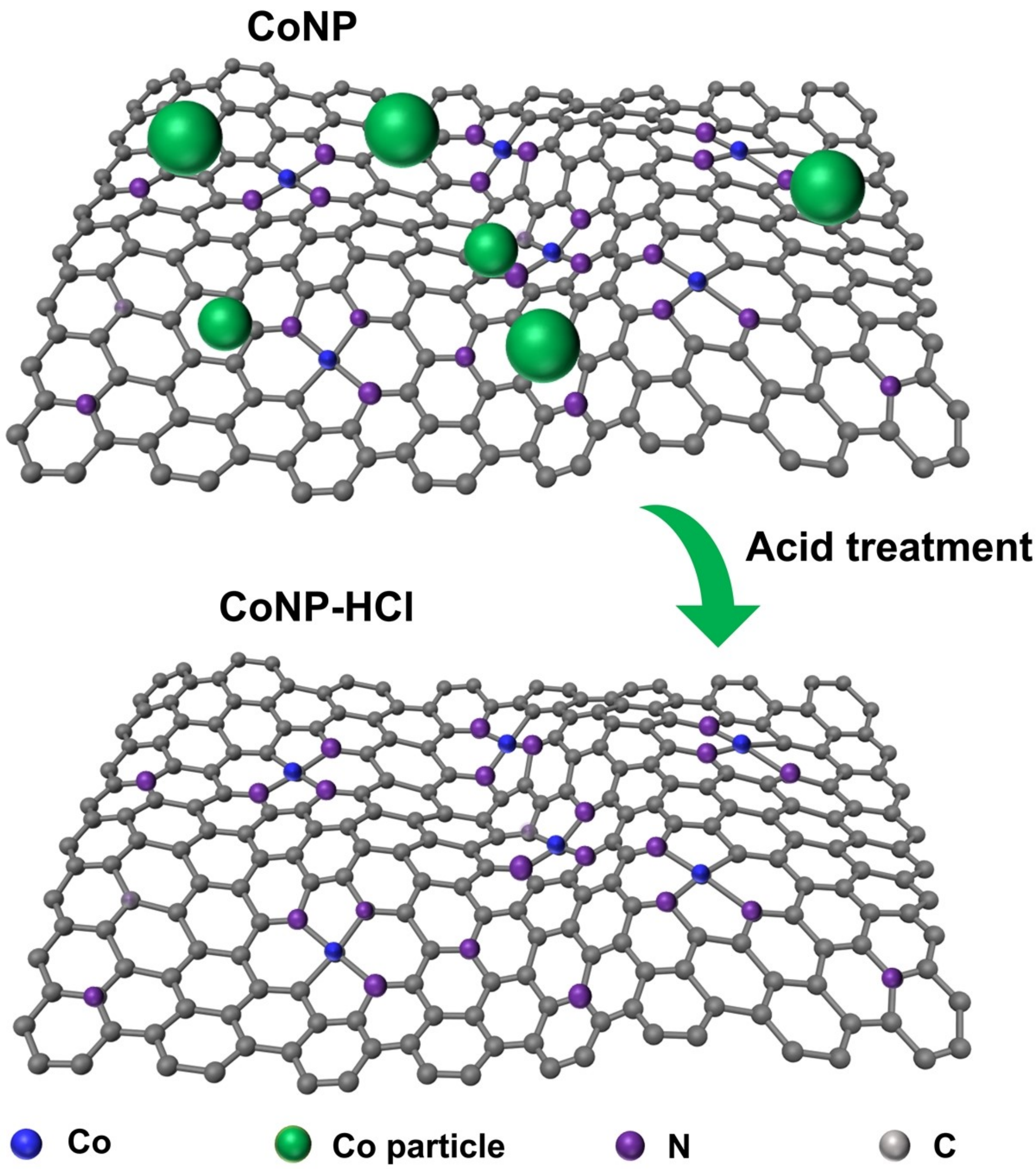


Figure S9. Schematic illustrations of the acid treatment process of CoNP. The CoNP (0.50g) was added to 20mL of 2M hydrochloric acid aqueous solution and stirred for 12h. CoNP-HCl was obtained by filtration, washed with deionized water, and dried in vacuum at 70^{o}C for 12 h.

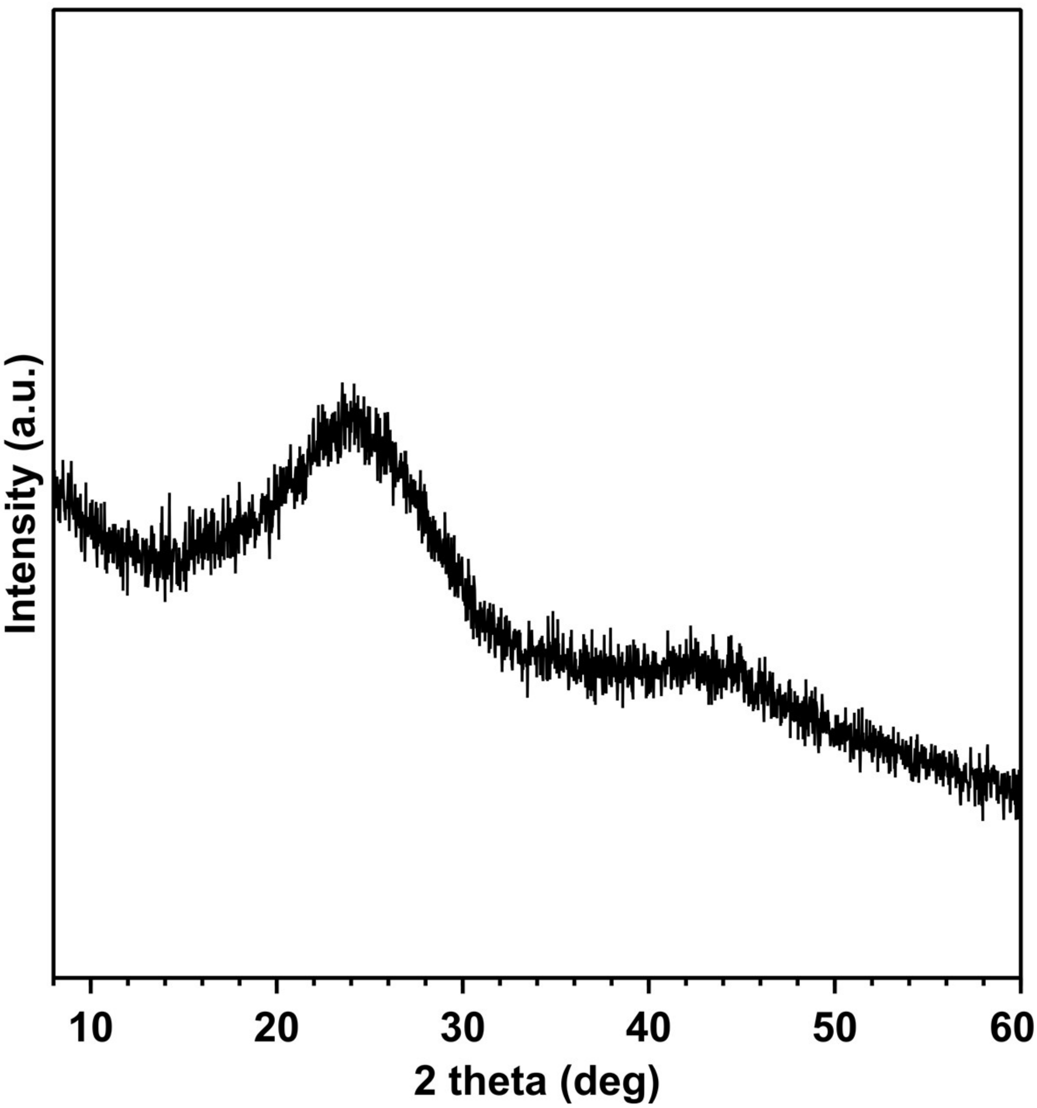


Figure S10. XRD pattern of the CoN3 catalyst after four cycles.

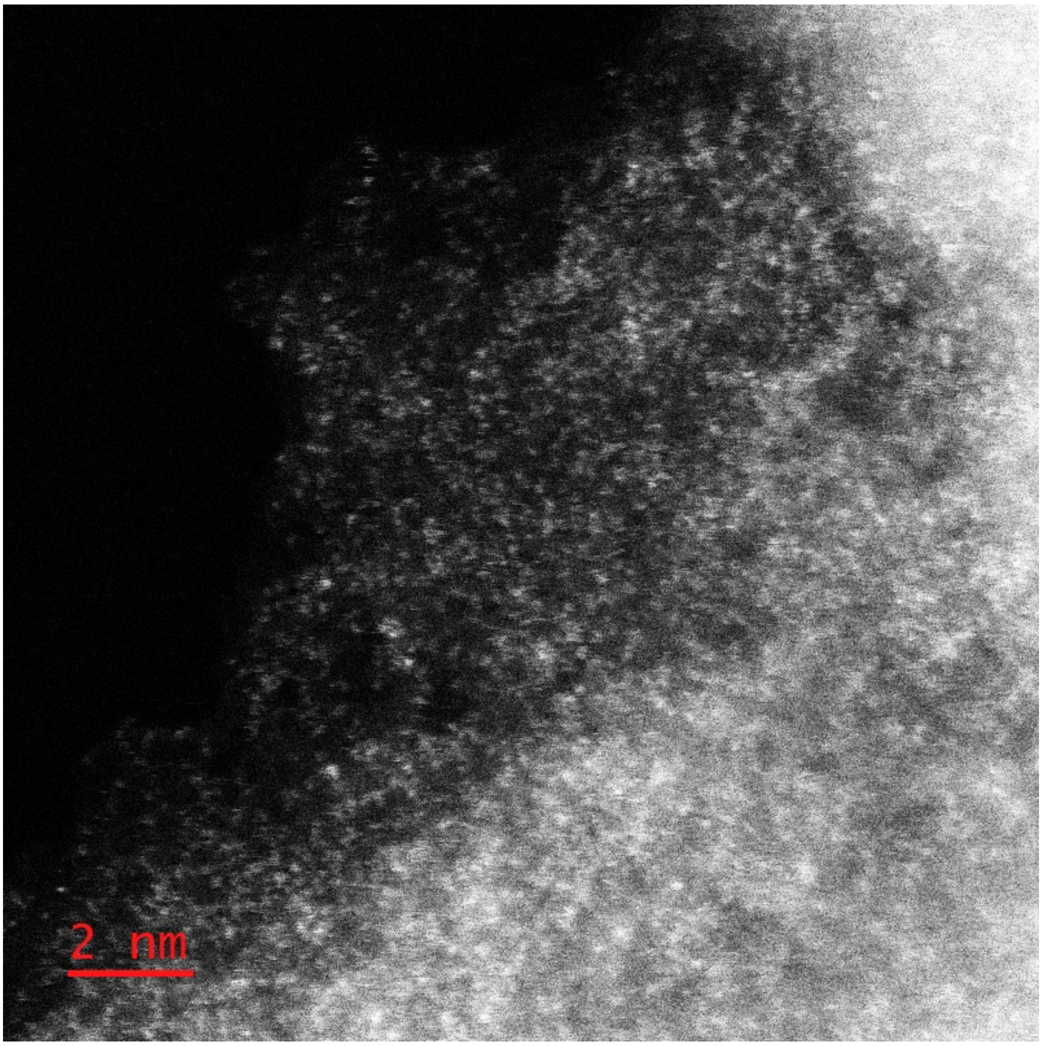


Figure S11. HAADF-STEM image of the CoN3 catalyst after four cycles.

