# Electronic Supplementary Information

## Manganese Complex-Catalyzed Oxidation and Oxidative Kinetic Resolution of Secondary Alcohols by Hydrogen Peroxide

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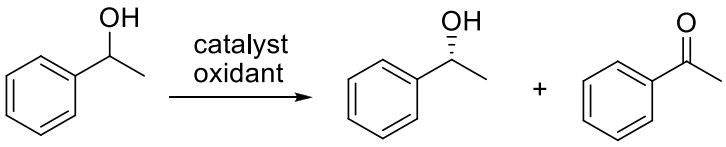
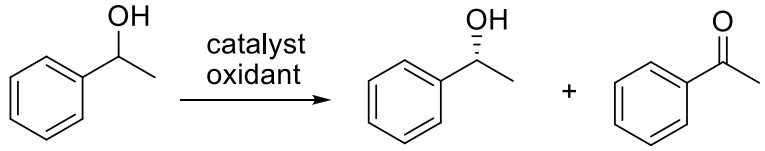
**Table S1** Oxidative kinetic resolution (OKR) of 1-phenylethanol catalyzed by manganese complex with N4 ligand[a]




| entry | catalyst | T ($^{o}$C) | oxidant | conversion (%)[b] | *ee* (%)[b] |
|---|---|---|---|---|---|
| 1 | **1** | 0 | $H_2O_2$ | 54 | 50 |
| 2 | **2** | 0 | $H_2O_2$ | 57 | 64 |
| 3 | **3** | 0 | $H_2O_2$ | trace | - |
| 4 | **2** | 25 | $H_2O_2$ | 55 | 58 |
| 5 | **2** | -20 | $H_2O_2$ | 58 | 63 |
| 6 | **2** | -40 | $H_2O_2$ | 51 | 52 |
| 8 | **2** | 0 | 70% TBHP | 58 | 65 |
| 9 | **2** | 0 | *m*-CPBA | 50 | 55 |
| 10[c] | **2** | 0 | oxone | 20 | 16 |
| 11 | **2** | 0 | $PhI(OAc)_2$ | 58 | 70 |

[a] Reaction conditions: An $CH_3CN$ (1.0 or 1.5 mL) solution containing 1-phenylethanol (0.50 mmol), catalyst (0.20 mol%), and $H_2SO_4$ (1.0 mol%) was added into the Schleck tube at 0 $^{o}$C. Then, an $CH_3CN$ (0.50 mL) solution containing oxidant (0.60 equiv.) was added dropwise into the Schleck tube by using a syringe pump for 1 h (for $H_2O_2$ and TBHP) or added at once and stirred for 1 h (for *m*-CPBA, oxone, and PhIOAc). [b] The conversion yields of 1-phenylethanol and the *ee* values of unreacted 1-phenylethanol were determined by GC with a CP-Chirasil-Dex CB column. [c] 0.30 equiv. of oxone was added.

**Table S2** Screening the amount of the acid and reaction time for oxidative kinetic resolution of 1-phenylethanol catalyzed by **2**[a]




| entry | $H_2SO_4$ (mol%) | t (h) | conversion (%)[b] | ee (%)[b] |
|---|---|---|---|---|
| 1 | 1.0 | 1 | 69 | 90 |
| 2[c] | 500 | 1 | 70 | 37 |
| 3[d] | 1.0 | 1 | 3 | trace |
| 4 | 1.0 | 0.50 | 61 | 70 |
| 5 | 1.0 | 2.0 | 74 | 92 |
| 6 | 0.25 | 1 | 52 | 57 |
| 7 | 0.50 | 1 | 65 | 84 |
| 8 | 3.0 | 1 | 66 | 79 |

[a] Reaction conditions: An $CH_3CN$ (1.0 mL) solution containing 1-phenylethanol (0.50 mmol), catalyst (0.20 mol%), and $H_2SO_4$ (0.25 – 3.0 mol%) was added into the Schleck tube at 0 °C. Then, an $CH_3CN$ (0.50 mL) solution containing 30% $H_2O_2$ (0.80 equiv.) was added dropwise into the Schleck tube by using a syringe pump for 1 h (except for entries 4 and 5). [b] The conversion yields of 1-phenylethanol and the *ee* values of unreacted 1-phenylethanol were determined by GC with a CP-Chirasil-Dex CB column. [c] 5.0 equiv. (500 mol%) of AcOH was used instead of $H_2SO_4$. [d] 1.0 mol% of AcOH was used instead of $H_2SO_4$.

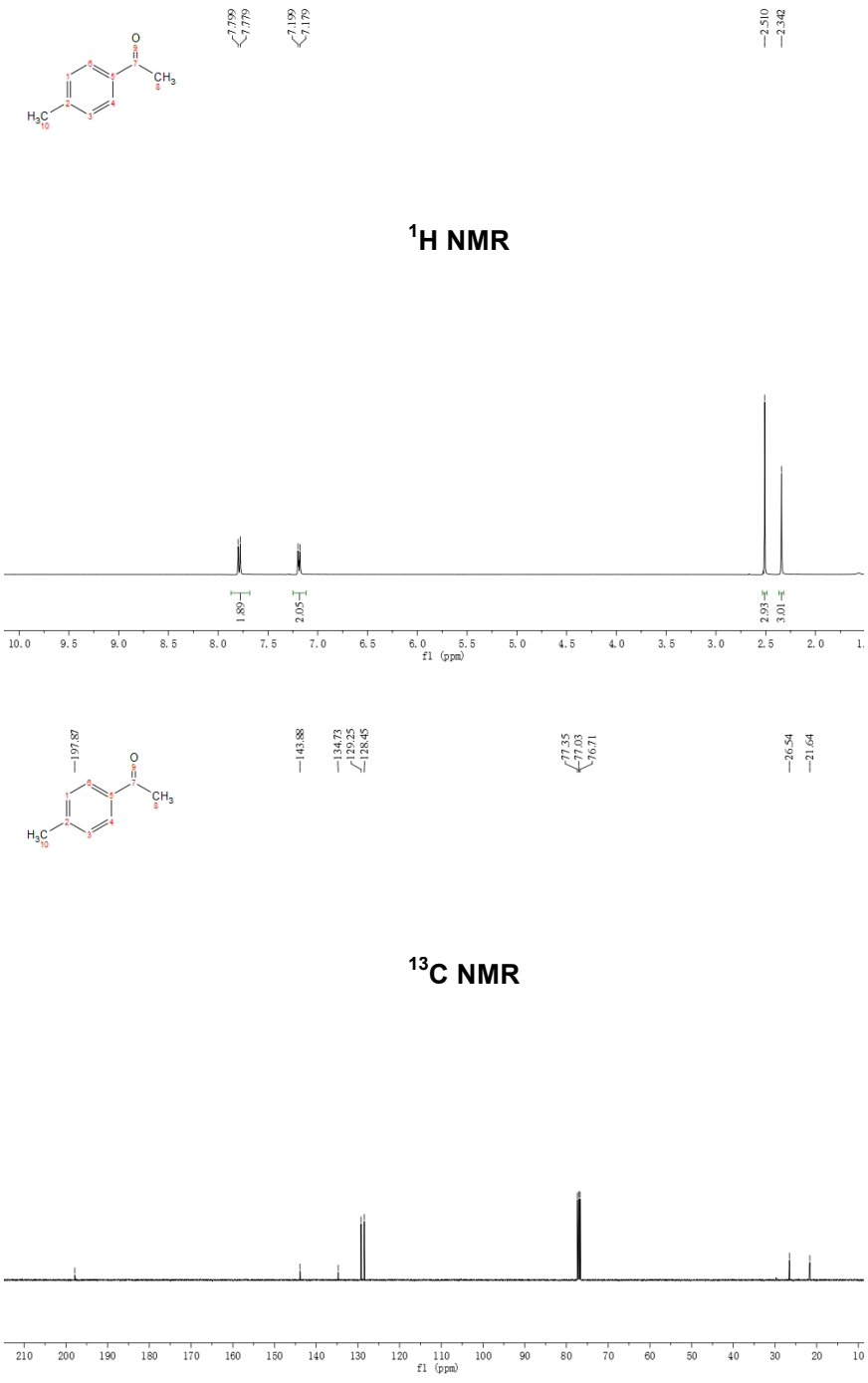
**Table S3** Comparison of the reaction energy barriers for the α-CH activation of both *S*- and *R*-1-phenylethanol (*S*-Sub and *R*-Sub, respectively) by the high-valent $[(\text{P-MCP})\text{Mn}^{5+}(\text{O}^{2-})(\text{SO}_4{}^{2-})]^+$ species (**I**). Energies were calculated using the B3LYP functional at different levels (i.e., B1 represents a LACVP(Mn), 6-31G*(C, H, O, N, and S) basis set, and B2 represents a LACV3P(Mn), 6-311+G**(C, H, O, N, and S) basis set). Absolute energies are in a.u. unit and relative ones are in kcal/mol

| | OPT/B1 | Δ*E* | OPT+ZPE | Δ*E* | SPE/B2 | Δ*E* | SPE+ZPE | Δ*E* | ZPE/B1 |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | ***S*-enantiomer** | | | | |
| $^3$**I**+*S*-Sub | -2724.214617 | 0.0 | -2723.404002 | 0.0 | -2724.896918 | 0.0 | -2724.086303 | 0.0 | 0.810615 |
| $^5$**I**+*S*-Sub | -2724.199664 | 9.4 | -2723.389608 | 9.0 | -2724.881228 | 9.8 | -2724.071172 | 9.5 | 0.810056 |
| $^3$**TS**$_S$ | -2724.194168 | 12.8 | -2723.386492 | 11.0 | -2724.881688 | 9.6 | -2724.074012 | **7.7** | 0.807676 |
| $^5$**TS**$_S$ | -2724.196030 | 11.7 | -2723.389233 | 9.3 | -2724.884267 | 7.9 | -2724.077470 | **5.5** | 0.806797 |
| | | | | | ***R*-enantiomer** | | | | |
| $^3$**I**+*R*-Sub | -2724.214613 | 0.0 | -2723.404005 | 0.0 | -2724.896919 | 0.0 | -2724.086311 | 0.0 | 0.810608 |
| $^5$**I**+*R*-Sub | -2724.199660 | 9.4 | -2723.389611 | 9.0 | -2724.881229 | 9.8 | -2724.071180 | 9.5 | 0.810049 |
| $^3$**TS**$_R$ | -2724.187034 | 17.3 | -2723.379333 | 15.5 | -2724.877133 | 12.4 | -2724.069432 | **10.6** | 0.807701 |
| $^5$**TS**$_R$ | -2724.192413 | 13.9 | -2723.386093 | 11.2 | -2724.881785 | 9.5 | -2724.075465 | **6.8** | 0.806320 |

**Table S4** Mulliken spin densities and charges of the oxidant-substrate complex (**I** + *S*-/*R*-Sub) as well as the transition states in the α-CH activation of both *S*- and *R*-1-phenylethanol by the [(P-MCP)$Mn^{5+}(O^{2-})(SO_4^{2-})]^+$ species (**I**) calculated at the UB3LYP/LACVP(Mn), 6-31G*(C, H, O, N, and S) level in solvent

| | spin density | | | | | | charge | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Mn | P-MCP | O | $SO_4$ | H | PA-H | Mn | P-MCP | O | $SO_4$ | H | PA-H |
| | | | | | | ***S*-enantiomer** | | | | | | |
| $^3$**I**+*S*-Sub | 2.84 | -0.18 | -0.44 | -0.21 | 0.00 | 0.00 | 0.82 | 1.49 | -0.34 | -0.97 | 0.13 | -0.13 |
| $^5$**I**+*S*-Sub | 2.79 | -0.19 | 0.87 | 0.52 | 0.00 | 0.00 | 0.82 | 1.44 | -0.39 | -0.88 | 0.13 | -0.13 |
| $^3$**TS**$_S$ | 2.81 | -0.16 | -0.35 | -0.07 | 0.01 | -0.24 | 0.83 | 1.48 | -0.48 | -1.03 | 0.19 | 0.01 |
| $^5$**TS**$_S$ | 2.68 | -0.11 | 0.59 | 0.07 | 0.09 | 0.68 | 0.82 | 1.34 | -0.61 | -1.17 | 0.35 | 0.27 |
| | | | | | | ***R*-enantiomer** | | | | | | |
| $^3$**I**+*R*-Sub | 2.84 | -0.18 | -0.44 | -0.21 | 0.00 | 0.00 | 0.82 | 1.49 | -0.34 | -0.97 | 0.13 | -0.13 |
| $^5$**I**+*R*-Sub | 2.79 | -0.19 | 0.87 | 0.52 | 0.00 | 0.00 | 0.82 | 1.44 | -0.39 | -0.88 | 0.13 | -0.13 |
| $^3$**TS**$_R$ | 2.95 | -0.17 | -0.49 | -0.14 | 0.01 | -0.15 | 0.88 | 1.51 | -0.50 | -0.99 | 0.26 | -0.15 |
| $^5$**TS**$_R$ | 2.63 | -0.12 | 0.62 | 0.10 | 0.09 | 0.69 | 0.80 | 1.36 | -0.59 | -1.16 | 0.33 | 0.26 |

## Additional Data: NMR Spectra of the Products




**$^{1}$H NMR**

**$^{13}$C NMR**

**Fig. S1** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*p*-tolyl)ethan-1-one produced in the catalytic oxidation of 1-(*p*-tolyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, $J$ = 8.0 Hz, 2H), 7.19 (d, $J$ = 8.0 Hz, 2H), 2.51 (s, 3H), 2.34 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 197.9, 143.9, 134.7, 129.3, 128.5, 26.5, 21.6.

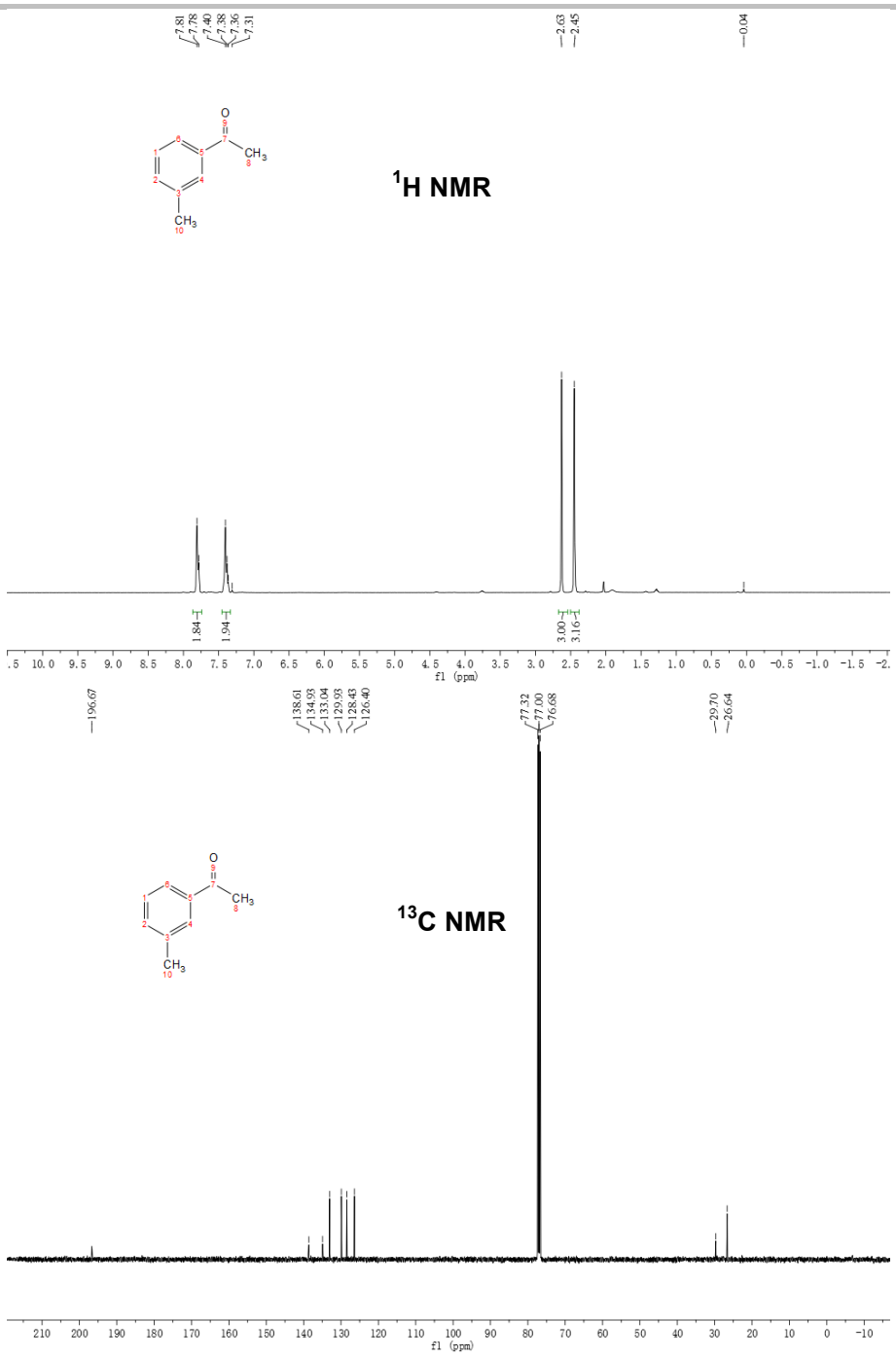



**Fig. S2** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*m*-tolyl)ethan-1-one produced in the catalytic oxidation of 1-(*m*-tolyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, $J$ = 7.6 Hz, 1H), 7.42 (t, $J$ = 7.2 Hz, 1H), 7.31 (m, 2H), 2.62 (s, 3H), 2.57 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.7, 138.6, 134.9, 133.0, 129.9, 128.4, 126.4, 29.7, 26.6.

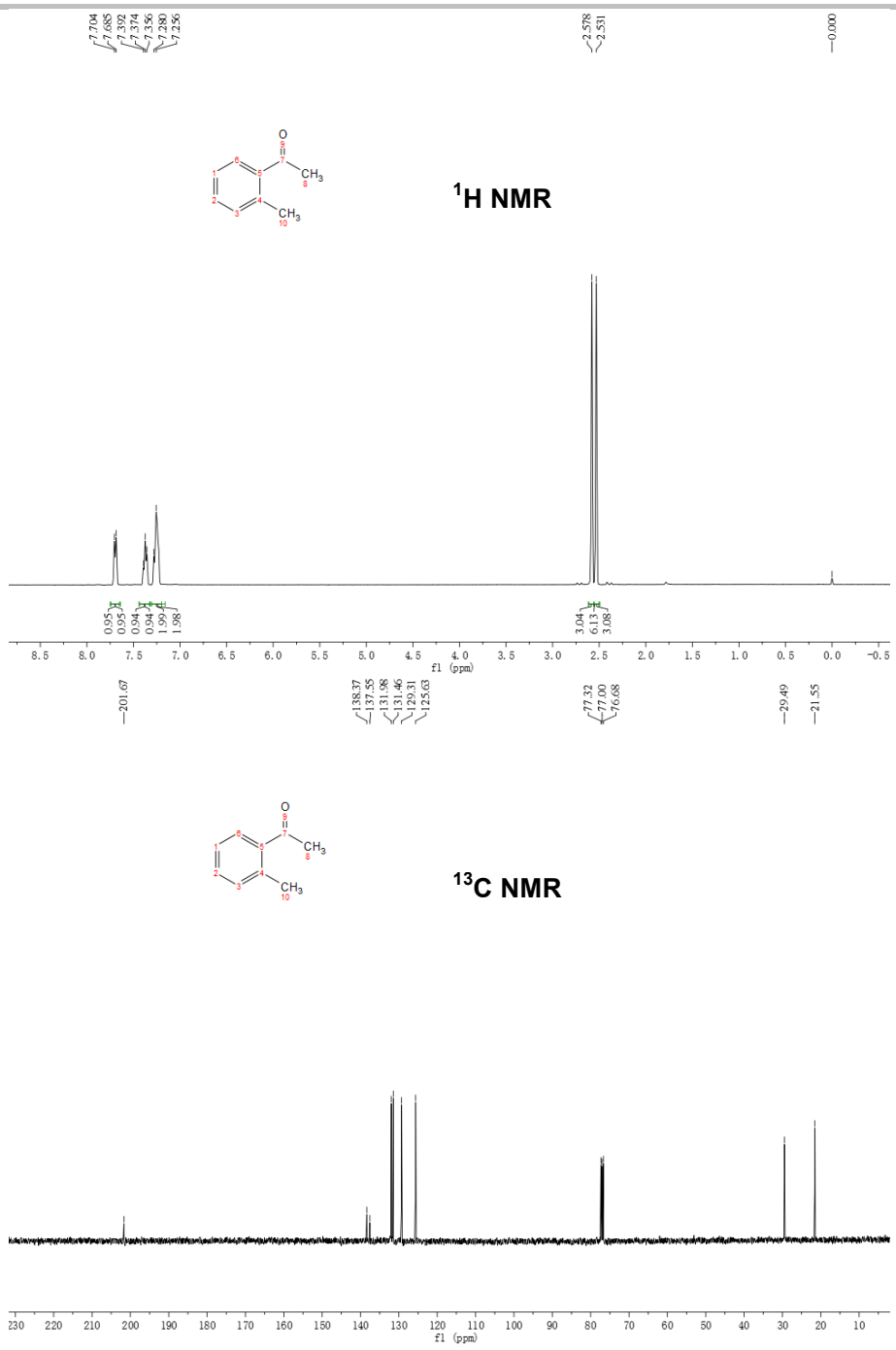



**Fig. S3** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*o*-tolyl)ethan-1-one produced in the catalytic oxidation of 1-(*o*-tolyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, $J$ = 7.6 Hz, 1H), 7.37 (t, $J$ = 7.2 Hz, 1H), 7.27 (d, $J$ = 9.6 Hz, 2H), 2.58 (s, 3H), 2.53 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 201.7, 138.4, 137.6, 132.0, 131.5, 129.3, 125.6, 29.5, 21.6.

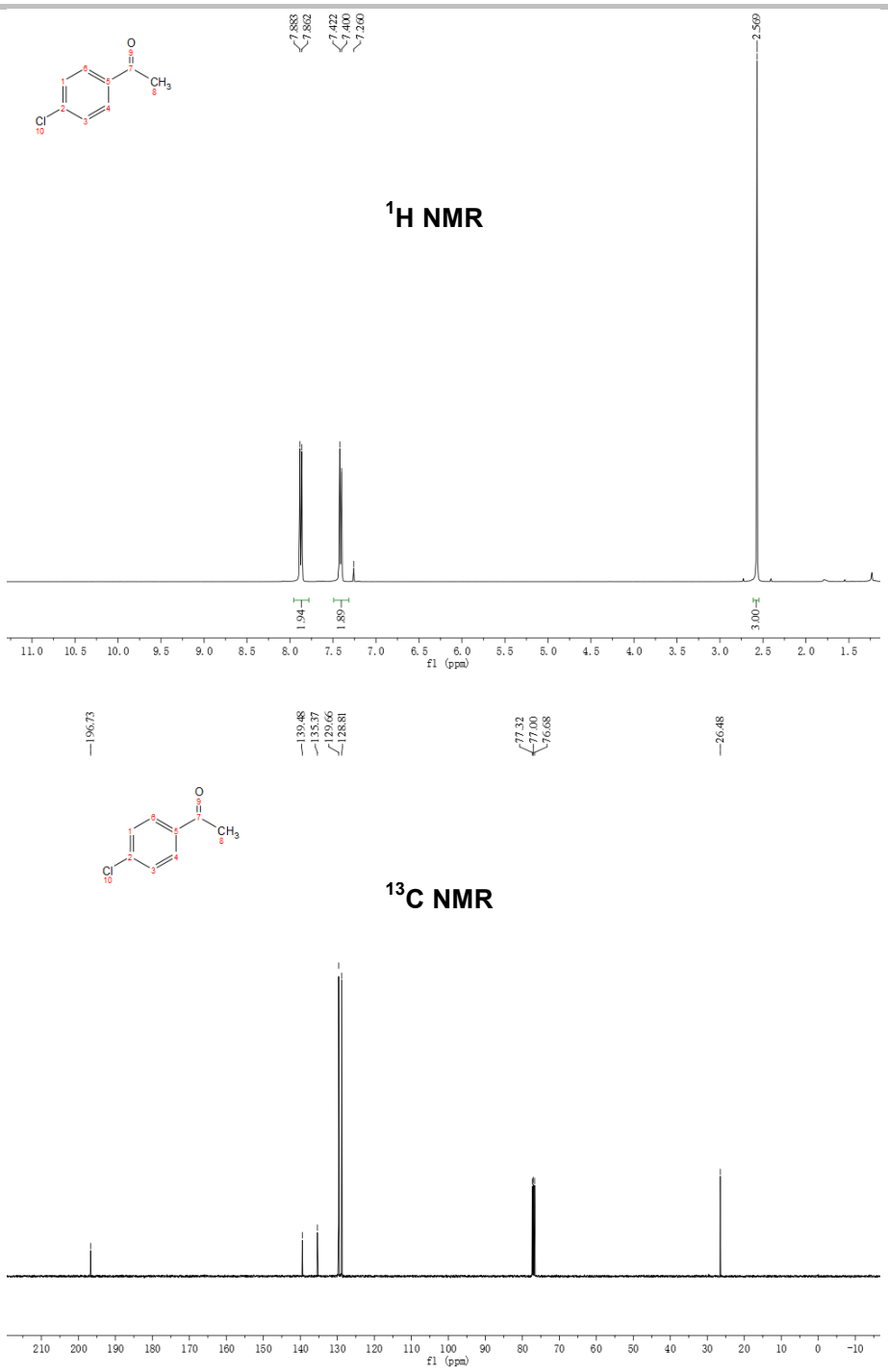



**Fig. S4** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*p*-chlorophenyl)ethan-1-one produced in the catalytic oxidation of 1-(*p*-chlorophenyl)ethan-1-ol (0.50 mmol) by **1** (0.03 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, $J$ = 8.4 Hz, 2H), 7.43 (d, $J$ = 8.8 Hz, 2H), 2.59 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.8, 139.6, 135.4, 129.7, 128.9, 26.5.

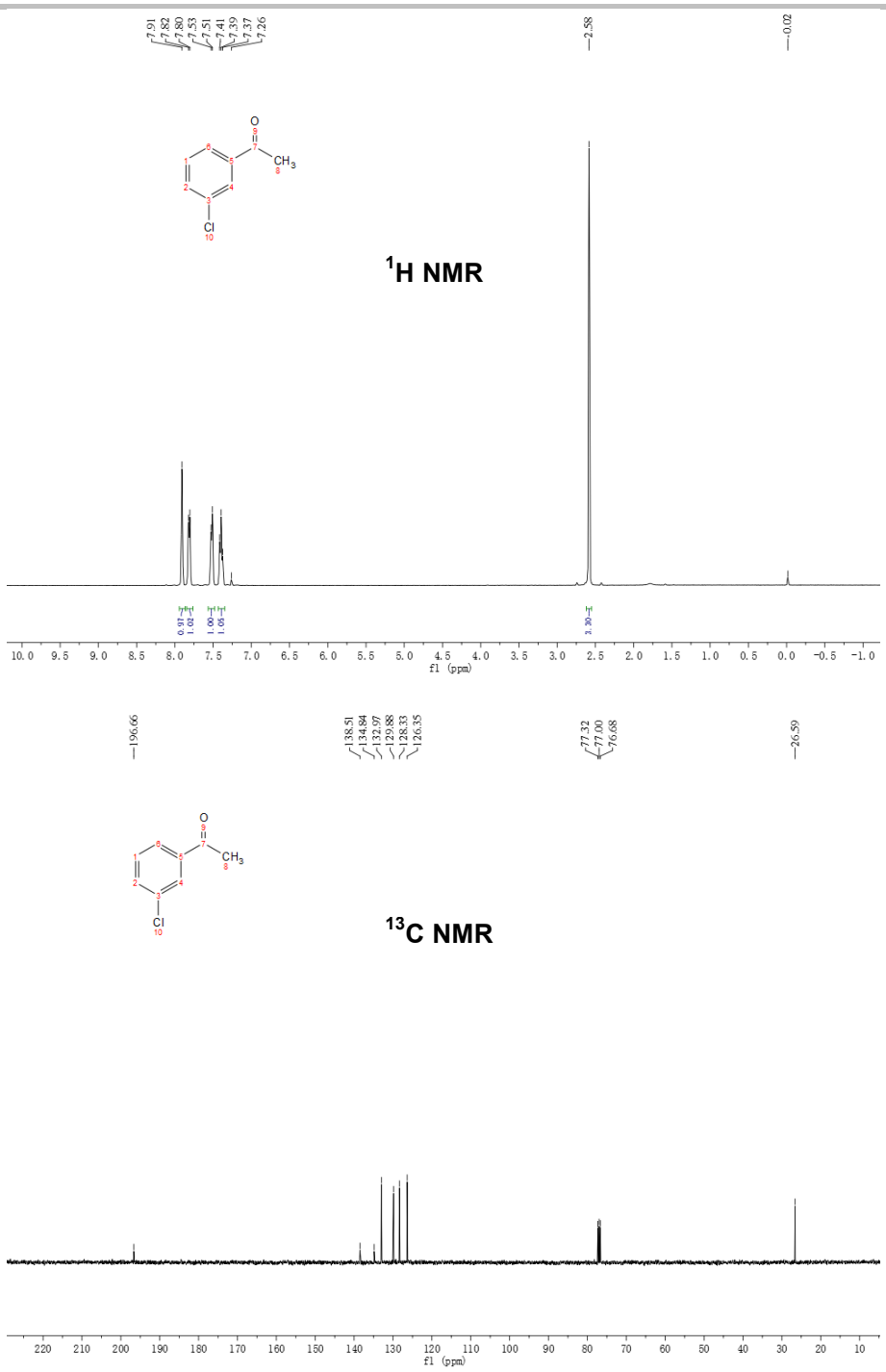



**Fig. S5** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*m*-chlorophenyl)ethan-1-one produced in the catalytic oxidation of 1-(*m*-chlorophenyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.81 (d, $J$ = 7.6 Hz, 1H), 7.52 (d, $J$ = 7.6 Hz, 1H), 7.39 (t, $J$ = 7.6 Hz, 1H), 2.58 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.7, 138.5, 134.8, 133.0, 129.9, 128.3, 126.4, 26.6.