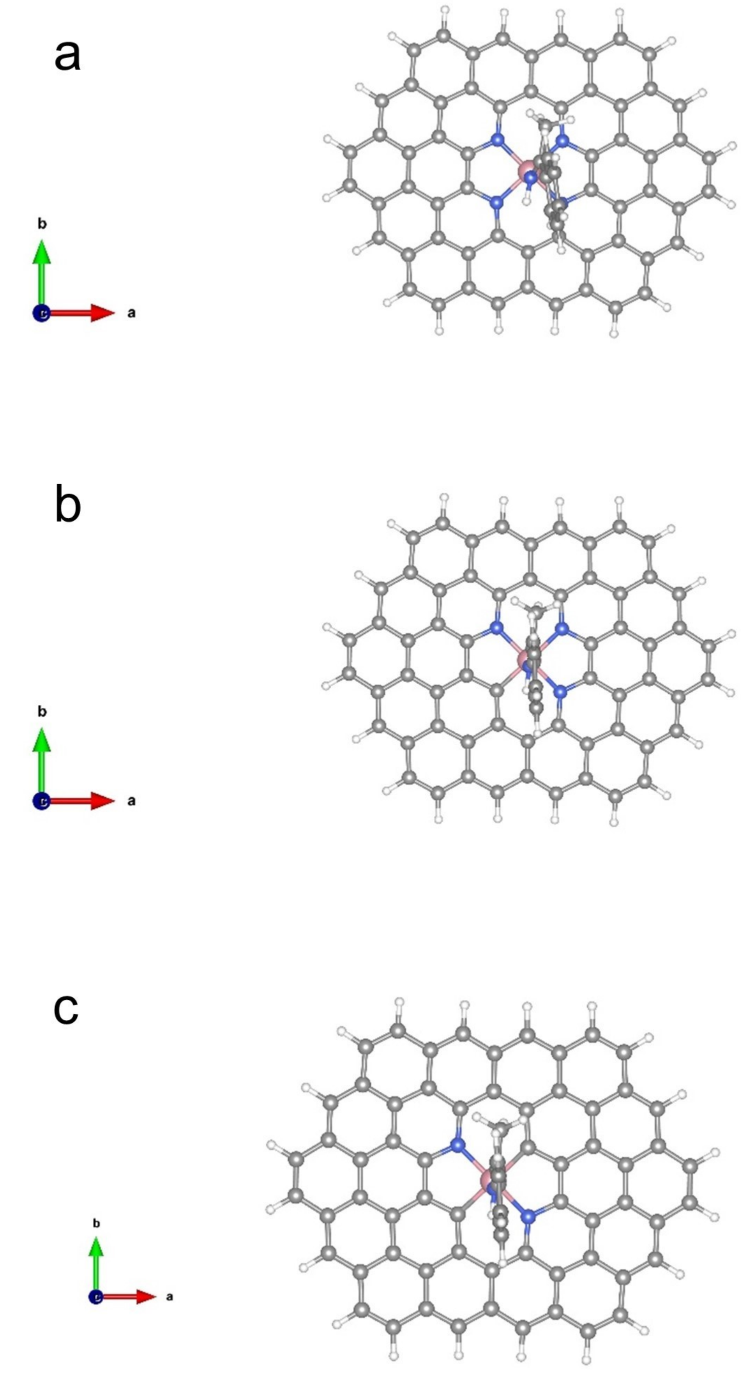


Figure S12. The top views of final state for the direct dissociation of imine **1i** over (a) CoN4, (b) CoN3 and (c) CoN2.

Table S1. The metal content of Co in the catalyst measured by ICP-OES.

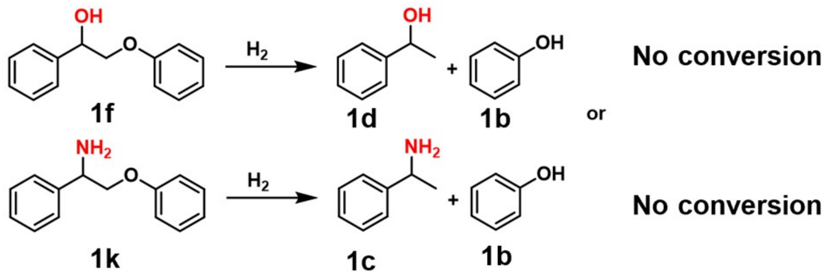
Entry	Catalyst	Content/wt.%
1	CoNP	40.5
2	CoN4	1.6
3	CoN3	1.6
4	CoN2	2.0

Table S2. Curve Parameters for Co K-edge EXAFS for CoN4, CoN3 and CoN2.

Sample	Shell	CN	$\sigma^2/(10^{-3}Å^2)$	$\Delta E_{0/eV}$	R/Å	R factor
CoN4	Co-N	4.0(5)	1.5	-9.6	1.86(4)	0.018
CoN3	Co-N	3.2(4)	3.2	-7.0	1.89(4)	0.032
CoN2	Co-N	2.5(5)	1.2	-5.4	1.92(5)	0.034

The passive electron factors ($S0^2$) were set from fitting the experimental data of Co foil while the Co-Co coordination number (CN) was fixed. S_0^2 was fixed at 0.93. Data ranges: $3 \leq k \leq 7.1$ Å^{-1}, $1.0 \leq R \leq 2.7$ Å. CN: coordination number. R: bond distance. σ^2: Debye-Waller factors. ΔE_0: the inner potential correction.

Table S3. Catalytic performances of Co-based catalysts for the hydrogenolysis of 1f and 1k.



Entry	Catalyst	Conv. (%) of 1f	Conv. (%) of 1k
1	CoNP	-	-
2	CoN4	-	-
3	CoN3	-	-
4	CoN2	-	-

Reaction conditions: acetophenone, 0.2 mmol; 7 M ammonia solution in methanol, 2 mL; H_2, 1.0 MPa; catalyst, 15 mg; 140 °C; 6 h. Yields were determined by GC with dodecane as an internal standard.

No conversion was detected for substrate 1f or 1k under reaction conditions.

Table S4. Comparison of dissociation energy of C_{β}-O bond.

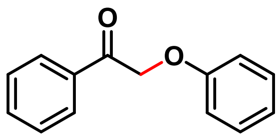
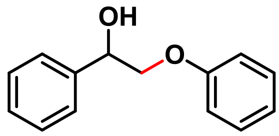
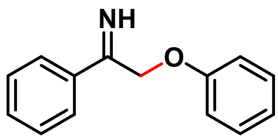
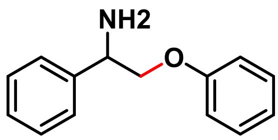
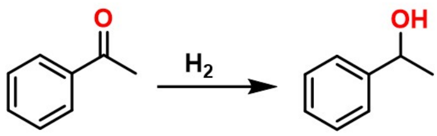
Entry	Compound	BDE (kJ mol^{-1})
1		255.1
2		294.1
3		255.6
4		291.6

Table S5. Catalytic performances of CoSA catalysts for the hydrogenation of 1e.



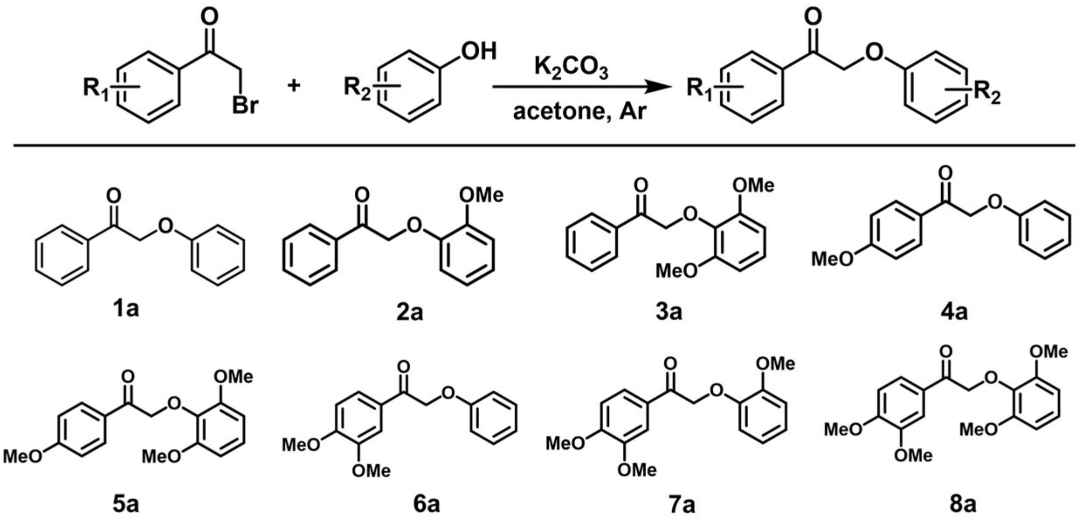
1e 1d

Entry	Catalyst	Conv. (%) of 1e	Yeild (%) of 1d
2	CoN4	2	1
3	CoN3	18	18
4	CoN2	17	17

Reaction conditions: acetophenone, 0.2 mmol; methanol, 2 mL; H_2, 1.0 MPa; catalyst, 15 mg; 140 ^{o}C; 4 h. Yields were determined by GC with p-xylene as an internal standard.

Procedure for preparation of oxidized lignin model compounds.

Oxidized lignin model compounds were prepared by reference.[2] Phenol (10.5 mmol) and K_2CO_3 (10.7 mmol) in acetone (22 mL) was added into 50 mL 3-neck- boiling flask in Ar atmosphere and stirred at room temperature for 30 min. To this solution, 2-bromoacetophenone (10.0 mmol) was added. The resulting suspension was stirred at RT for 16 h, after which the suspension (K_2CO_3) was filtered and solution was concentrated in a rotary evaporator. The solid obtained was dissolved in ethyl acetate and washed with NaOH aqueous (5%, 30 mL) and water (30 mL) in separatory funnel. The organic phase was dried over anhydrous Na_2SO_4. The crude product was recrystallized from ethanol to give 2-phenoxy-1-phenylethanone. For the other methoxyl substituted substrates, the preparation procedure is the same as described above, except that using different stating materials.