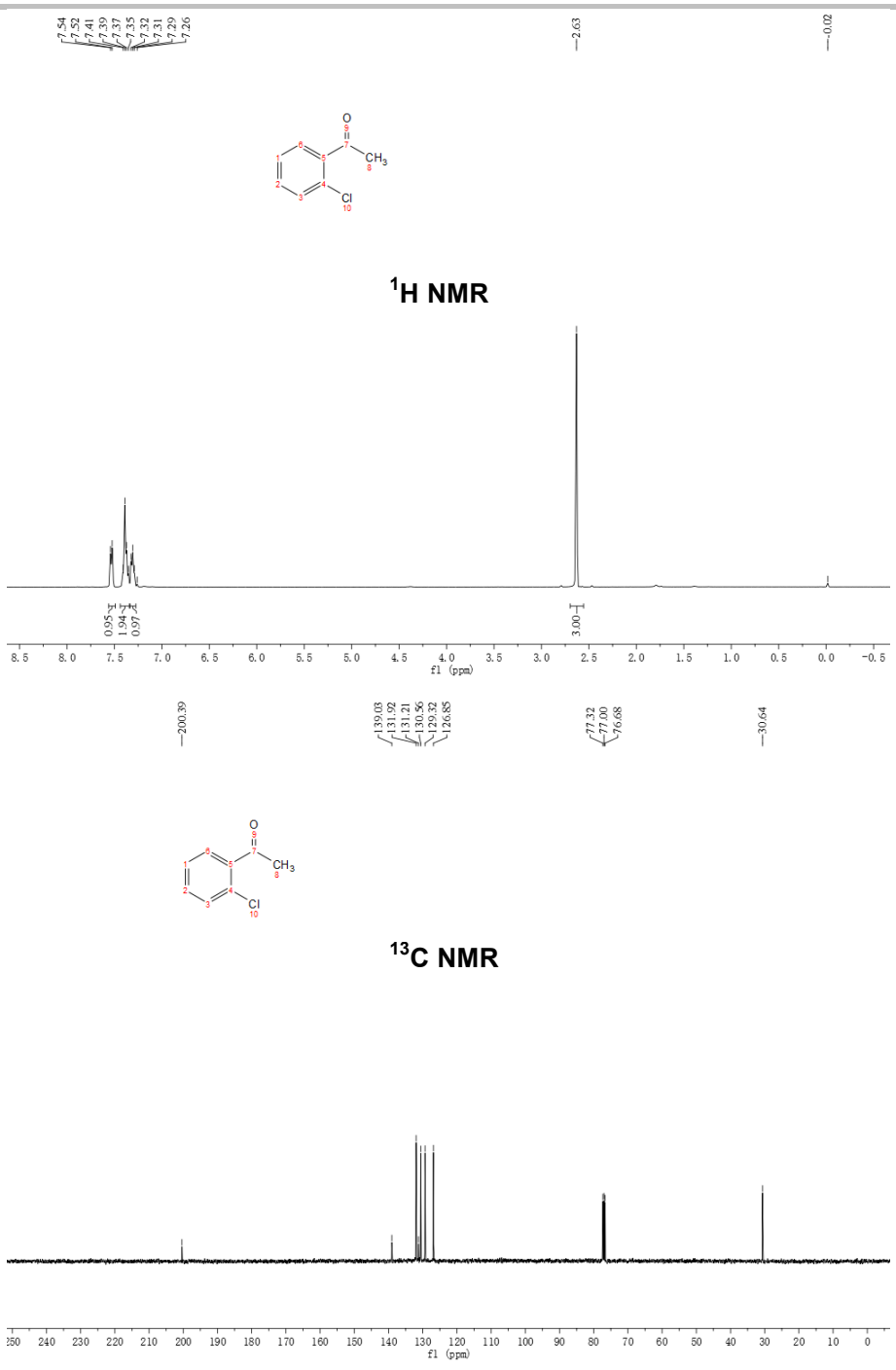



**Fig. S6** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*o*-chlorophenyl)ethan-1-one produced in the catalytic oxidation of 1-(*o*-chlorophenyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, $J$ = 7.2 Hz, 1H), 7.40-7.35 (m, 2H), 7.29 (t, $J$ = 6.8 Hz, 1H), 2.63 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 200.4, 139.0, 131.9, 131.2, 130.6, 129.3, 126.9, 30.6.

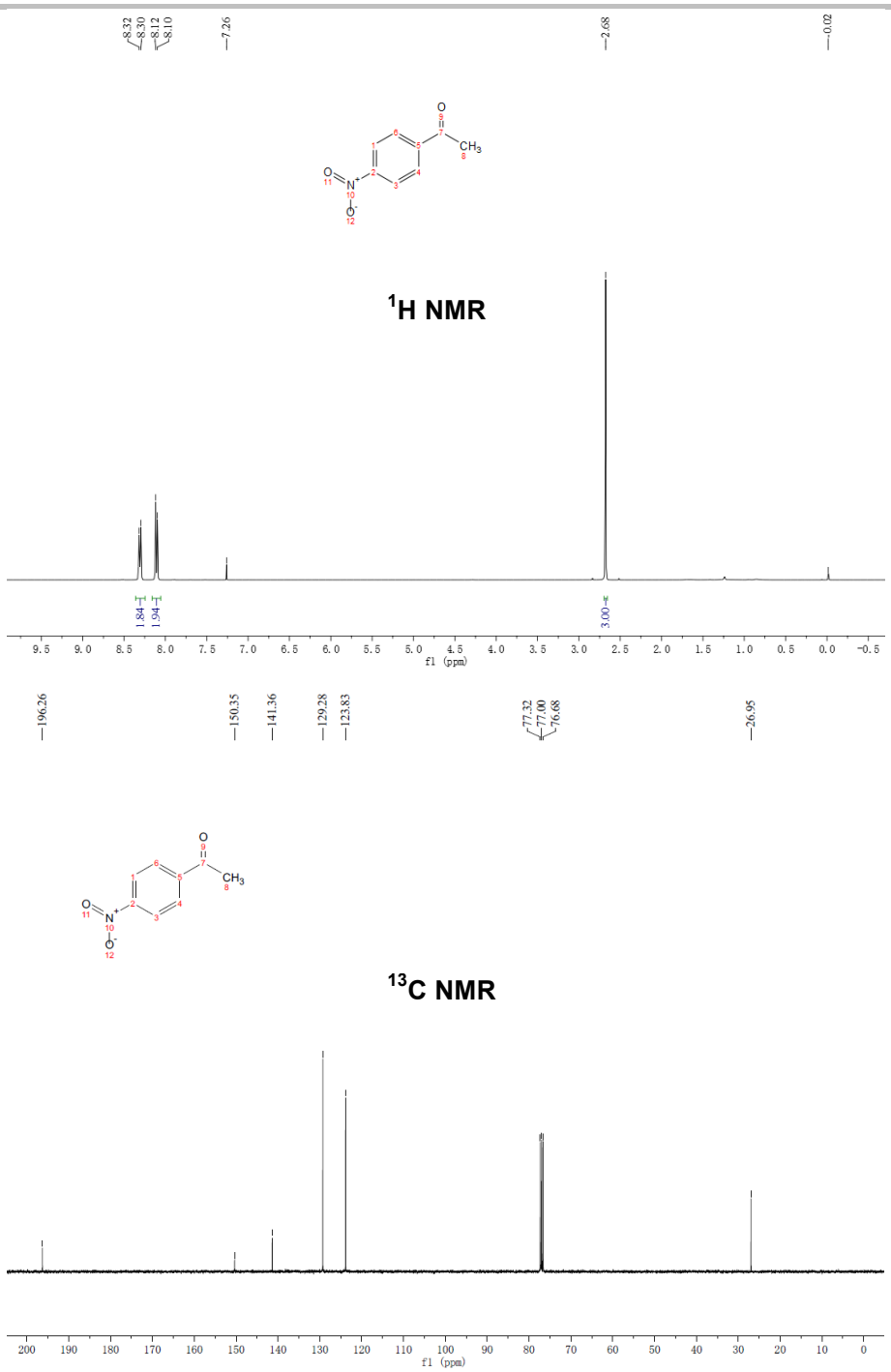



**Fig. S7** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*p*-nitrophenyl)ethan-1-one produced in the catalytic oxidation of 1-(*p*-nitrophenyl)ethan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, $J$ = 7.2 Hz, 2H), 8.11 (d, $J$ = 8.4 Hz, 2H), 2.68 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.3, 150.4, 141.4, 129.3, 123.8, 27.0.

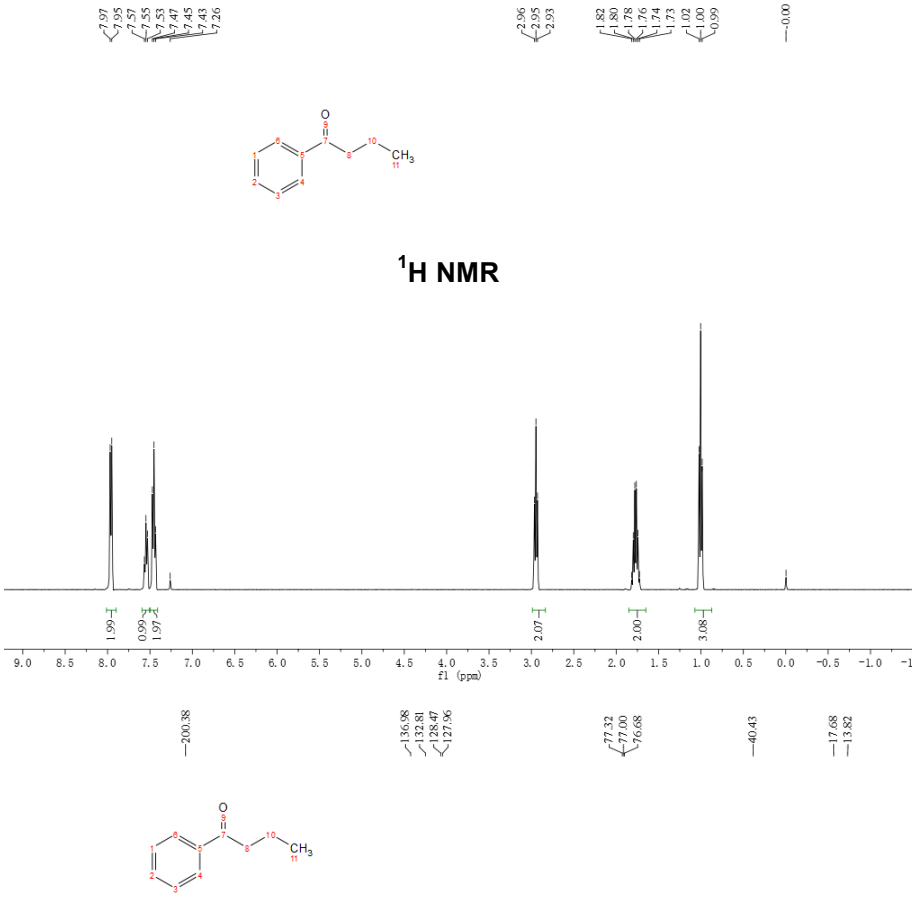



**Fig. S8** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-phenylbutan-1-one produced in the catalytic oxidation of 1-phenylbutan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, $J$ = 7.6 Hz, 2H), 7.55 (t, $J$ = 7.2 Hz, 1H), 7.45 (t, $J$ = 7.2 Hz, 2H), 2.95 (t, $J$ = 7.2 Hz, 2H), 1.77 (m, 2H), 1.00 (t, $J$ = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 200.5, 137.1, 132.9, 128.6, 128.0, 40.5, 17.8, 13.9.

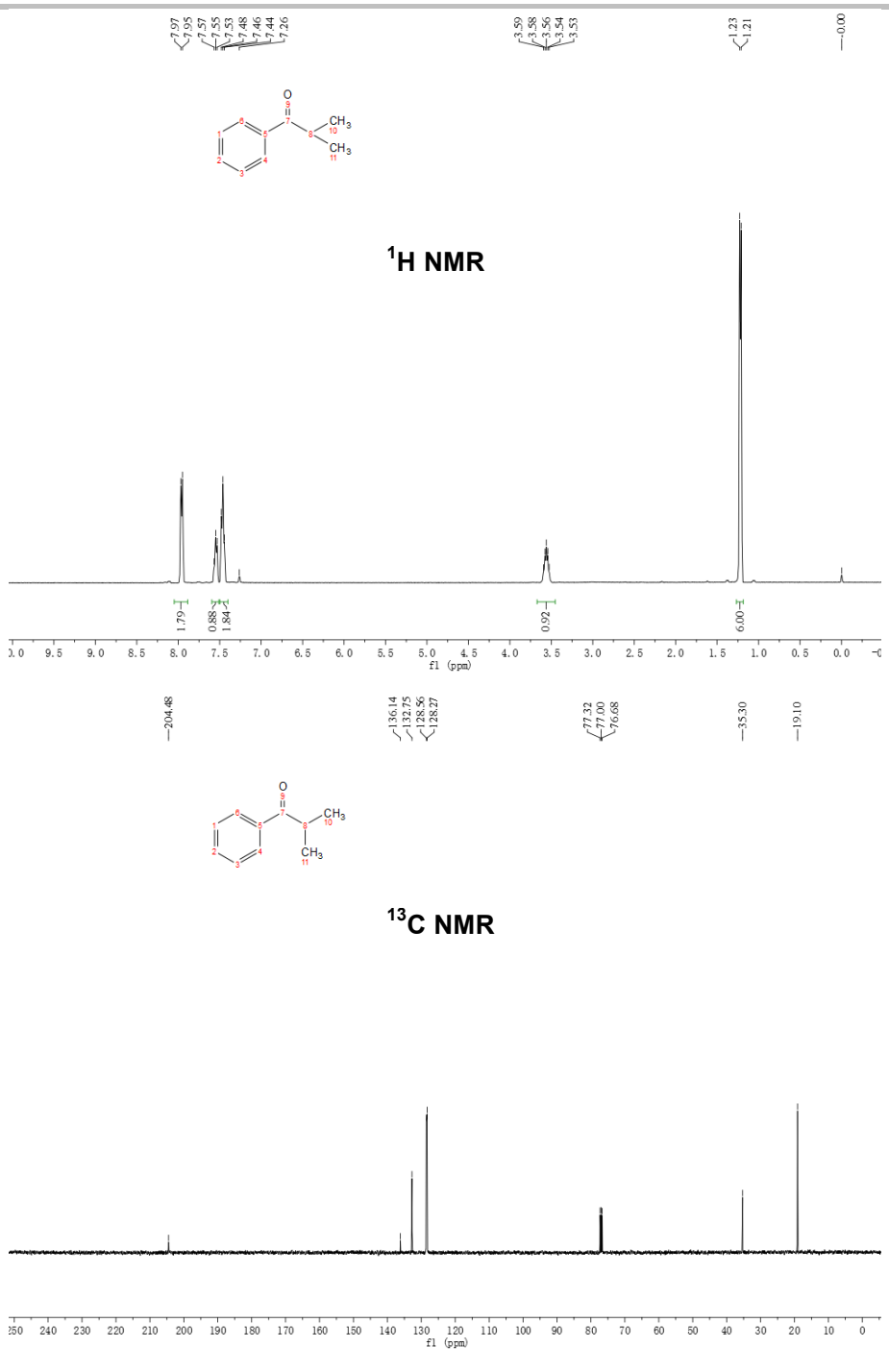



**Fig. S9** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 2-methyl-1-phenylpropan-1-one produced in the catalytic oxidation of 2-methyl-1-phenylpropan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 °C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, $J$ = 7.6 Hz, 2H), 7.55 (t, $J$ = 7.2 Hz, 1H), 7.46 (t, $J$ = 7.2 Hz, 2H), 3.56 (m, 1H), 1.22 (d, $J$ = 6.8 Hz, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 204.5, 136.2, 132.8, 128.6, 128.3, 35.4, 19.2.

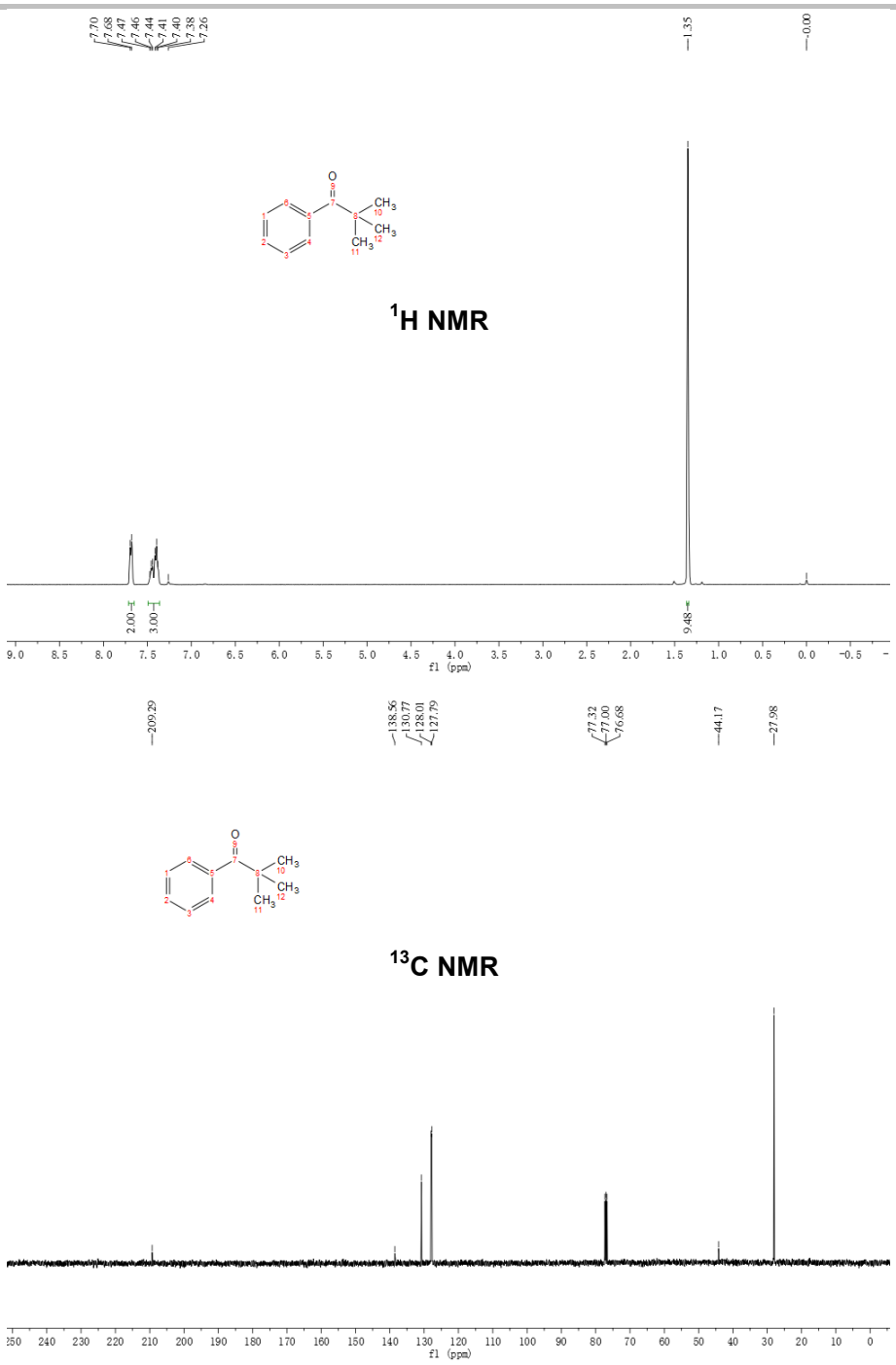



**Fig. S10** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 2,2-dimethyl-1-phenylpropan-1-one produced in the catalytic oxidation of 2,2-dimethyl-1-phenylpropan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at room temperature for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, $J$ = 7.2 Hz, 2H), 7.43 (m, 3H), 1.35 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 209.3, 138.6, 130.8, 128.0, 127.8, 44.2, 28.0.

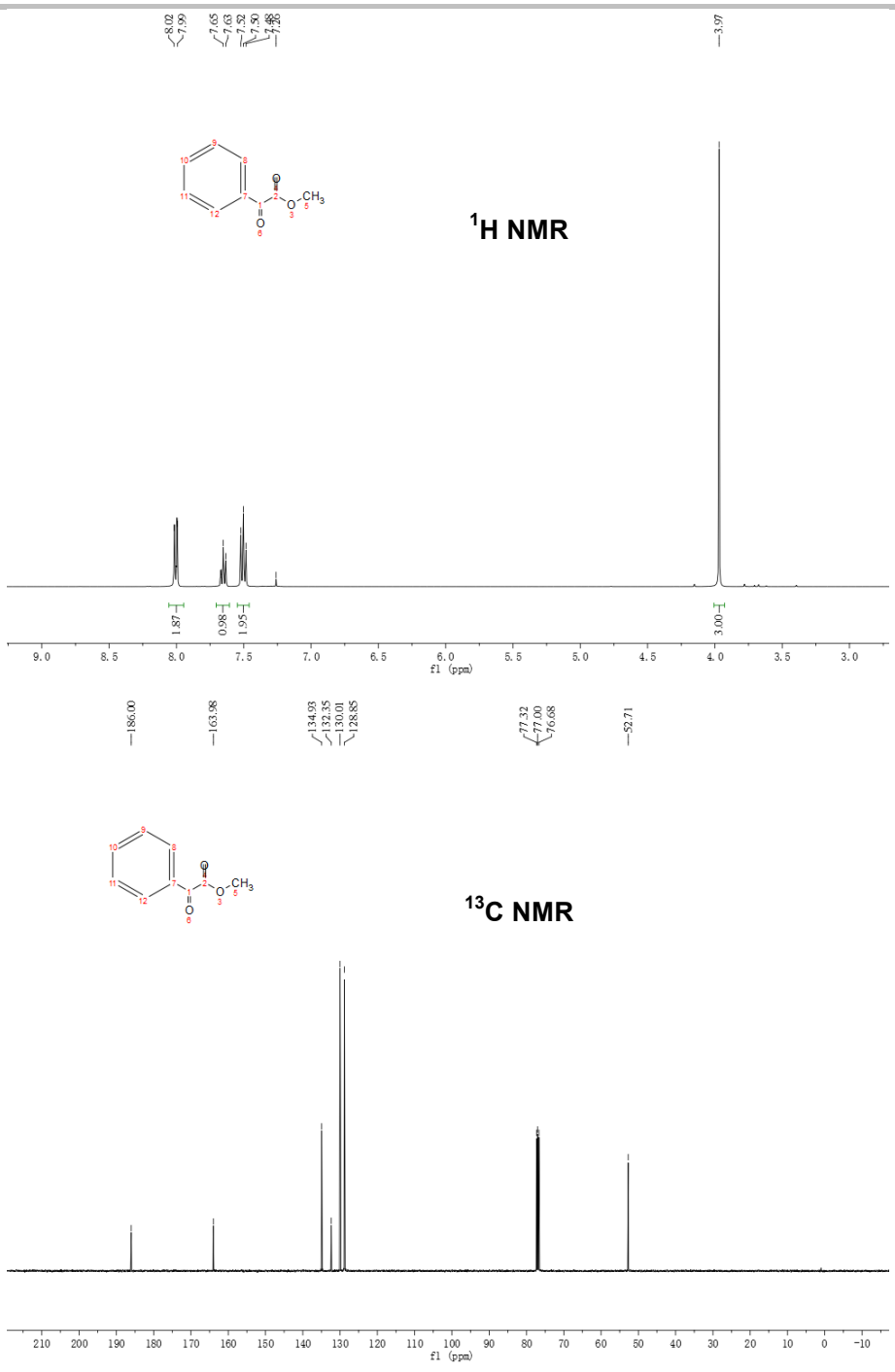



**Fig. S11** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of methyl 2-oxo-2-phenylacetate produced in the catalytic oxidation of methyl 2-hydroxy-2-phenylacetate (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, $J$ = 9.6 Hz, 2H), 7.65 (t, $J$ = 7.2 Hz, 1H), 7.50 (t, $J$ = 8.0 Hz, 2H), 3.97 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 186.1, 164.1, 135.0, 132.4, 130.1, 128.9, 52.8.

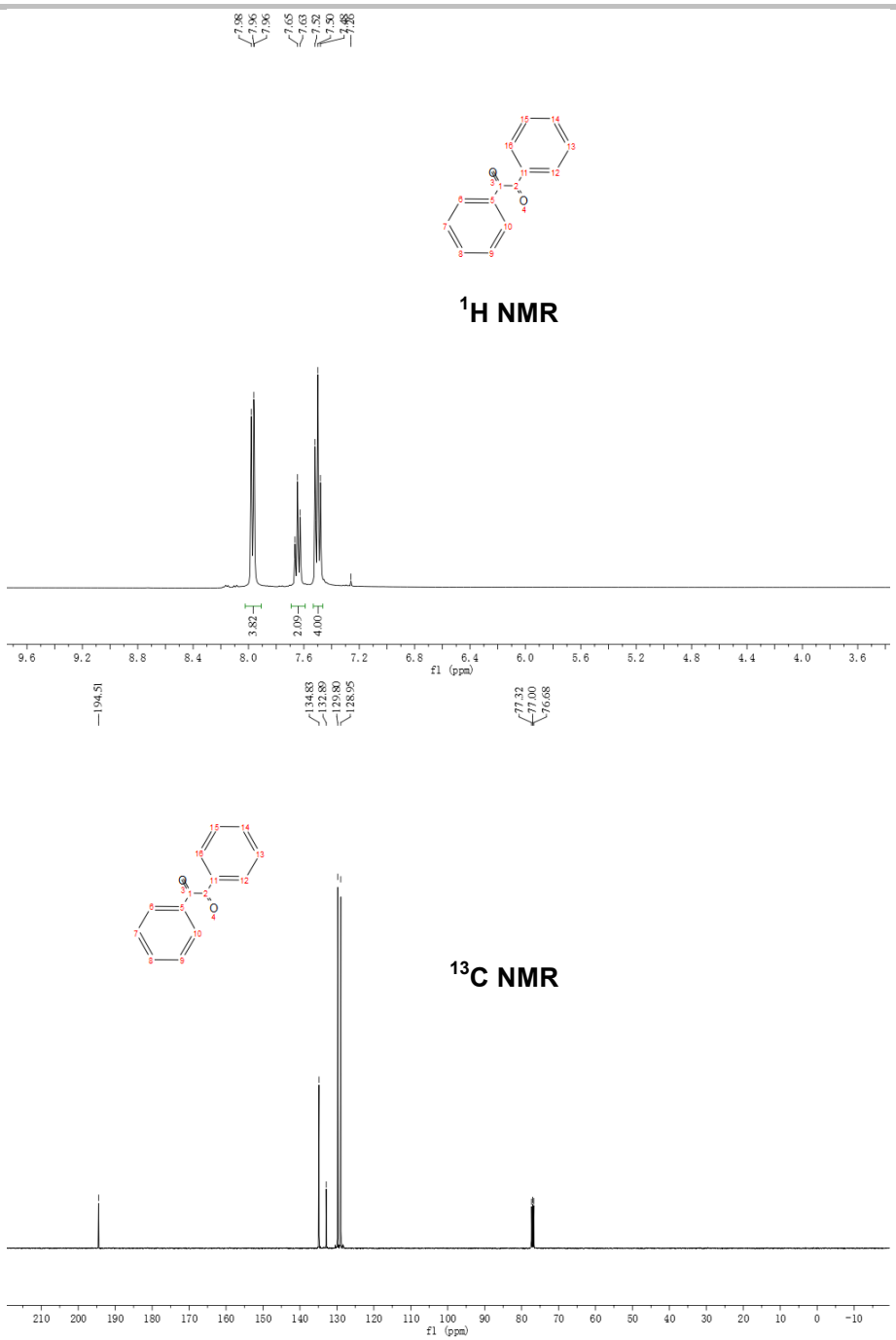



**Fig. S12** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of benzil produced in the catalytic oxidation of 2-hydroxy-1,2-diphenylethan-1-one (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.02–7.91 (m, 4H), 7.65 (t, $J$ = 7.6 Hz, 2H), 7.50 (t, $J$ = 8.0 Hz, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 194.6, 134.9, 133.0, 129.9, 129.1.