^{1}H and ^{13}C NMR spectra of substrate 2a

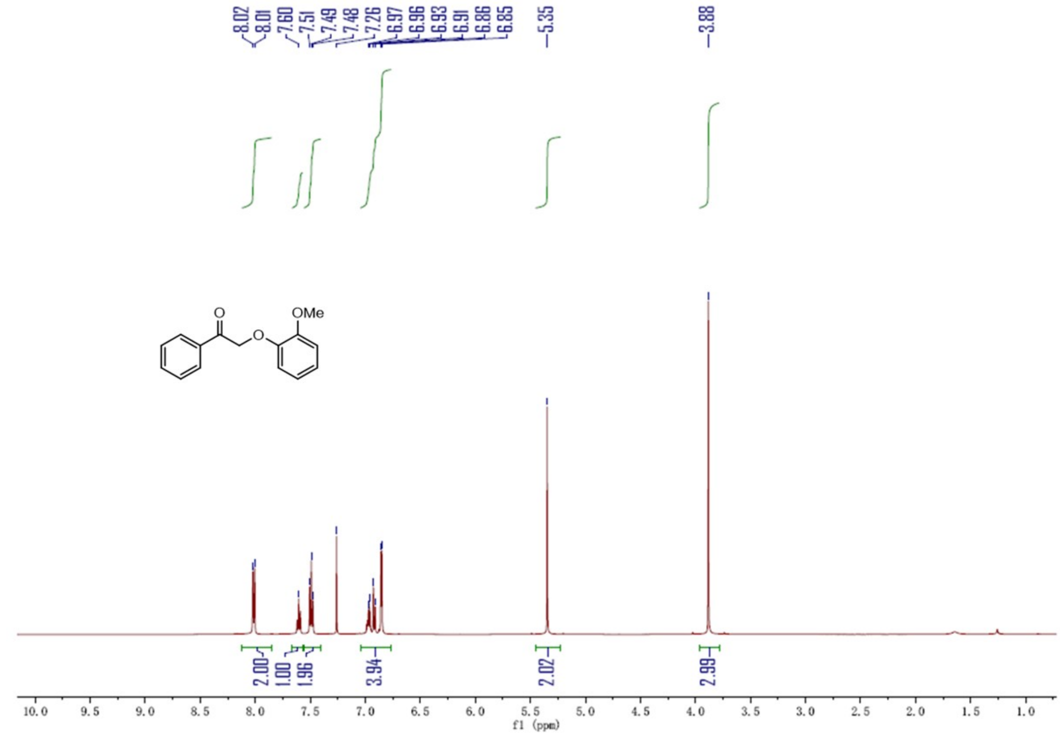


Figure S13. ^{1}H NMR of 2-(2-Methoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

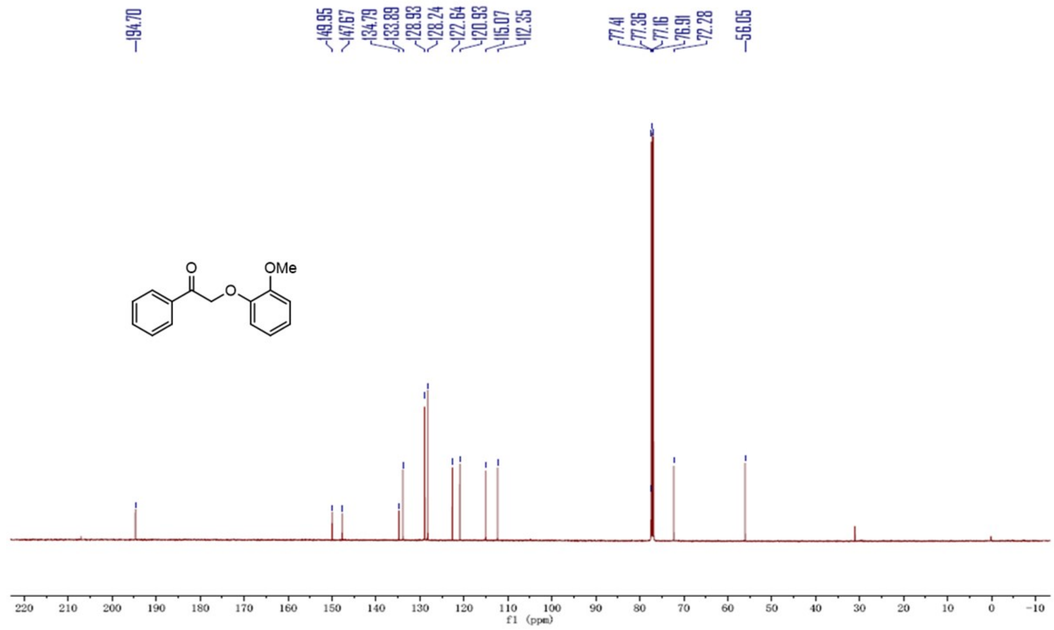


Figure S14. ^{13}C NMR of 2-(2-Methoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

^{1}H and ^{13}C NMR spectra of substrate 3a

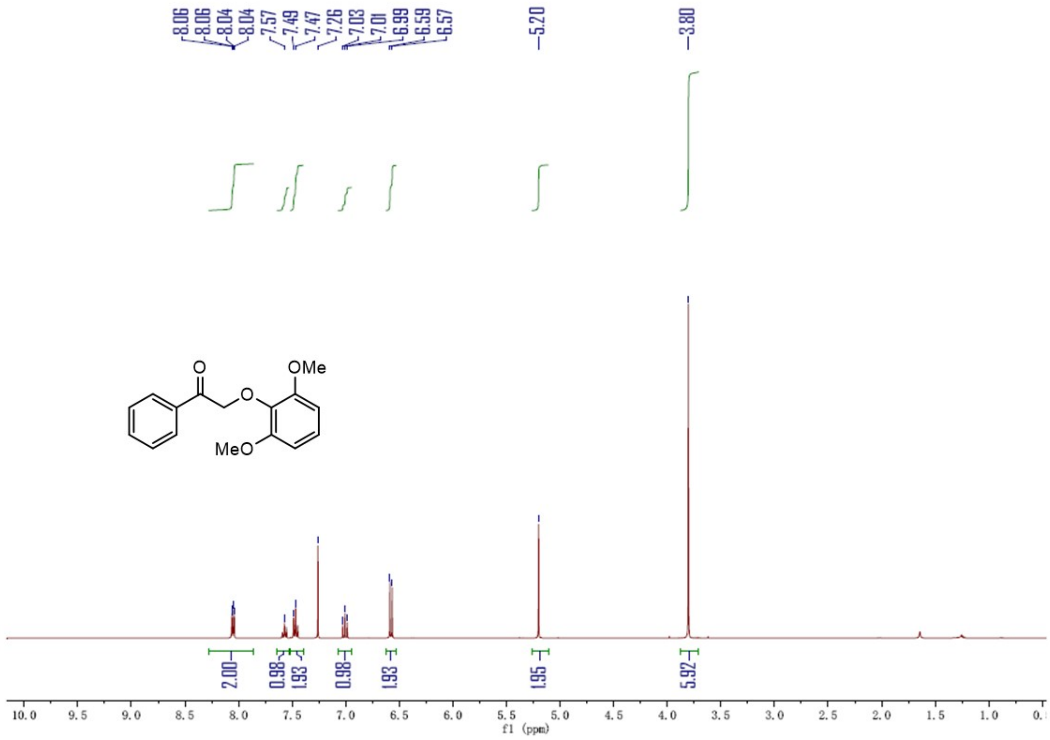


Figure S15. ^{1}H NMR of 2-(2,6-Dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

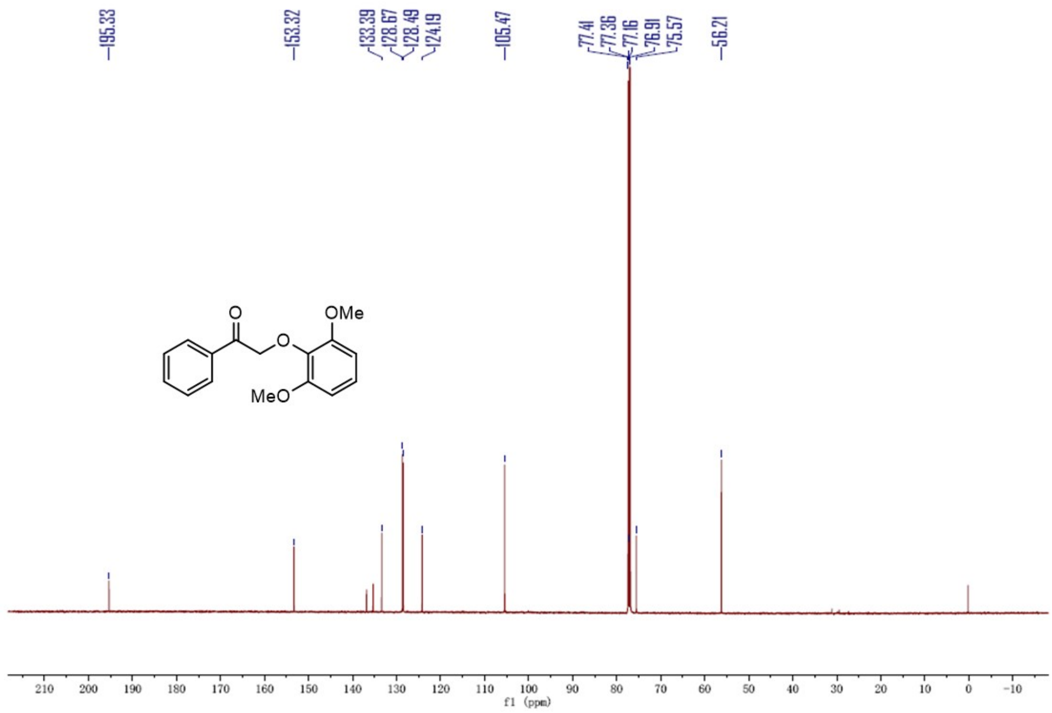


Figure S16. ^{13}C NMR of 2-(2,6-Dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

^{1}H and ^{13}C NMR spectra of substrate 4a

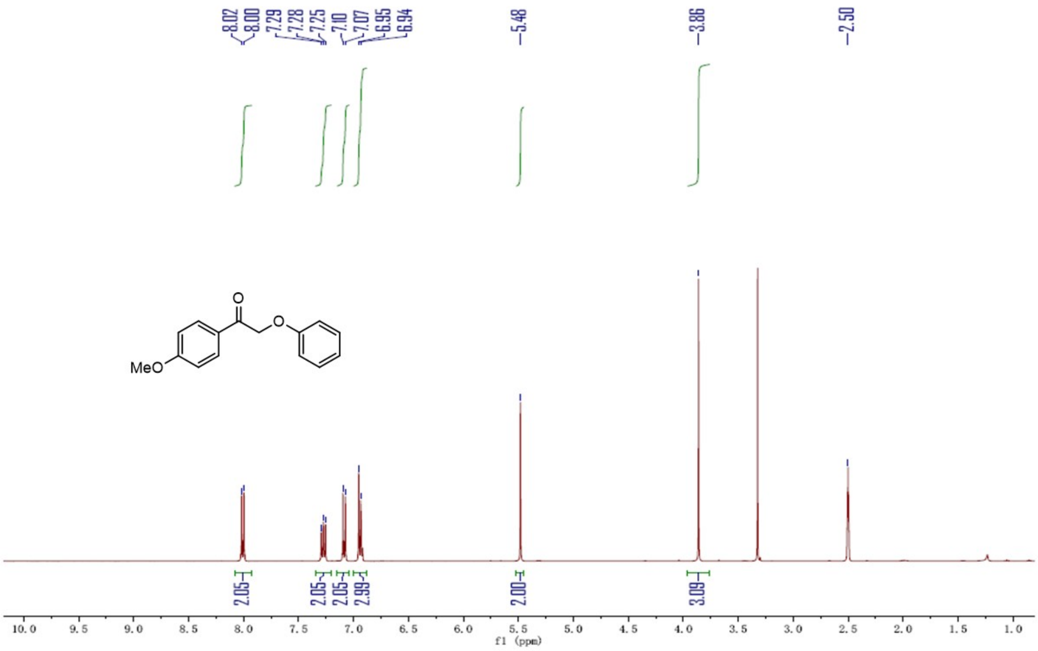


Figure S17. ^{1}H NMR of 1-(4-Methoxyphenyl)-2-phenoxyethan-1-one in $(CD_3)_2SO$.