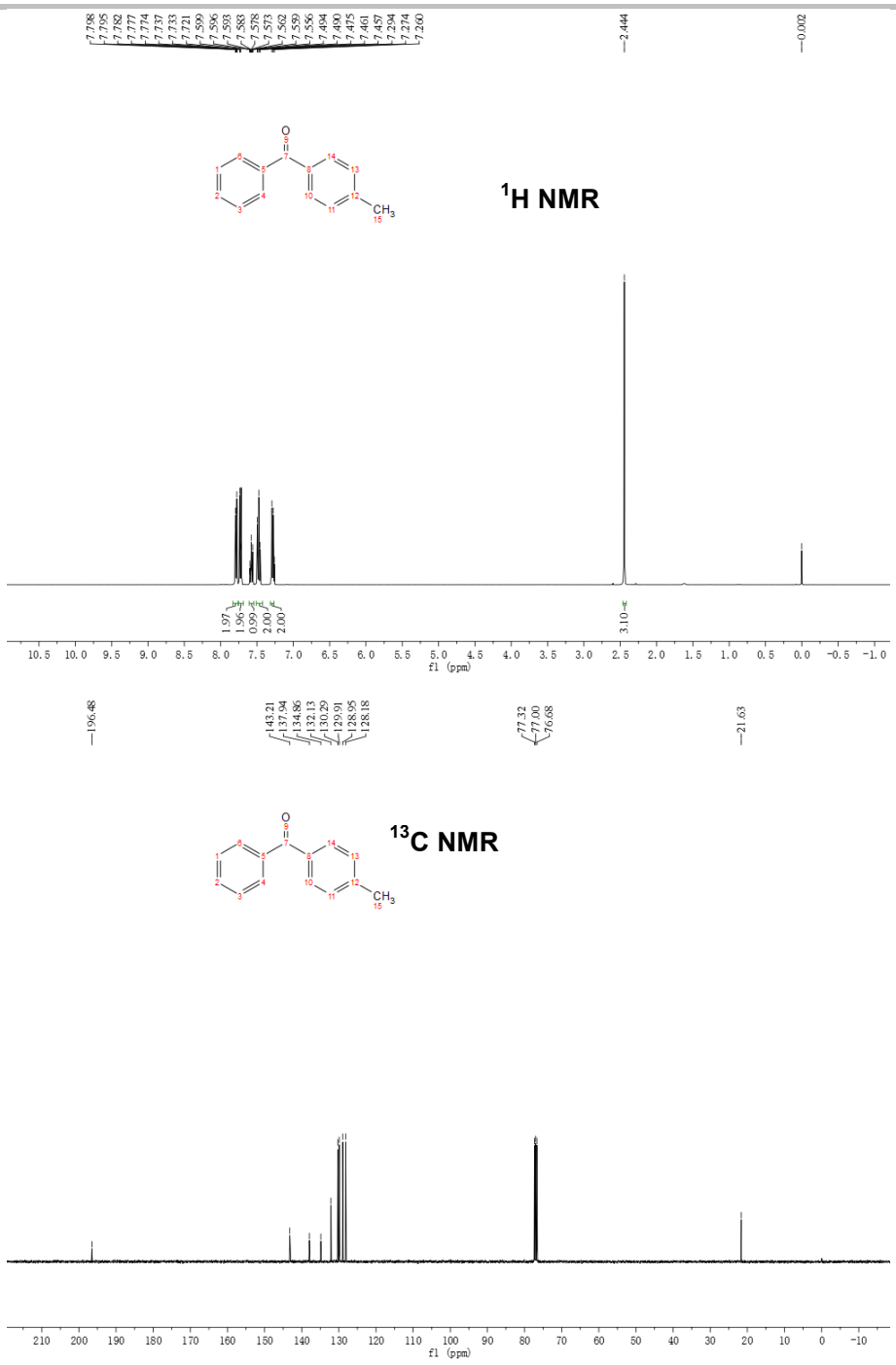



**Fig. S13** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of phenyl(*p*-tolyl)methanone produced in the catalytic oxidation of phenyl(*p*-tolyl)methanol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.80–7.77 (m, 2H), 7.74–7.72 (m, 2H), 7.59–7.55 (m, 1H), 7.49–7.46 (m, 2H), 7.28 (d, $J$ = 8.0 Hz, 2H), 2.44 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 196.5, 143.2, 137.9, 134.9, 132.1, 130.3, 129.9, 129.0, 128.2, 21.6.

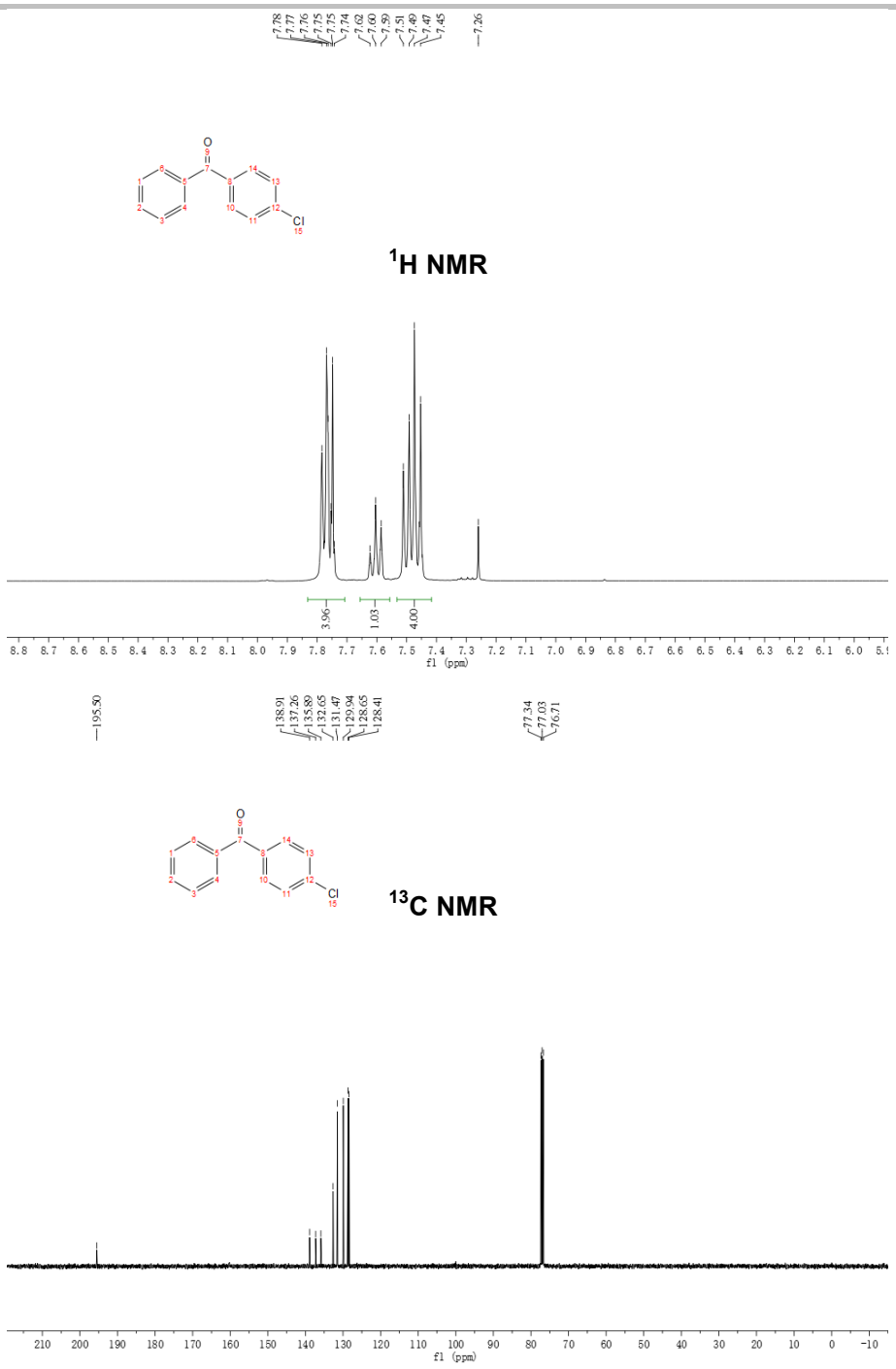



**Fig. S14** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of (*p*-chlorophenyl)(phenyl)methanone produced in the catalytic oxidation of (*p*-chlorophenyl)(phenyl)methanol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.79–7.75 (m, 4H), 7.63–7.57 (m, 1H), 7.52–7.45 (m, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.5, 138.9, 137.2, 135.9, 132.6, 131.5, 129.9, 128.6, 128.4.

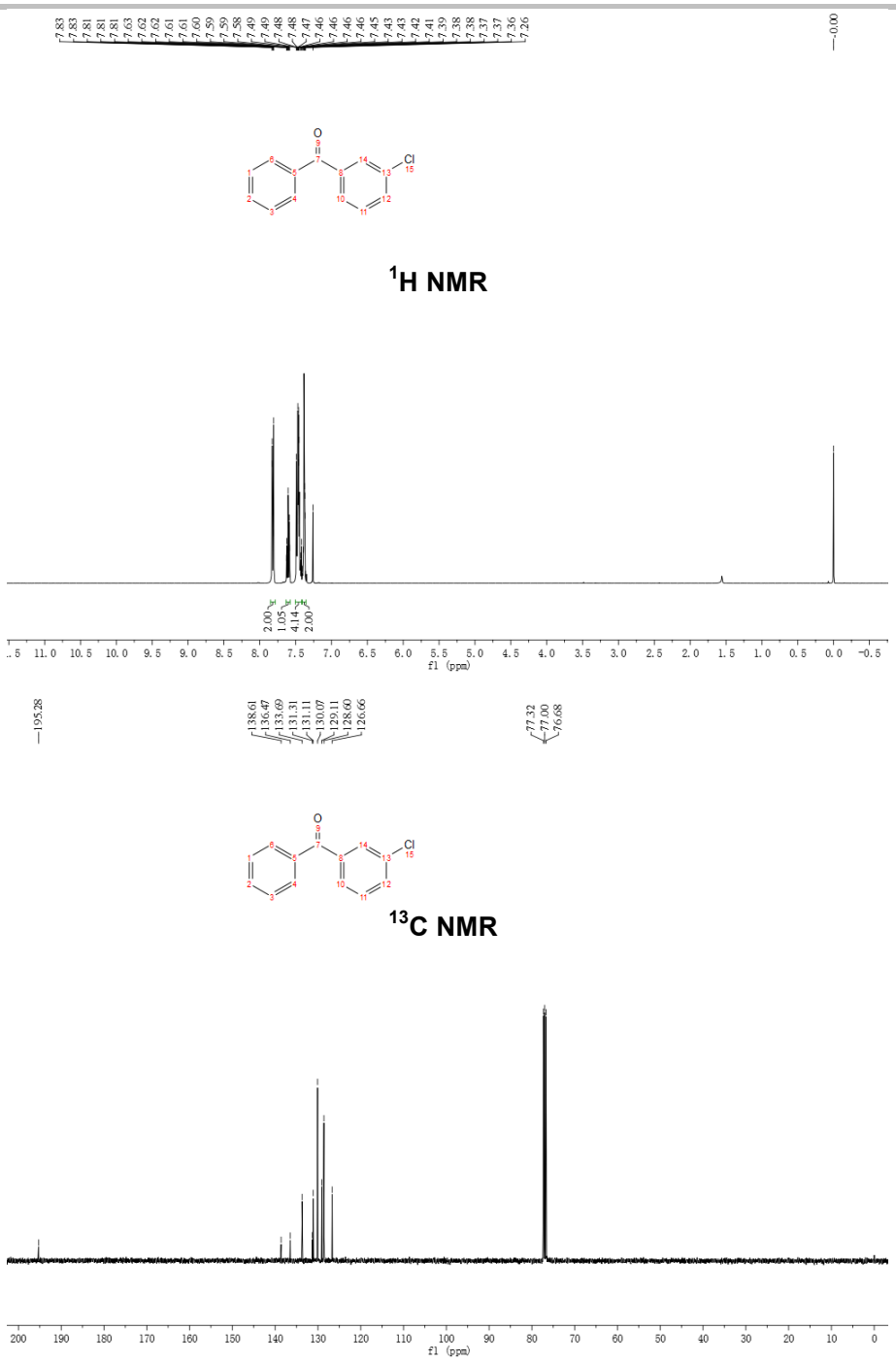



**Fig. S15** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of (*m*-chlorophenyl)(phenyl)methanone produced in the catalytic oxidation of (*m*-chlorophenyl)(phenyl)methanol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.83–7.81 (m, 2H), 7.62–7.58 (m, 1H), 7.49–7.42 (m, 4H), 7.41–7.36 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 195.3, 138.6, 136.5, 133.7, 131.3, 131.1, 130.1, 129.1, 128.6, 126.7.