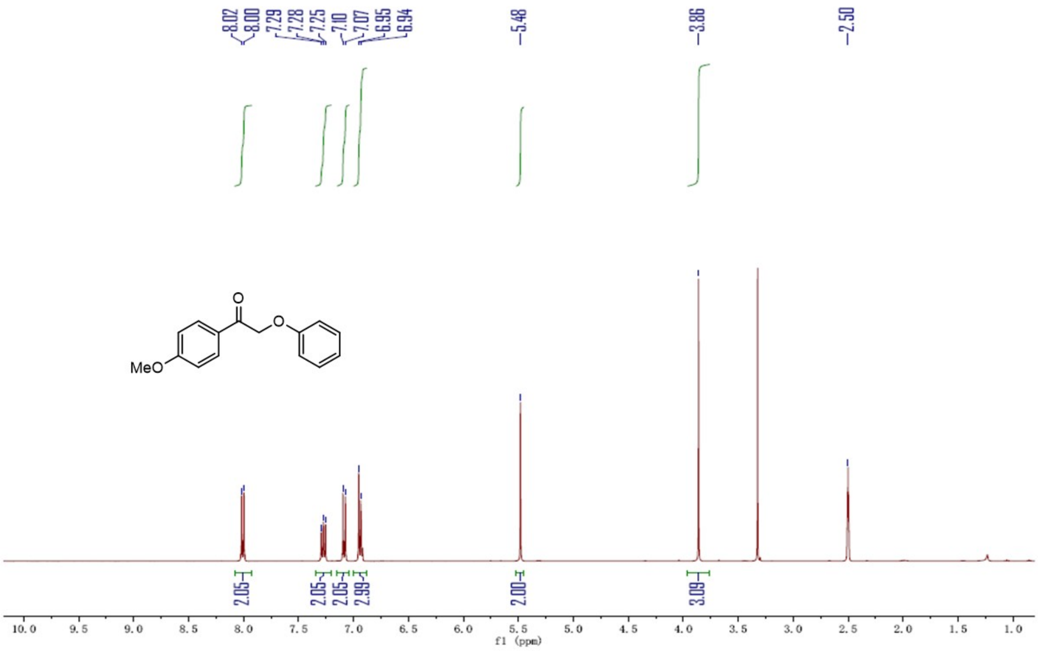


Figure S18. ^{13}C NMR of 1-(4-Methoxyphenyl)-2-phenoxyethan-1-one in $(CD_3)_2SO$.

^{1}H and ^{13}C NMR spectra of substrate 5a

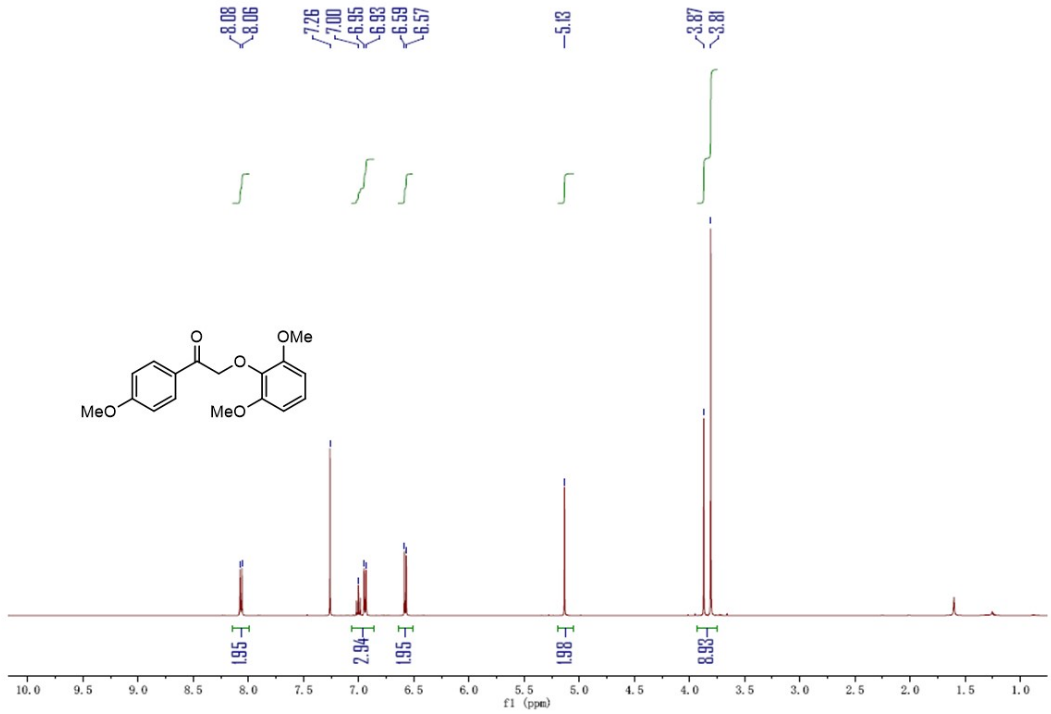


Figure S19. ^{1}H NMR of 2-(2,6-Dimethoxyphenoxy)-1-(4-methoxyphenyl)ethan-1-one in $CDCl_3$.

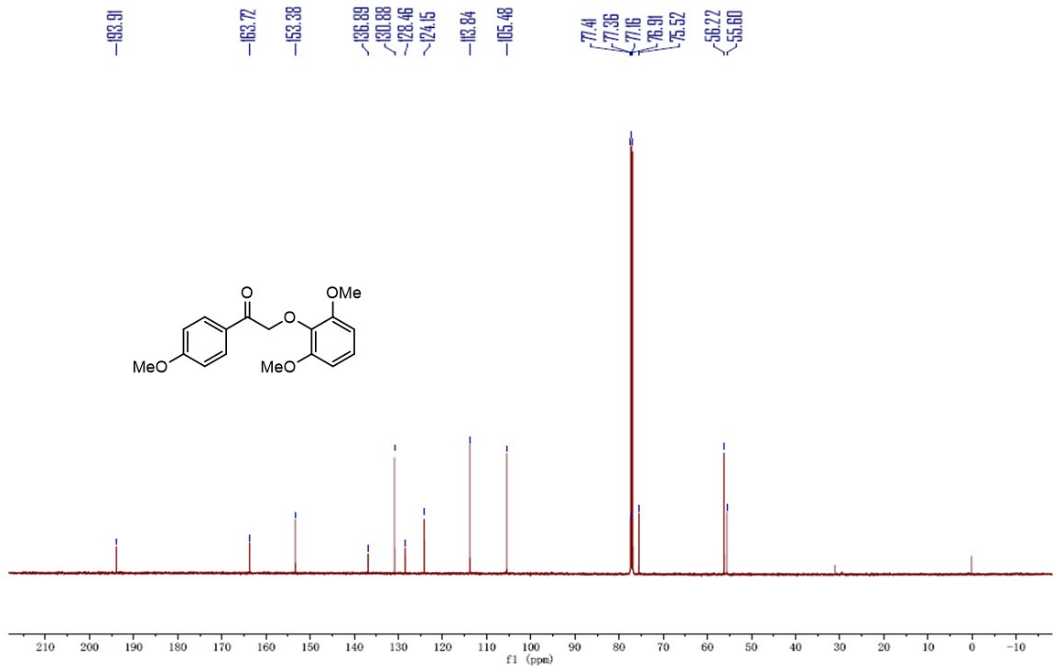


Figure S20. ^{13}C NMR of 2-(2,6-Dimethoxyphenoxy)-1-(4-methoxyphenyl)ethan-1-one in $CDCl_3$.

^{1}H and ^{13}C NMR spectra of substrate 6a

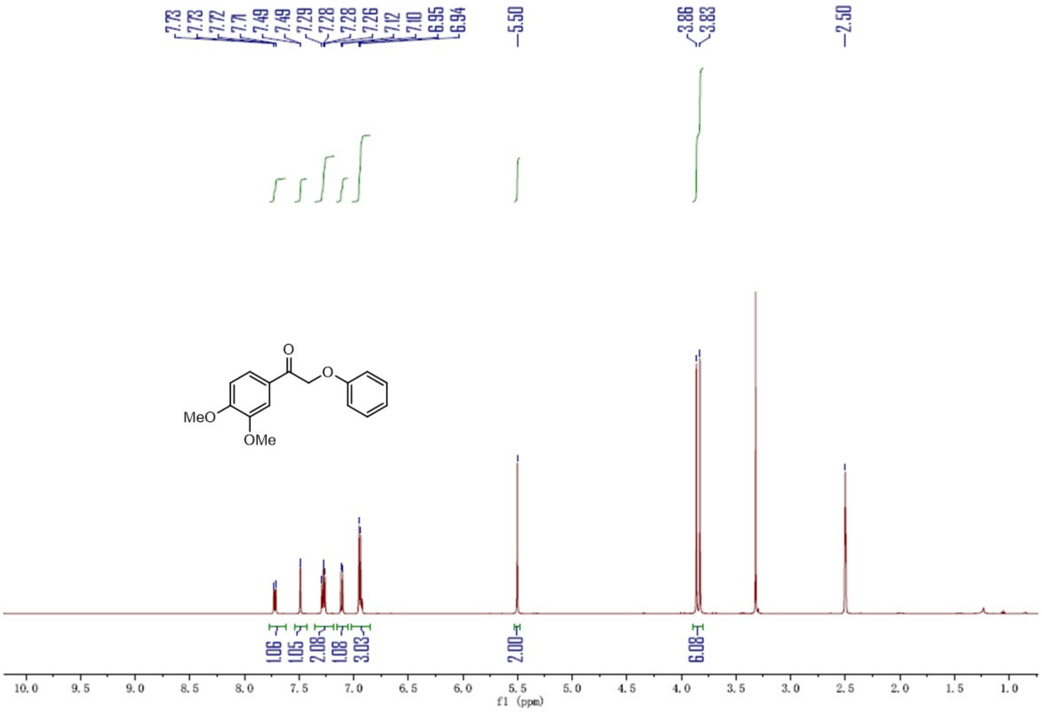


Figure S21. ^{1}H NMR of 1-(3,4-Dimethoxyphenyl)-2-phenoxyethan-1-one in $(CD_3)_2SO$.