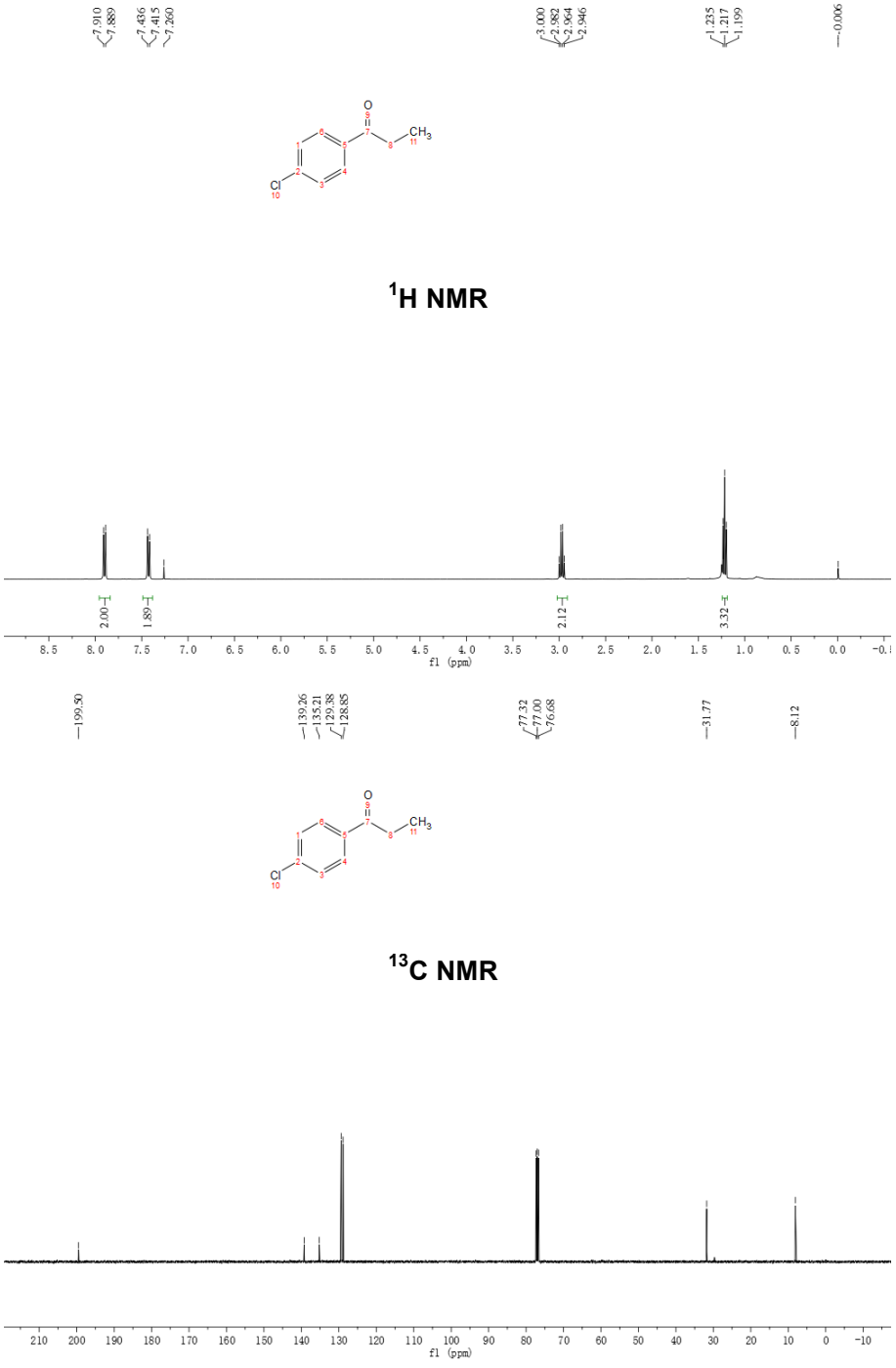
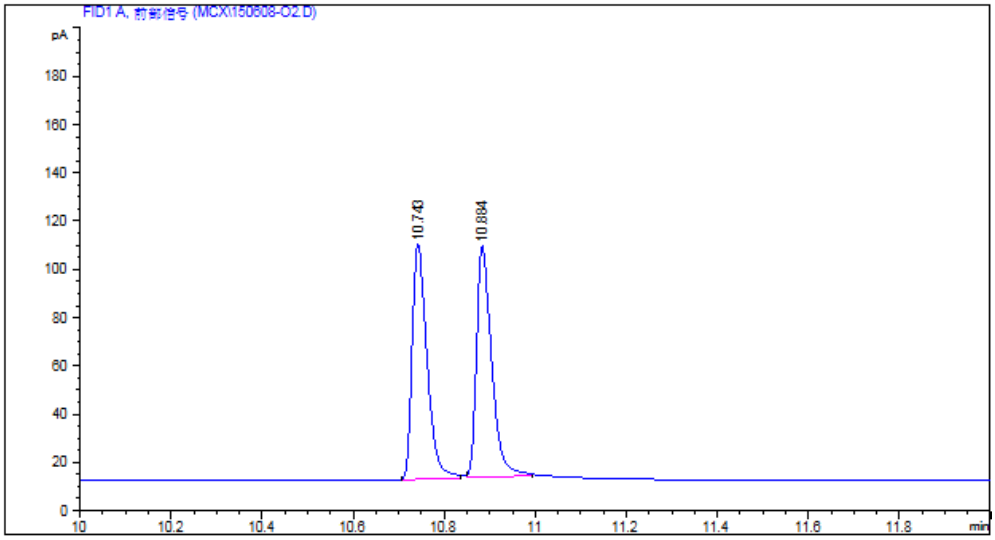
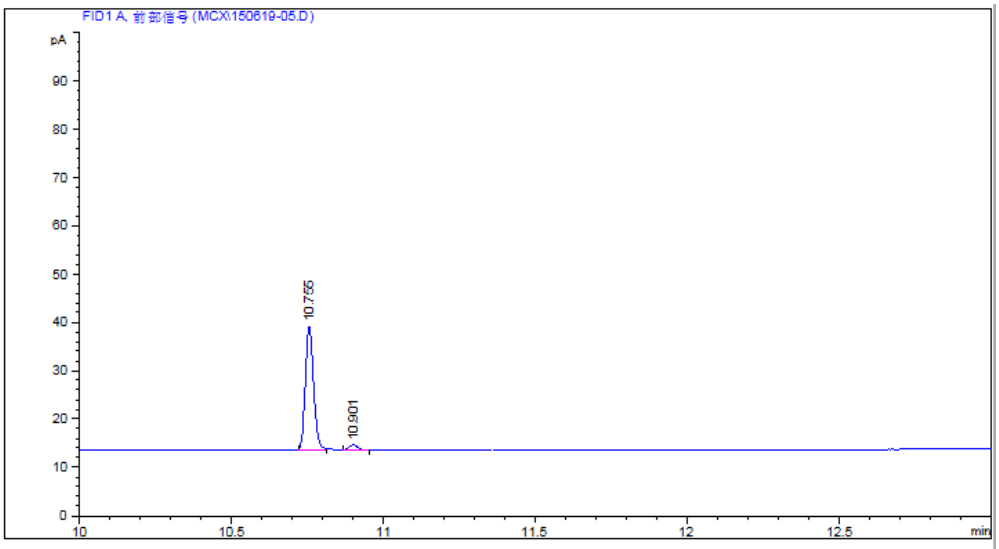



**Fig. S16** $^{1}$H (top) and $^{13}$C (bottom) NMR spectra of 1-(*p*-chlorophenyl)propan-1-one produced in the catalytic oxidation of 1-(*p*-chlorophenyl)propan-1-ol (0.50 mmol) by **1** (0.30 mol%) and $H_2O_2$ (1.2 equiv. based on the substrate concentration) in the presence of $H_2SO_4$ (0.30 mol%) in $CH_3CN$ at 25 $^{o}$C for 1 h. NMR spectra were recorded in $CDCl_3$ at 25 °C: $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, $J$ = 8.4 Hz, 2H), 7.43 (d, $J$ = 8.4 Hz, 2H), 2.97 (q, $J$ = 7.2 Hz, 2H), 1.22 (t, $J$ = 7.2 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 199.5, 139.3, 135.2, 129.4, 128.9, 31.8, 8.2.

## Additional Data: GC Chromatograms in the OKR of Secondary Alcohols

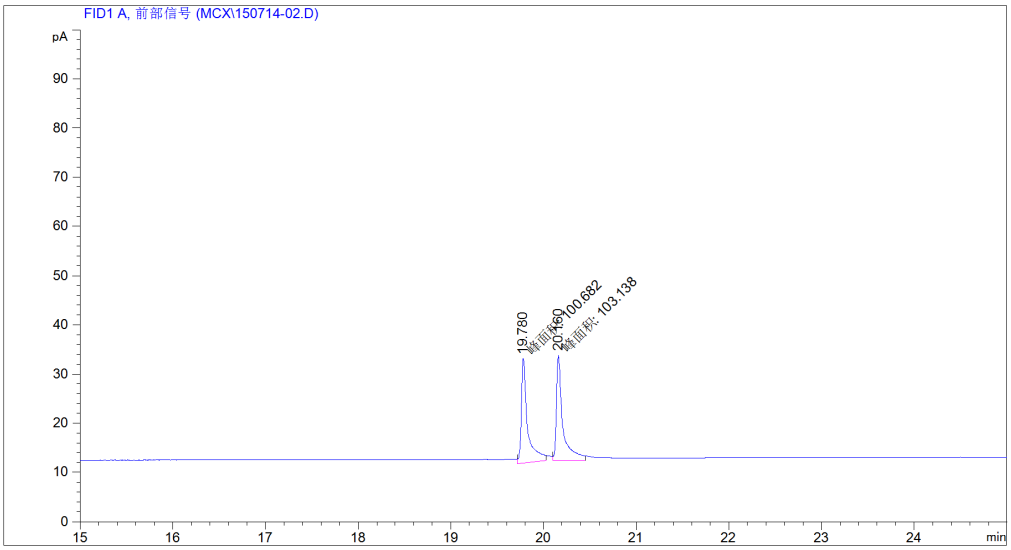



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 10.743 | 221.32146 | 50.09376 |
| 2 | 10.884 | 220.49294 | 49.90624 |

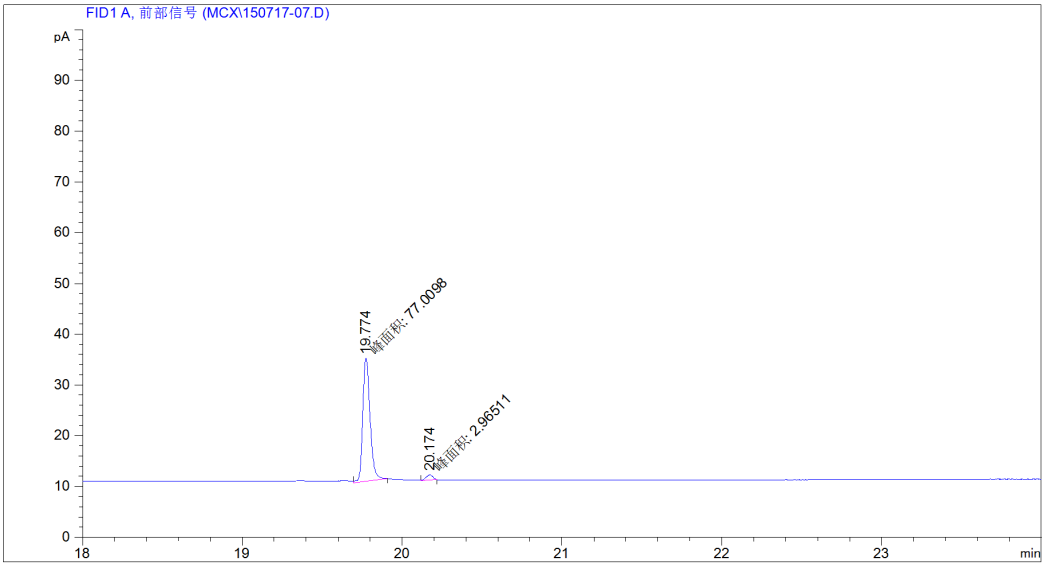



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 10.755 | 48.22452 | 96.18677 |
| 2 | 10.901 | 1.91181 | 3.81323 |

**Fig. S17** GC chromatograms of racemic 1-phenylethanol (top) as an authentic compound and the unreacted 1-phenylethanol (bottom) remained in the oxidative kinetic resolusion (OKR) of 1-phenylethanol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 10.76, $t_R$(minor) = 10.90.

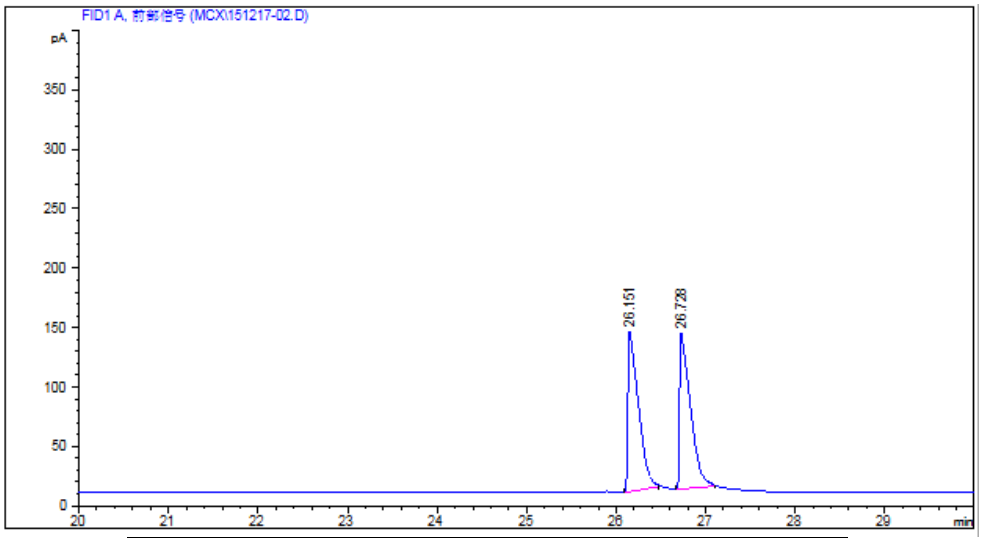



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 19.780 | 21.27739 | 49.39753 |
| 2 | 21.160 | 21.35649 | 50.60247 |

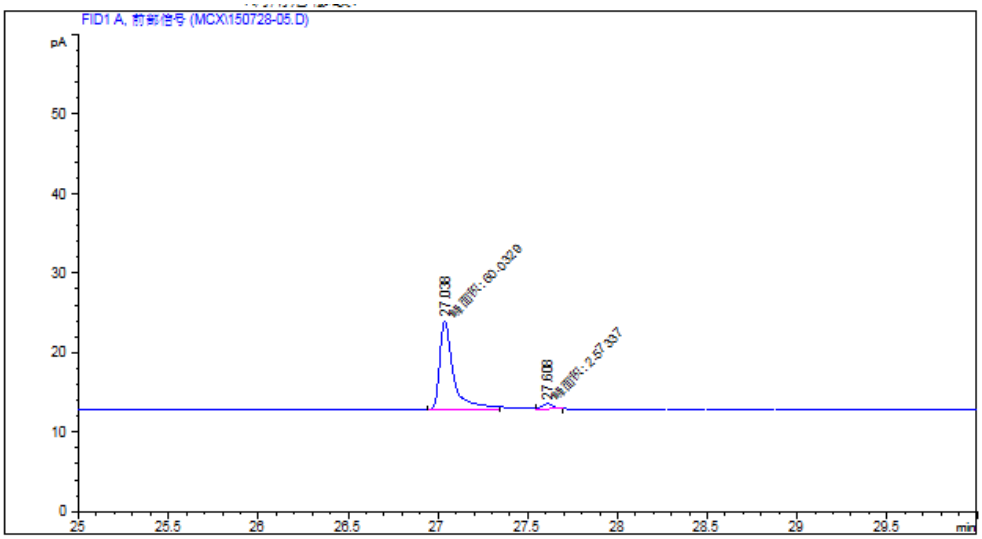



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 19.774 | 77.00982 | 96.29245 |
| 2 | 20.174 | 2.96511 | 3.70755 |

**Fig. S18** GC chromatograms of racemic 1-(*p*-chlorophenyl)ethan-1-ol (top) as an authentic compound and the unreacted 1-(*p*-chlorophenyl)ethan-1-ol (bottom) remained in the OKR of 1-(*p*-chlorophenyl)ethan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 19.77, $t_R$(minor) = 20.17.