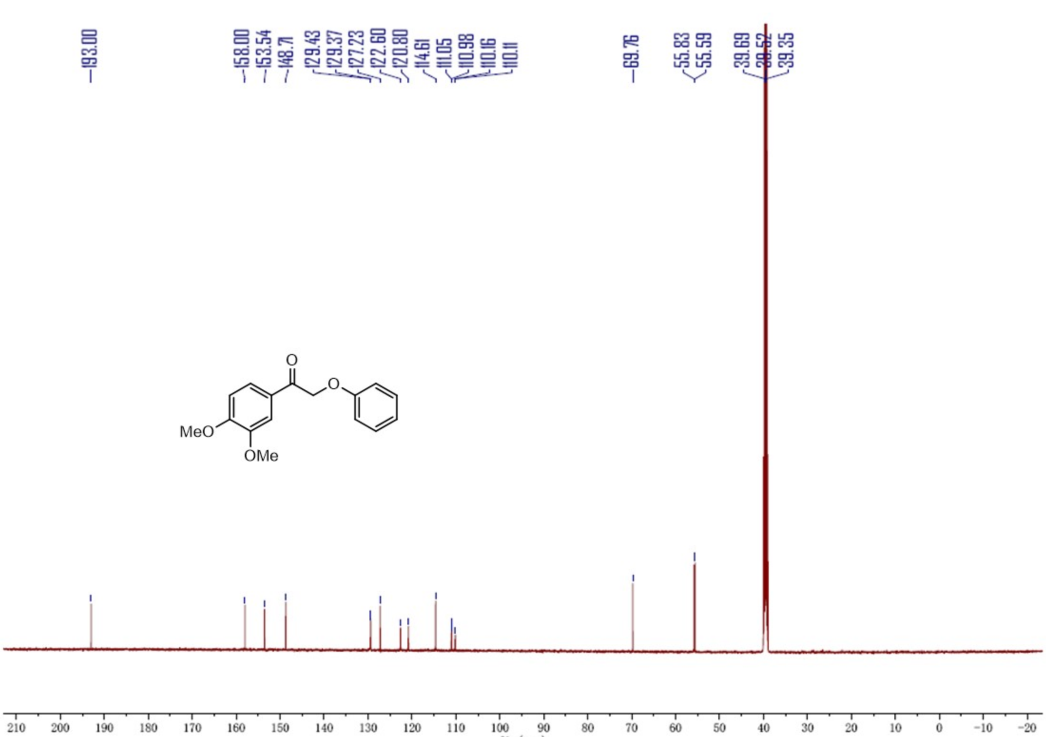


Figure S22. ^{13}C NMR of 1-(3,4-Dimethoxyphenyl)-2-phenoxyethan-1-one in (CD_3)2SO.

^{1}H and ^{13}C NMR spectra of substrate 7a

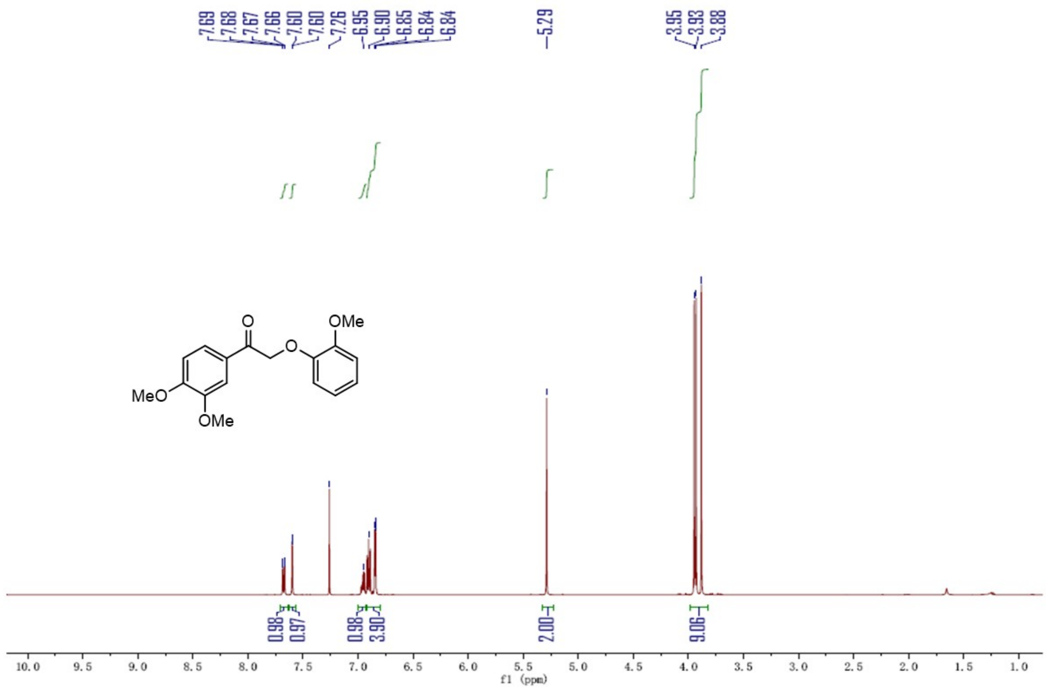


Figure S23. ^{1}H NMR of 1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)ethan-1-one in $CDCl_3$.

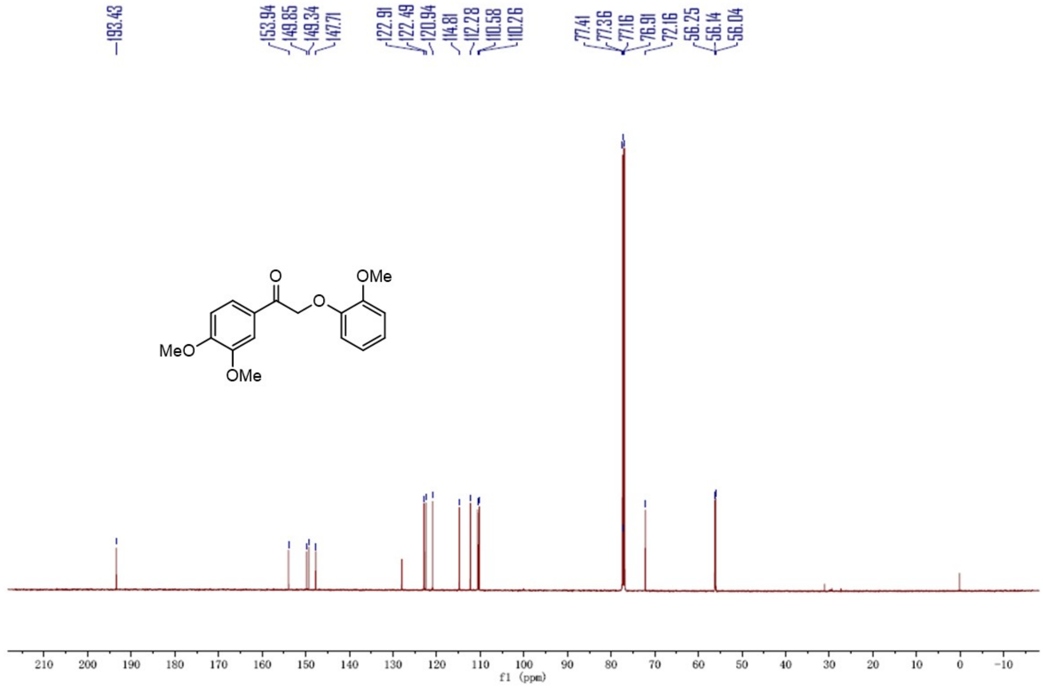


Figure S24. ^{13}C NMR of 1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)ethan-1-one in $CDCl_3$.

^{1}H and ^{13}C NMR spectra of substrate 8a

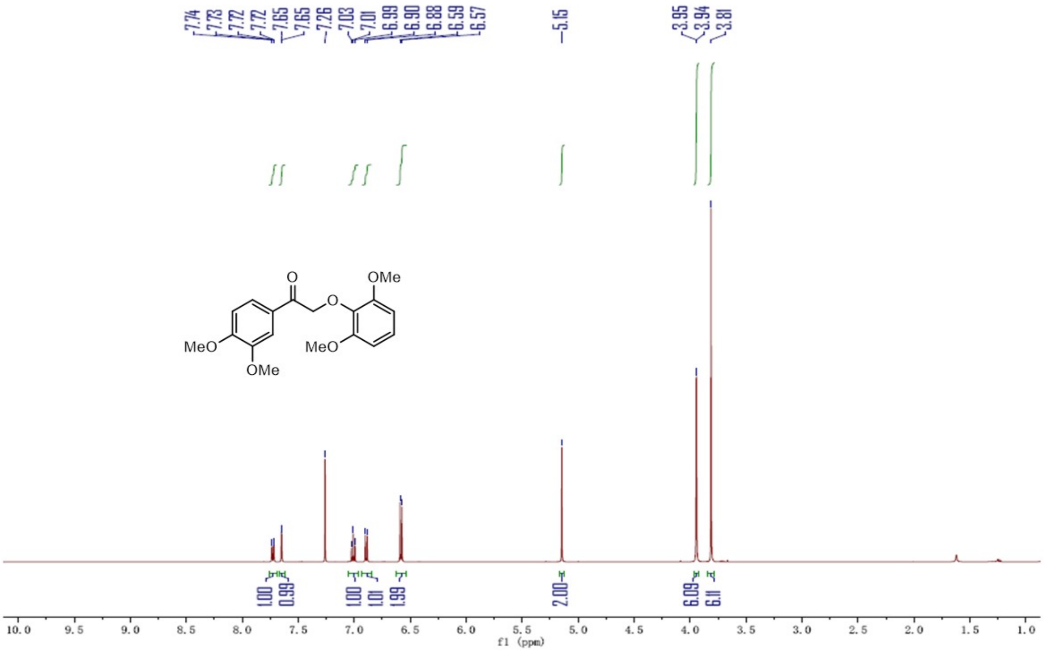


Figure S25. ^{1}H NMR of 2-(2,6-Dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$.

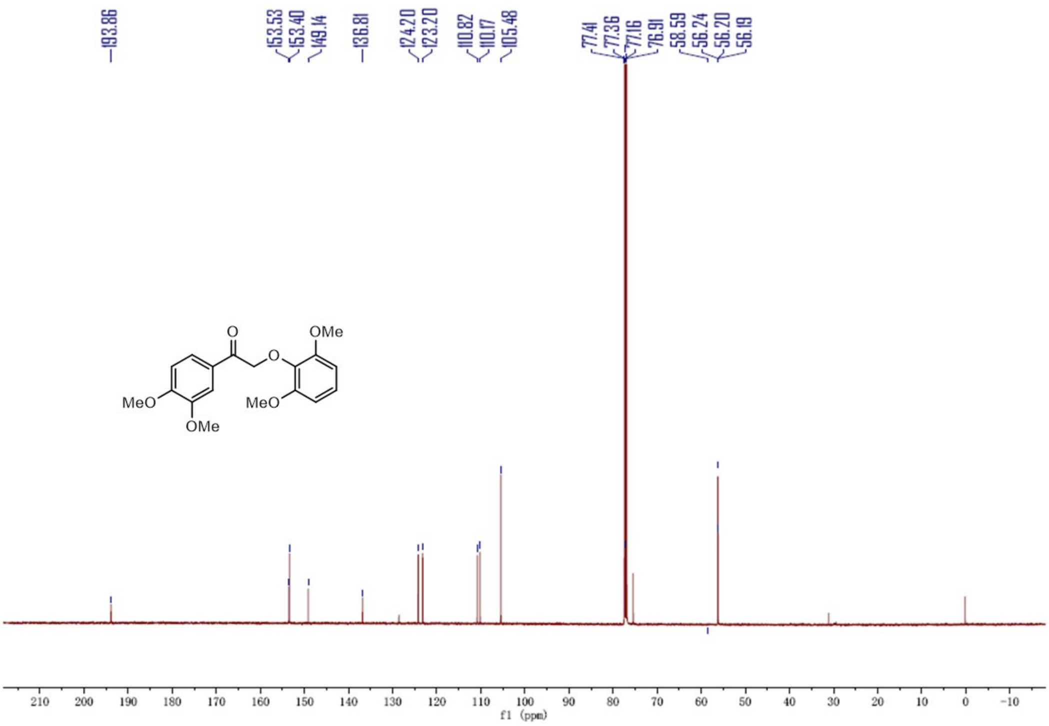
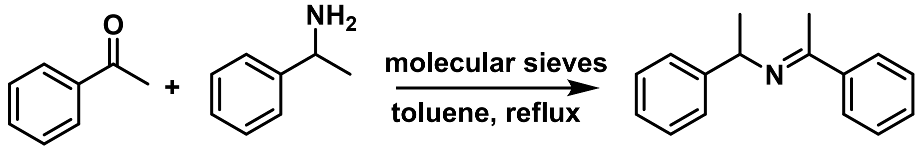


Figure S26. ^{13}C NMR of 2-(2,6-Dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$.

Procedure for preparation of 1-phenyl-N-(1-phenylethyl)ethan-1-imine. 1-phenyl-N-(1-phenylethyl)ethan-1-imine was prepared by previous report.[3] In a Dean-Stark apparatus, a 125 mL toluene solution of 10 ml acetophenone and 11 ml 1-phenylethanamine in the presence of 4 molecular sieves was refluxed for 12 h. The reaction mixture was then filtered and the solvent was removed under reduced pressure. The crude product was further purified by decompression distillation at 140°C.



^{1}H and ^{13}C NMR spectra of substrate 1-phenyl-N-(1-phenylethyl)ethan-1-imine

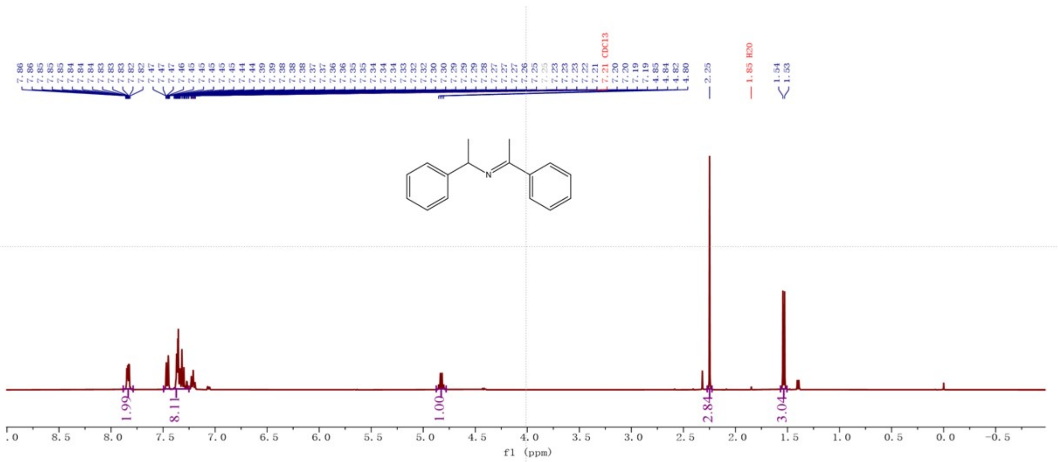


Figure S27. ^{1}H NMR of 1-phenyl-N-(1-phenylethyl)ethan-1-imine in $CDCl_3$.

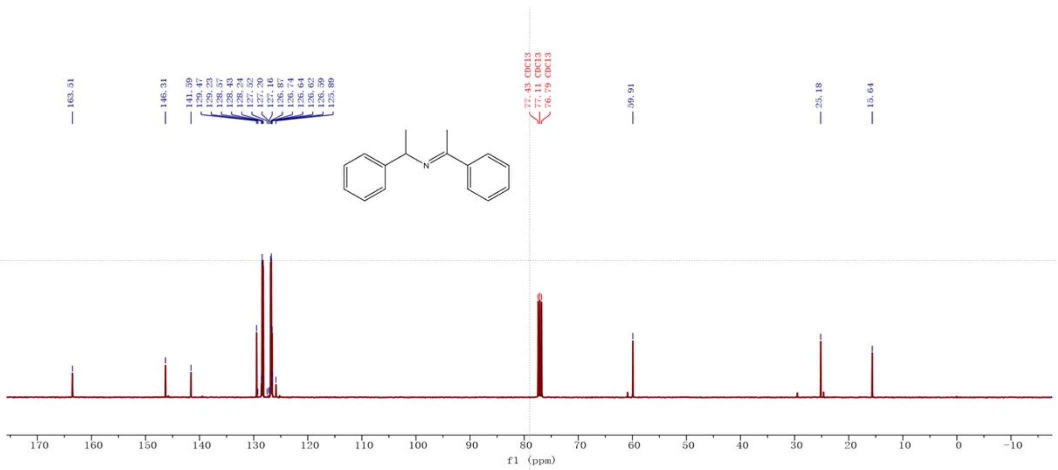
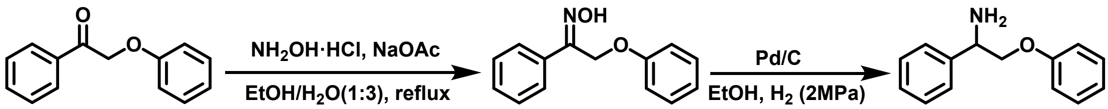


Figure S28. ^{13}C NMR of 1-phenyl-N-(1-phenylethyl)ethan-1-imine in $CDCl_3$.

Procedure for preparation of 2-phenoxy-1-phenylethan-1-one oxime.

Step1: 2-phenoxy-1-phenylethan-1-one oxime was prepared by previous report.[4] To a solution of **1a** (10 mmol) in EtOH:H2O (1:3, 80 mL) was added $NH_2OH{\cdot}HCl$ (15 mmol), $NaOAc{\cdot}3H_2O$ (25 mmol) at room temperature. The mixture was heated to reflux. After the reaction, the mixture was extracted with ethyl acetate for three times and washed with saturated brine. The organic phase was dried by anhydrous $MgSO_4$. The solution was concentrated under reduced pressure. The solid was precipitated by dropping a concentrated solution into a large amount of petroleum ether. Finally, the product was obtained by filtration and drying to remove the excess solvent.

Step2: 0.2 g of 2-phenoxy-1-phenylethan-1-one oxime, 2 mL of ethanol and 10 mg of Pt/C catalyst were added to an autoclave reactor, filled with 2 MPa H_2 and stirred at room temperature for 24 h. The catalyst was filtered off and the solvent was removed by distillation under reduced pressure to obtain 2-phenoxy-1-phenylethanamine. 2-phenoxy-1-phenylethanamine was treated with hydrochloric acid to obtain the corresponding salt which were also subjected to NMR analysis.



^{1}H and ^{13}C NMR spectra of substrate 2-phenoxy-1-phenylethanamine.

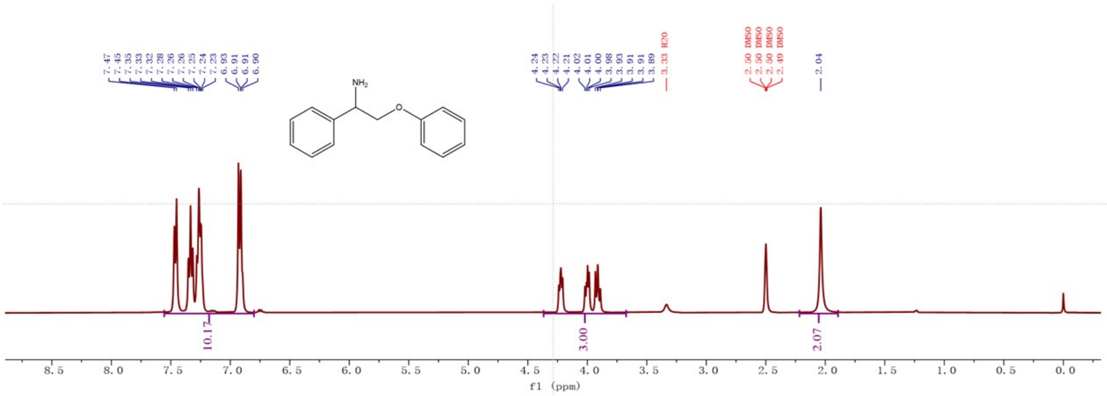


Figure S29. ^{1}H NMR of 2-phenoxy-1-phenylethanamine in DMSO-d_6.