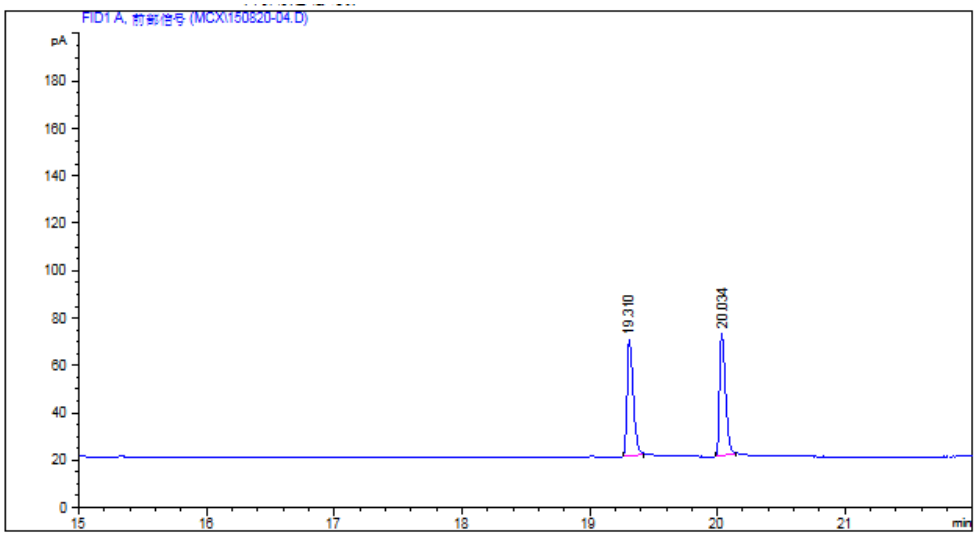



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 26.151 | 1103.08179 | 50.06979 |
| 2 | 26.728 | 1100.00684 | 49.93021 |

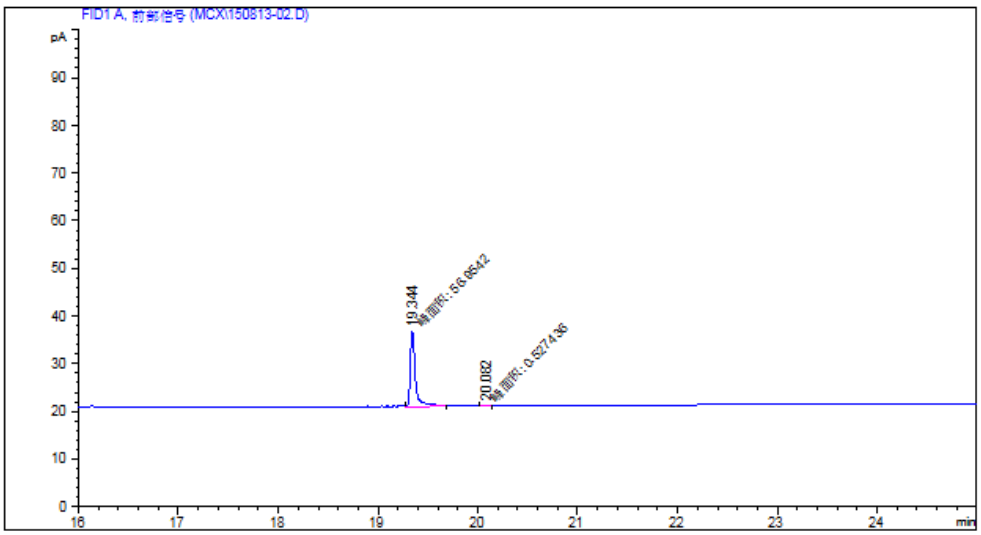



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 27.038 | 60.03294 | 95.88960 |
| 2 | 27.608 | 2.57337 | 4.11040 |

**Fig. S19** GC chromatograms of racemic 1-(*m*-chlorophenyl)ethan-1-ol (top) as an authentic compound and the unreacted 1-(*m*-chlorophenyl)ethan-1-ol (bottom) remained in the OKR of 1-(*m*-chlorophenyl)ethan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.90 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 27.04, $t_R$(minor) = 27.61.

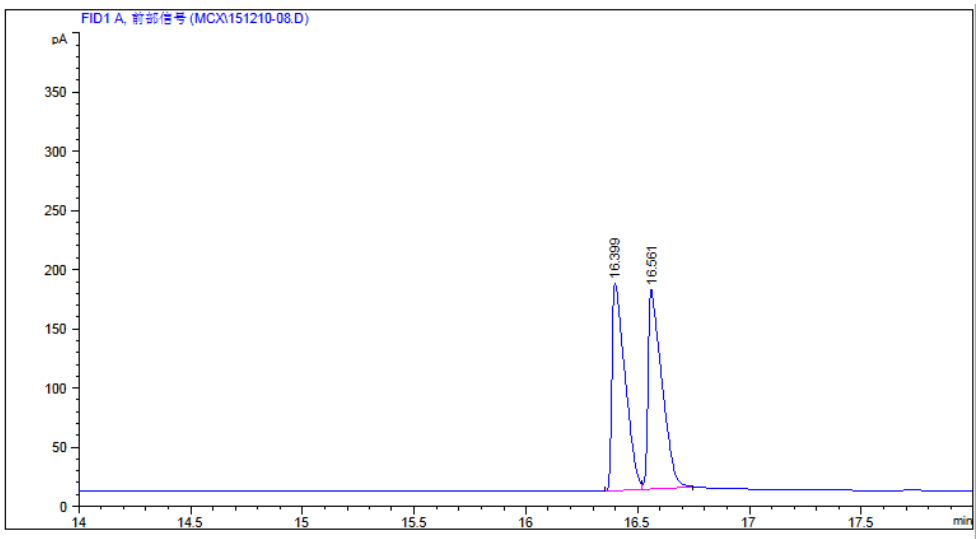



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 19.310 | 164.51648 | 49.72251 |
| 2 | 20.034 | 166.35277 | 50.27749 |

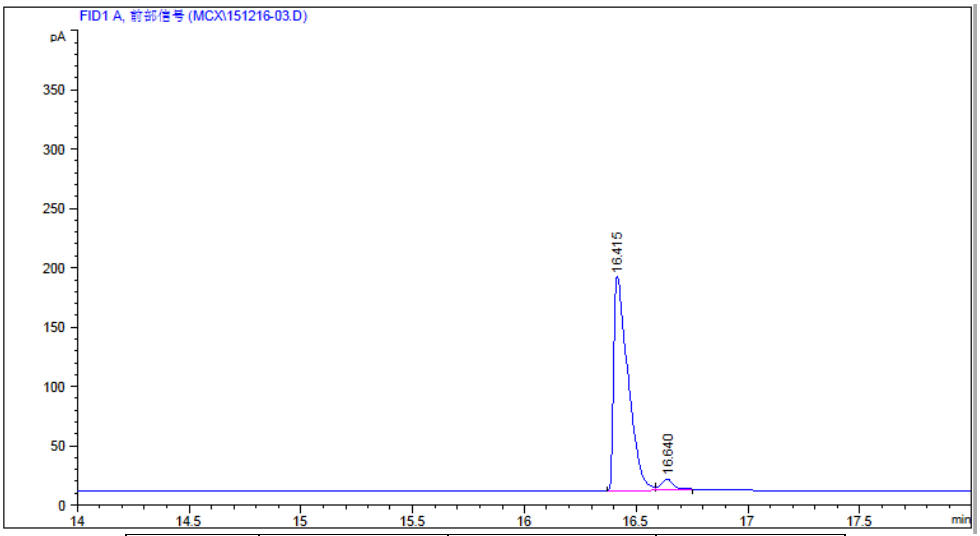



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 19.344 | 56.95418 | 99.08243 |
| 2 | 20.082 | 5.27436e-1 | 0.91757 |

**Fig. S20** GC chromatograms of racemic 1-(*o*-chlorophenyl)ethan-1-ol (top) as an authentic compound and the unreacted 1-(*o*-chlorophenyl)ethan-1-ol (bottom) remained in the OKR of 1-(*o*-chlorophenyl)ethan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.90 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 19.34, $t_R$(minor) = 20.08.

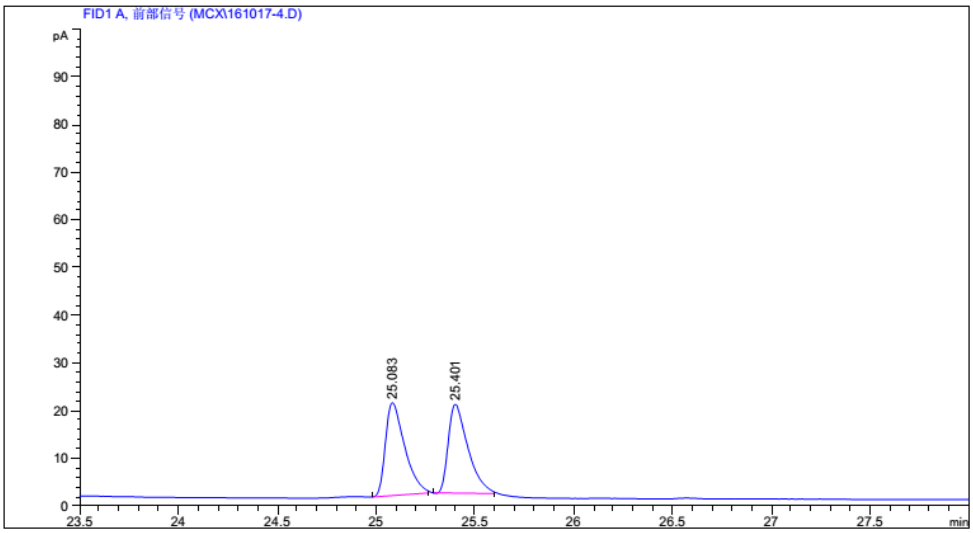



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 16.399 | 713.44073 | 49.62795 |
| 2 | 16.561 | 724.13788 | 50.37205 |

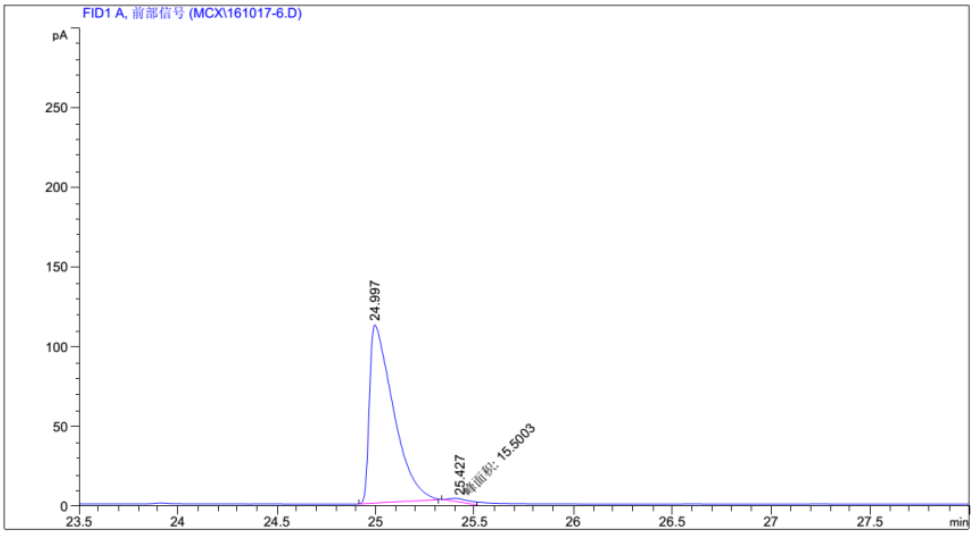



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 16.415 | 807.34265 | 95.85714 |
| 2 | 16.640 | 34.89264 | 4.14286 |

**Fig. S21** GC chromatograms of racemic 1-phenylpropan-1-ol (top) as an authentic compound and the unreacted 1-phenylpropan-1-ol (bottom) remained in the OKR of 1-phenylpropan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 16.42, $t_R$(minor) = 16.64.