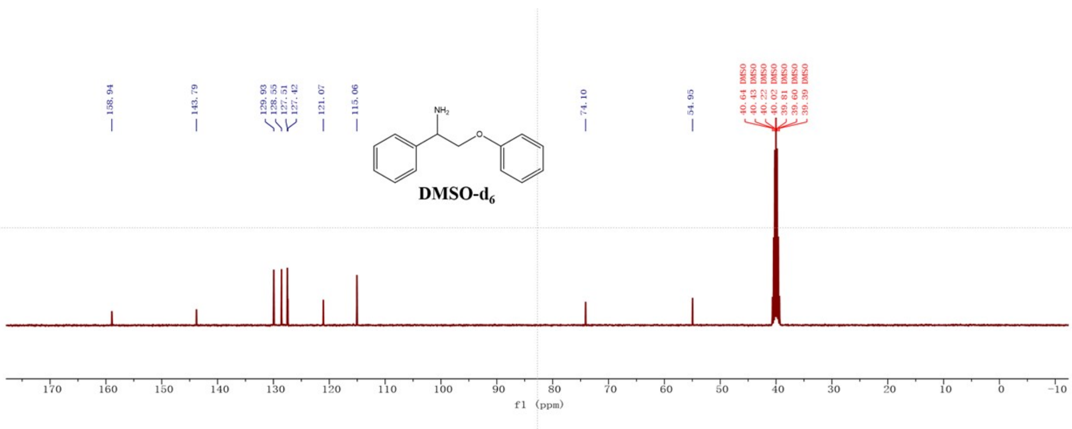


Figure S30. ^{13}C NMR of 2-phenoxy-1-phenylethanamine in DMSO-d_6.

^{1}H and ^{13}C NMR spectra of substrate 2-phenoxy-1-phenylethanamine hydrochloride.

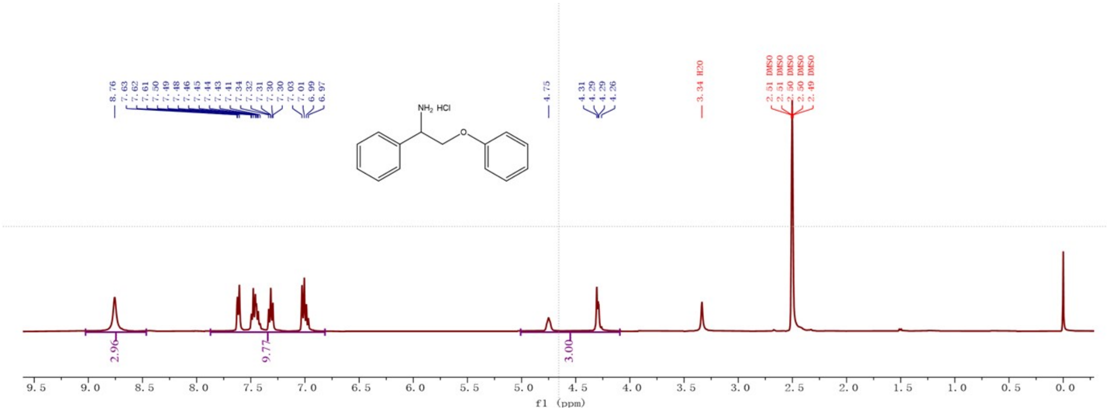


Figure S31. ^{1}H NMR of 2-phenoxy-1-phenylethanamine hydrochloride in DMSO-d_6.

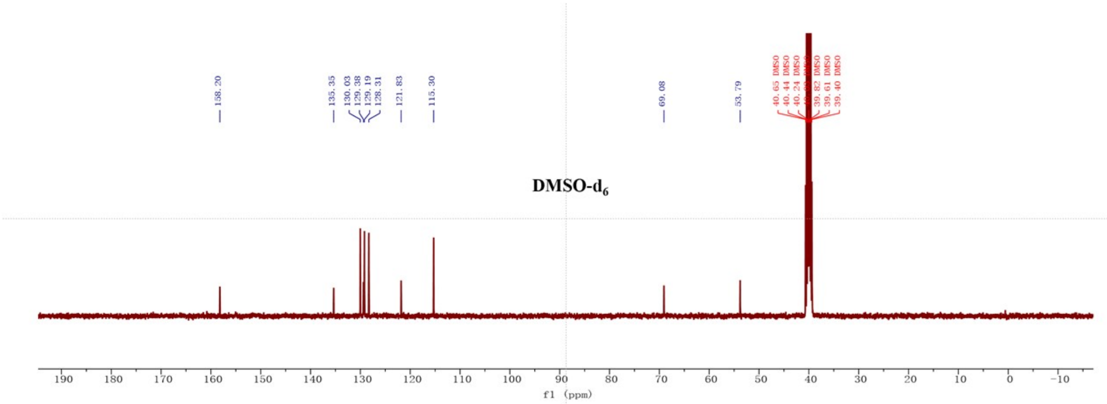


Figure S32. ^{13}C NMR of 2-phenoxy-1-phenylethanamine hydrochloride in DMSO-d_6.

Refences

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Structure Information

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0.2949360404340188	0.7029497393167552	0.3037687175873400	T	T	T

0.3905635838129112	0.6399411660085210	0.2992375289801790	T	T	T
0.3439266948455019	0.7271897776106816	0.3042942101818386	T	T	T
0.3343645036954425	0.4463863502403126	0.2908714870055287	T	T	T
0.4429489313038750	0.7217084098204536	0.3021130775606369	T	T	T
0.3931496711427630	0.6972360433254241	0.3019594640385325	T	T	T
0.3863130670387627	0.3058114203765122	0.2833580617748023	T	T	T
0.3860766342066249	0.3632357654959130	0.2858998334556448	T	T	T
0.3356691353755197	0.3899095344447550	0.2881358783247997	T	T	T
0.5898345620172533	0.4701900518341692	0.2845239331010922	T	T	T
0.4338517750021589	0.4493476711139644	0.2889562225313748	T	T	T
0.5429977080092387	0.5521260178347865	0.2903154590798929	T	T	T
0.5400102796321785	0.4468591510752398	0.2851956064338378	T	T	T
0.4339786214117831	0.5532211592378574	0.2941493119468119	T	T	T
0.4875924252493639	0.4998676465733624	0.2899500884994289	T	T	T

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H	C	N	Co
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Selective dynamics
Direct

0.3463265555164212	0.7711223915347676	0.3064308247566157	T	T	T
0.4445424225505454	0.7664132204144378	0.3042672096928423	T	T	T
0.5392940926956660	0.7645292640718264	0.3021144364077588	T	T	T
0.6387002363359646	0.7664849153219866	0.3000548295697675	T	T	T
0.7249676981084405	0.7188004307309718	0.2952765500290929	T	T	T
0.7756043363132027	0.6323559834541673	0.2893868722186837	T	T	T
0.8258689123182524	0.5434233337258791	0.2842768611283933	T	T	T
0.8238501459909237	0.4450093053348530	0.2797198007647602	T	T	T
0.7708564385428036	0.3584674523112915	0.2768168555399957	T	T	T
0.7170867591396920	0.2729470616074345	0.2747564531441751	T	T	T
0.6285747526060587	0.2288328258275335	0.2750619730053934	T	T	T
0.5305359742853681	0.2335797245135039	0.2771601729219065	T	T	T
0.4359010419411452	0.2354807948077589	0.2792765605591692	T	T	T
0.3365560659097817	0.2334652977354631	0.2812719442332959	T	T	T
0.2502435482964221	0.2811398664373373	0.2847164702325192	T	T	T
0.1994987957913469	0.3676591512663453	0.2886864789209247	T	T	T
0.1491706301740933	0.4565961120542910	0.2923409703153679	T	T	T
0.1511059707895629	0.5549963706731652	0.2968709927782510	T	T	T
0.2041187583121550	0.6415729312393362	0.3012872470175317	T	T	T
0.2579507069698666	0.7270517482278979	0.3054663289062676	T	T	T

0.3355846710134733	0.2771352283937813	0.2831378546814999	T	T	T
0.5327428857593881	0.2772020124250885	0.2786645863262708	T	T	T
0.6316055324988383	0.2724079434680321	0.2763298929215264	T	T	T
0.4349314183325350	0.2791645106962786	0.2810916081428425	T	T	T
0.1886031666410347	0.5325615984373809	0.2958758577298261	T	T	T
0.1875206239085033	0.4775441405781772	0.2933220200556968	T	T	T
0.2357070114687458	0.4464362557277788	0.2917884040700138	T	T	T
0.2372281004044890	0.3897986476306617	0.2893065423134444	T	T	T
0.2854777952126220	0.3610693844881931	0.2875571096330442	T	T	T
0.2877786591550065	0.3035445395667645	0.2850612918649573	T	T	T
0.6899095108644040	0.5252543230573550	0.2848309297300509	T	T	T
0.6410700982451796	0.5539803582222311	0.2872965858036108	T	T	T
0.6886899271903476	0.4682944596893296	0.2821146173236033	T	T	T
0.5918918254466763	0.5263606156489898	0.2870898807528703	T	T	T
0.7393479937600849	0.5536293043452245	0.2856575511538464	T	T	T
0.6397745597894133	0.6104698950889302	0.2906945064843031	T	T	T
0.7370763855710747	0.4382039857120389	0.2802397981974787	T	T	T
0.6389676835924913	0.4405116247161841	0.2818537971939125	T	T	T
0.7875002006805777	0.5224973257194667	0.2835984407760530	T	T	T
0.7378639065806213	0.6102432306396750	0.2887594131671695	T	T	T
0.7863909065081164	0.4674841470552083	0.2810308861769623	T	T	T
0.6896479020167536	0.6389749537236692	0.2912972297600471	T	T	T
0.6360861848454106	0.3842473475787812	0.2798422198182309	T	T	T
0.5401875298536969	0.6080541909113042	0.2935415593032814	T	T	T
0.5895590937725894	0.6374436357711002	0.2936992619769597	T	T	T
0.7338027638444251	0.3816883391022302	0.2781130500667734	T	T	T
0.5368141930322182	0.3912243272952849	0.2829268506507732	T	T	T
0.6848640043536111	0.3541079039303740	0.2778913617638882	T	T	T
0.5847113726535275	0.3596130627871833	0.2802796503686216	T	T	T
0.2379047470556151	0.5618664948167789	0.2971787555107082	T	T	T
0.2411779896284106	0.6183602738817368	0.2999396210566079	T	T	T
0.6874041140765476	0.6964484074209257	0.2947602689072309	T	T	T
0.4854877287753615	0.3643445158152901	0.2833992354495391	T	T	T
0.5822911371143427	0.3021834757323261	0.2783557255928746	T	T	T
0.4896289079600204	0.6357219890402627	0.2966613230831989	T	T	T
0.5892358837110975	0.6947850261101058	0.2970542454983261	T	T	T
0.6804936880474292	0.2967601152850329	0.2761430459565772	T	T	T
0.2863287834123560	0.5318039627175313	0.2954761512721512	T	T	T
0.4382599696322562	0.6088617575299370	0.2967158127029384	T	T	T
0.4846069922289461	0.3068471043841803	0.2810037524089513	T	T	T
0.6396253845894101	0.7228513271663312	0.2974503624753487	T	T	T
0.2851314131066537	0.4748480535565840	0.2927821372222414	T	T	T
0.4349364568833682	0.3920358596500723	0.2860838432637697	T	T	T
0.3843597992109494	0.5307072261394647	0.2941327184520889	T	T	T

0.2901263915085862	0.6459273946800620	0.3009515181325608	T	T	T
0.3831822162807221	0.4737645037730072	0.2914012603983587	T	T	T
0.3360554578443397	0.5595943910715484	0.2962779755834525	T	T	T
0.4905301116470339	0.6931990322041355	0.2995873413322552	T	T	T
0.5402428873390391	0.7208646353497965	0.2997657533378296	T	T	T
0.3389332137221876	0.6158372072639441	0.2989309046094439	T	T	T
0.2945242968810970	0.7032240485604911	0.3037856674876166	T	T	T
0.3903384686317547	0.6404587229698853	0.2992747971748018	T	T	T
0.3434168370297385	0.7275685167785970	0.3043163171098671	T	T	T
0.3340048985497542	0.4461416182057706	0.2908645444376113	T	T	T
0.4423626136796716	0.7228141115616824	0.3021946343891497	T	T	T
0.3927786753447021	0.6978632110661160	0.3020027076410055	T	T	T
0.3859316826684308	0.3052617654366015	0.2833220158037359	T	T	T
0.3855722638730559	0.3626411214154046	0.2858756784958678	T	T	T
0.3353296620684162	0.3896209498090364	0.2881286705832073	T	T	T
0.5906980760158355	0.4694144382284701	0.2843959735548085	T	T	T
0.5420756118286684	0.5515867399475606	0.2902524428184998	T	T	T
0.4330275787321680	0.4485143563345814	0.2890378554875107	T	T	T
0.5411927643289024	0.4464495310594759	0.2850620971145104	T	T	T
0.4338815411540519	0.5536510329851314	0.2942110434207661	T	T	T
0.4875540058555194	0.5000216083551745	0.2901502118843342	T	T	T

CoN4-C8H9N
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H	C	N	Co
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Selective dynamics
Direct

0.3479101729579733	0.7711204981034432	0.3040980090172506	T	T	T
0.4466319962625361	0.7660420144595323	0.2988083700829155	T	T	T
0.5400274552854563	0.7645044815327980	0.2961230083536538	T	T	T
0.6388325570465736	0.7662459199270540	0.2959312268544446	T	T	T
0.7254758786928792	0.7191860338471863	0.2922467594920945	T	T	T
0.7766286600102311	0.6325983989569536	0.2861945933310047	T	T	T
0.8265045106514533	0.5440857534546641	0.2830962061308608	T	T	T
0.8246945208641040	0.4457973250574205	0.2793561366062509	T	T	T
0.7716719711218694	0.3592300223317207	0.2752659881705695	T	T	T
0.7174626730542638	0.2744641279966610	0.2732510415885935	T	T	T
0.6292476454969214	0.2303229085839008	0.2752566219804582	T	T	T
0.5306458834335082	0.2354310603198234	0.2791908506096279	T	T	T
0.4372979068251279	0.2370270599262012	0.2810936506048304	T	T	T

0.3384015981471350	0.2352430578286376	0.2811689817306470	T	T	T
0.2517520900888613	0.2823308299527106	0.2840772865417786	T	T	T
0.2006955527663968	0.3688852400960217	0.2892925357286353	T	T	T
0.1507390326315924	0.4572878529496725	0.2939232631716716	T	T	T
0.1524882450029711	0.5555563111239942	0.2982733198895282	T	T	T
0.2055615282532754	0.6421489622960551	0.3019593167218886	T	T	T
0.2597163231700953	0.7269091997204045	0.3056916699084721	T	T	T
0.5457598351874513	0.4257291954981953	0.6156498435347245	T	T	T
0.5321006788633739	0.5242870024440047	0.6088242316639301	T	T	T
0.5141877338612612	0.5661512184213340	0.5216432649688115	T	T	T
0.5245200067567255	0.4112079562682472	0.4455371123725952	T	T	T
0.5416262066212035	0.3697896523030619	0.5331077635168290	T	T	T
0.4895732297296195	0.5984971300916243	0.4472388422069867	T	T	T
0.5061471913562609	0.5901030208098957	0.3787933471281050	T	T	T
0.5569506711168986	0.5874097033261230	0.4287035015571696	T	T	T
0.4836940733521574	0.4513098479787391	0.3904405100317165	T	T	T
0.3372161667588459	0.2788476233921909	0.2834782404938599	T	T	T
0.5332094348038001	0.2790498673659679	0.2808120975175741	T	T	T
0.6320401571962477	0.2738898055001556	0.2765870701878148	T	T	T
0.4362860763782630	0.2806728587299790	0.2833317345870230	T	T	T
0.1900322261656349	0.5332450638961588	0.2967070006877868	T	T	T
0.1890438463963854	0.4783090977548589	0.2942793029844752	T	T	T
0.2372387044423304	0.4472717049706936	0.2921743675581017	T	T	T
0.2384171536495437	0.3909462304008211	0.2897243344039955	T	T	T
0.2866952875045303	0.3621077505921994	0.2878895478228550	T	T	T
0.2891666130466315	0.3048688092049158	0.2850105269464255	T	T	T
0.6905399120858701	0.5256882131814168	0.2830592594360399	T	T	T
0.6415309700524642	0.5544840104783091	0.2852479475651878	T	T	T
0.6895195668219836	0.4691176646284490	0.2811643101645403	T	T	T
0.5923490443726241	0.5272229540194689	0.2868180515116867	T	T	T
0.7400186508230189	0.5542855900316538	0.2834704443614334	T	T	T
0.6408378442360234	0.6109009227586185	0.2873059676268121	T	T	T
0.7379246014263917	0.4387993311897318	0.2791917484518132	T	T	T
0.6395152970241548	0.4420211364533393	0.2819923469512045	T	T	T
0.7881816365669848	0.5231378742627478	0.2820563827908156	T	T	T
0.7388488809558299	0.6106024191525771	0.2858339125074894	T	T	T
0.7871715923751286	0.4681759301482639	0.2799475289779818	T	T	T
0.6905706868003031	0.6394021875266088	0.2878046663900485	T	T	T
0.6367905025106337	0.3856649531995807	0.2802862803332575	T	T	T
0.5413726683901101	0.6070425402554490	0.2902391953421675	T	T	T
0.5904326594527597	0.6372025940109228	0.2893658316613737	T	T	T
0.7347390436834187	0.3825512216492256	0.2771074490074321	T	T	T
0.5376003286494474	0.3928127941665415	0.2857652785776971	T	T	T
0.6854177334881395	0.3554520756843886	0.2773699537825091	T	T	T

0.5855336640154107	0.3610387567892262	0.2817837495232419	T	T	T
0.2392932993504568	0.5626448188827867	0.2971826201613680	T	T	T
0.2425005494232305	0.6188736838102274	0.2998478084557249	T	T	T
0.6880756339038030	0.6966202916030892	0.2910440234997814	T	T	T
0.4863365883220609	0.3665564634422061	0.2867427874958506	T	T	T
0.5829675395514738	0.3037297424251005	0.2797005366044730	T	T	T
0.4910230579434685	0.6349467584923646	0.2928631440394643	T	T	T
0.5898781133560947	0.6945398360806828	0.2919482047264256	T	T	T
0.6809097129021026	0.2983153187094861	0.2754041543736168	T	T	T
0.2877439602523414	0.5324092990627083	0.2949827142978463	T	T	T
0.4397152007207288	0.6086951281775659	0.2944625600829523	T	T	T
0.4852755299334757	0.3087295851570932	0.2838463136436515	T	T	T
0.6400477615214004	0.7226589163315962	0.2930644925489227	T	T	T
0.2867333460936061	0.4758570809060239	0.2927465028754159	T	T	T
0.4359539988780926	0.3944417687947984	0.2889649506426789	T	T	T
0.3859969141845245	0.5306242676472435	0.2942128407740475	T	T	T
0.2917631886774485	0.6460271865729236	0.2999264764058332	T	T	T
0.3849861353339952	0.4742488176624122	0.2926087387871785	T	T	T
0.3377515882757610	0.5594970971741787	0.2952718617247709	T	T	T
0.4920216265752673	0.6928044968482046	0.2945295363252162	T	T	T
0.5409865633148730	0.7208726321785238	0.2941114289761344	T	T	T
0.3404517365198064	0.6158510504900769	0.2972646320814059	T	T	T
0.2962777926635368	0.7031420213365241	0.3027646486552833	T	T	T
0.3917175694111036	0.6404944476999478	0.2966115833636243	T	T	T
0.3451772839938909	0.7275732801839692	0.3019783060142683	T	T	T
0.3357530546488635	0.4470642317641768	0.2912853994482412	T	T	T
0.4440743294134057	0.7224497085196846	0.2974584376922420	T	T	T
0.3942862549103300	0.6977935779548173	0.2985360150444466	T	T	T
0.3873595312015362	0.3070007871221426	0.2847649026600124	T	T	T
0.3868442022301864	0.3643216610637278	0.2875028186135447	T	T	T
0.3364334650431828	0.3906437523273808	0.2888406028119804	T	T	T
0.5913704534190136	0.4708727085186794	0.2855501601077696	T	T	T
0.5373758407906294	0.4441593000903294	0.5769649292208791	T	T	T
0.5298010391687941	0.4993582993504677	0.5730876168875766	T	T	T
0.5197750033984709	0.5229733389592603	0.5235737436975550	T	T	T
0.5166614170604072	0.4919311147069419	0.4766839076709455	T	T	T
0.5247468595816932	0.4363800232814983	0.4812407058368929	T	T	T
0.5348761112933154	0.4128154673529050	0.5306702078447987	T	T	T
0.5066273023403416	0.5175122689029054	0.4240055701569757	T	T	T
0.5154010221093359	0.5765743125788443	0.4191737627960062	T	T	T
0.5435669253495423	0.5521053921438887	0.2905342285133405	T	T	T
0.5418180648114455	0.4475433566241278	0.2883721905453803	T	T	T
0.4356057193901321	0.5539566838989460	0.2945926868852735	T	T	T
0.4337646701552499	0.4492405303183883	0.2920170964480101	T	T	T

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   0.4906990832196971   0.4909674692155912   0.3823303197952794   T   T   T
   0.4889281806808056   0.5006962586350053   0.2990290491182224   T   T   T

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Selective dynamics
Direct
   0.3466671750083248   0.7710533218736424   0.3065154207201383   T   T   T
   0.4456242656224431   0.7656226678376399   0.3041390446327265   T   T   T
   0.5390198557659777   0.7638062936540485   0.3020466852647382   T   T   T
   0.6380278595161251   0.7657254121192313   0.3001202660986520   T   T   T
   0.7245238826646310   0.7184910891450490   0.2961138479945136   T   T   T
   0.7755486514951420   0.6318852276407082   0.2901154642903251   T   T   T
   0.8253400826497433   0.5435601003975711   0.2844810162653706   T   T   T
   0.8234012732554848   0.4452551183661657   0.2796830563291472   T   T   T
   0.7707510391063634   0.3589410683809243   0.2768684800178491   T   T   T
   0.7172019443314321   0.2740425268889897   0.2745307530025644   T   T   T
   0.6291855809236909   0.2293665020922482   0.2746493115788985   T   T   T
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Selective dynamics

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