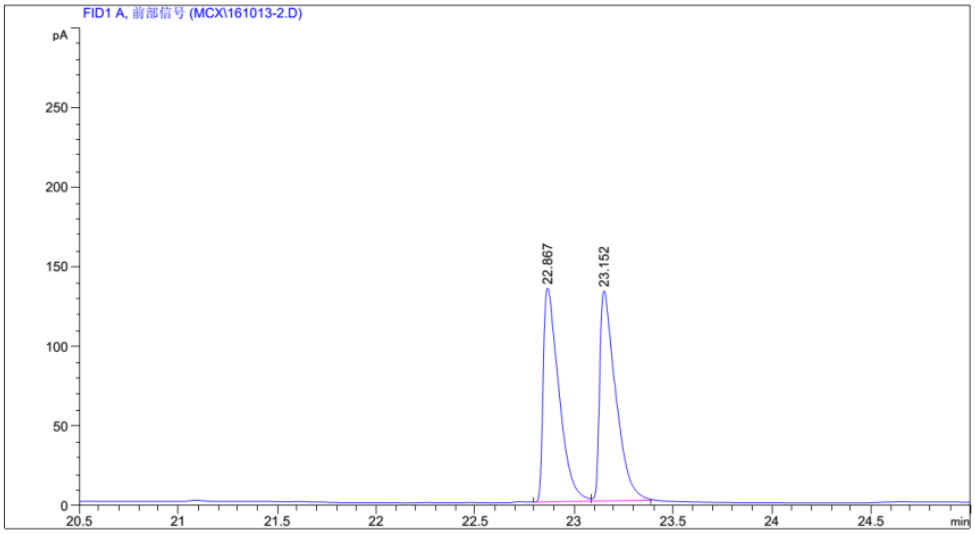



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 25.083 | 131.60493 | 50.56792 |
| 2 | 25.401 | 128.64888 | 49.43208 |

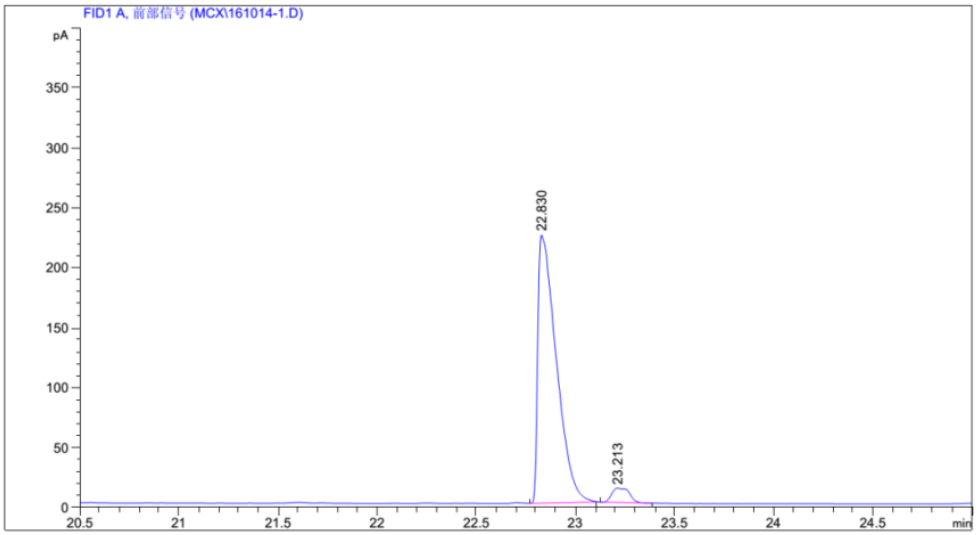



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 24.997 | 937.1784 | 98.37298 |
| 2 | 25.427 | 15.50025 | 1.62703 |

**Fig. S22** GC chromatograms of racemic 1-(*p*-bromophenyl)propan-1-ol (top) as an authentic compound and the unreacted 1-(*p*-bromophenyl)propan-1-ol (bottom) remained in the OKR of 1-(*p*-bromophenyl)propan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 25.00, $t_R$(minor) = 25.43.

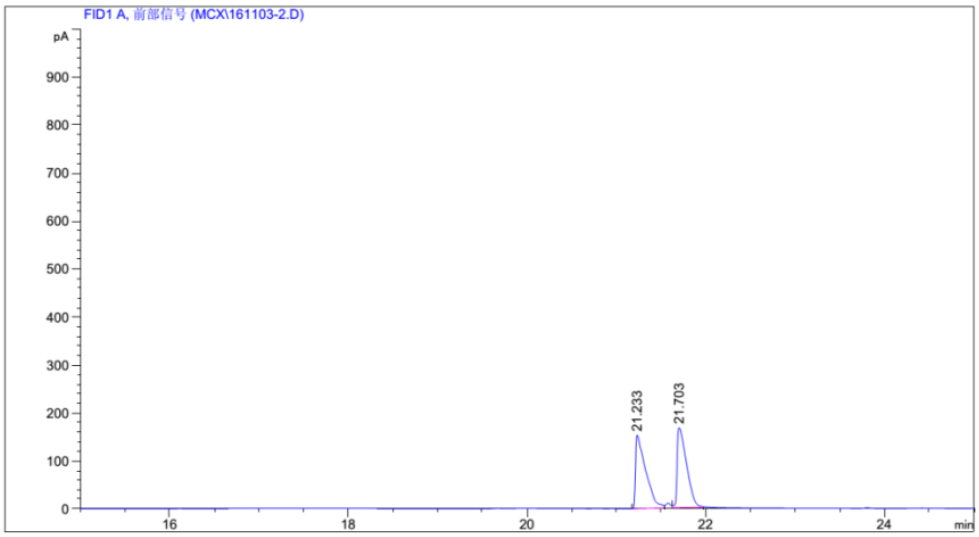



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 22.867 | 739.91113 | 49.89670 |
| 2 | 23.152 | 742.97467 | 50.10330 |

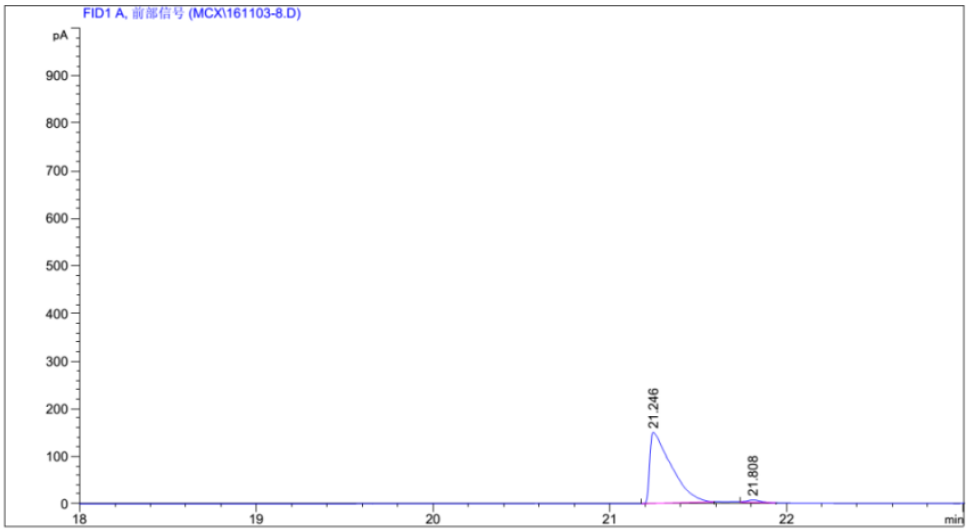



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 22.830 | 1447.52710 | 95.19693 |
| 2 | 23.213 | 73.03363 | 4.08307 |

**Fig. S23** GC chromatograms of racemic 1-(*p*-chlorophenyl)propan-1-ol (top) as an authentic compound and the unreacted 1-(*p*-chlorophenyl)propan-1-ol (bottom) remained in the OKR of 1-(*p*-chlorophenyl)propan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.70 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 5 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 22.83, $t_R$(minor) = 23.21.

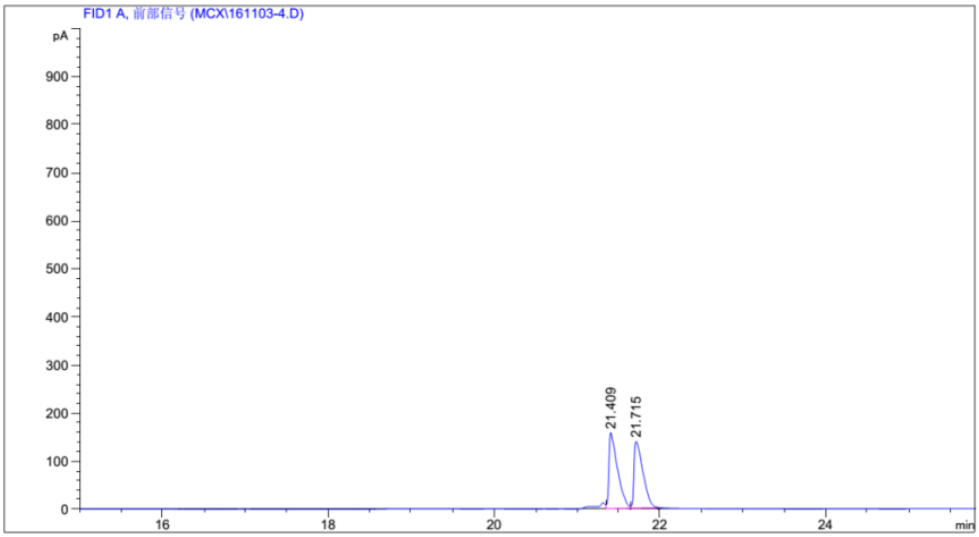



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 21.233 | 1213.78870 | 49.90455 |
| 2 | 21.703 | 1218.43164 | 50.09545 |

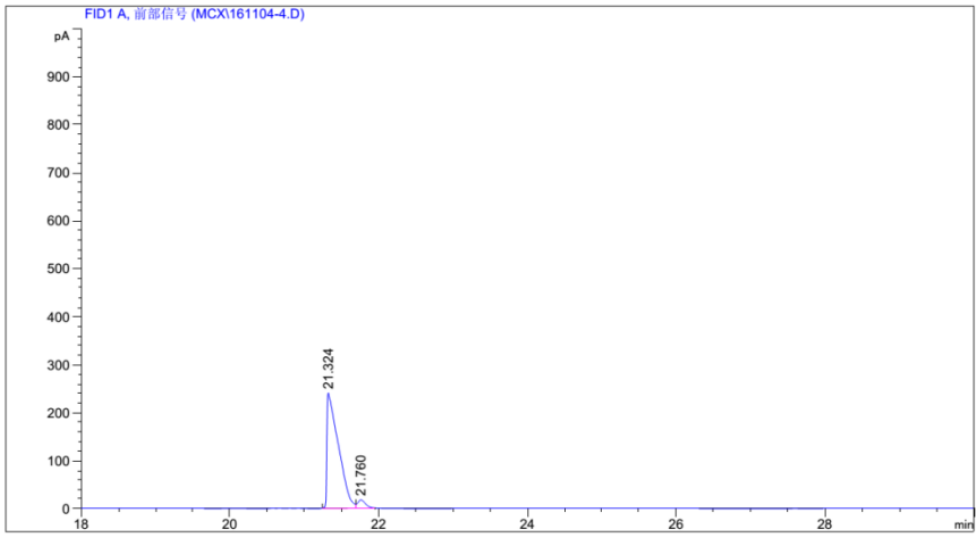



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 21.246 | 1253.60645 | 98.01667 |
| 2 | 21.808 | 25.36625 | 1.98333 |

**Fig. S24** GC chromatograms of racemic 1-(*p*-fluorophenyl)propan-1-ol (top) as an authentic compound and the unreacted 1-(*p*-fluorophenyl)propan-1-ol (bottom) remained in the OKR of 1-(*p*-fluorophenyl)propan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 4 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 21.25, $t_R$(minor) = 21.81.

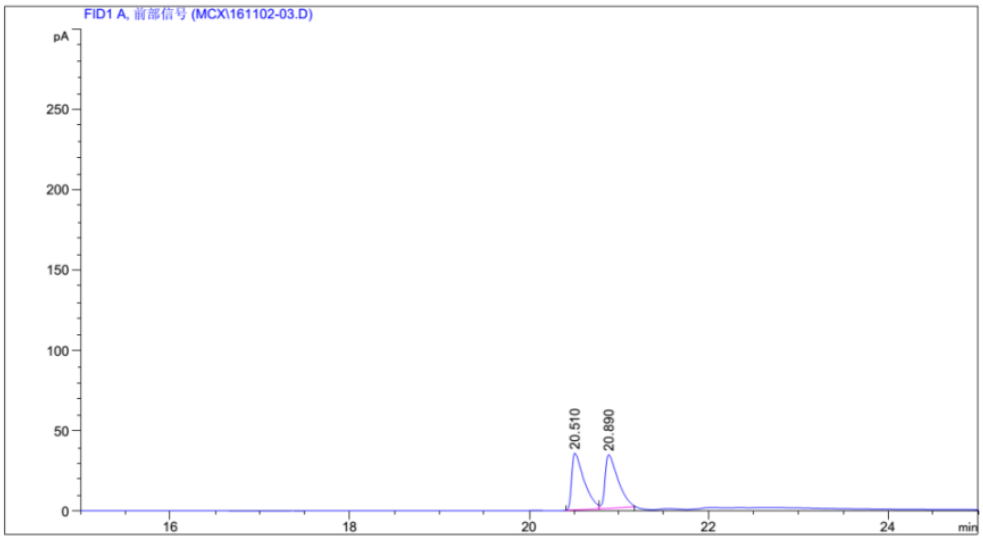



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 21.409 | 1131.69263 | 51.99319 |
| 2 | 21.715 | 1044.92416 | 48.00681 |

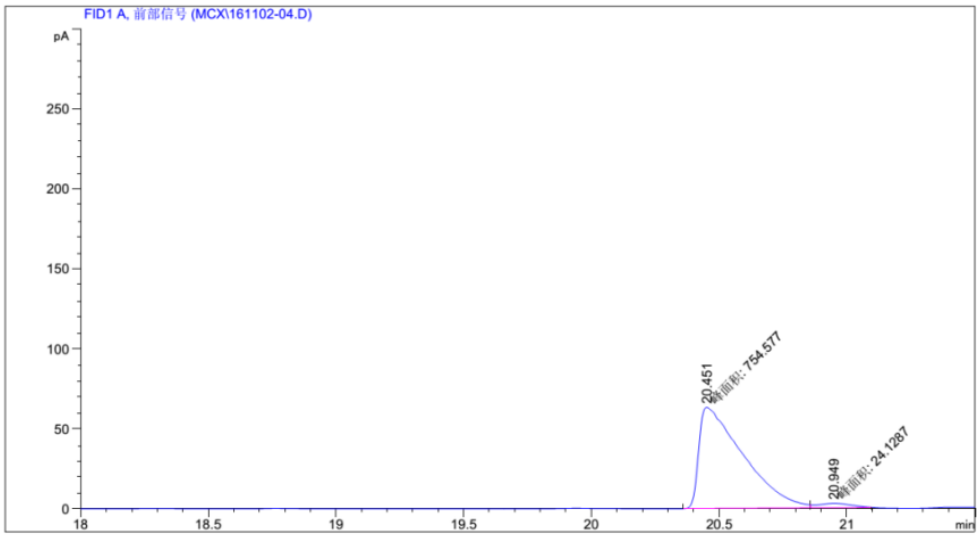



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 21.324 | 2582.07959 | 95.27065 |
| 2 | 21.760 | 128.17767 | 4.72935 |

**Fig. S25** GC chromatograms of racemic 1-(*m*-fluorophenyl)propan-1-ol (top) as an authentic compound and the unreacted 1-(*m*-fluorophenyl)propan-1-ol (bottom) remained in the OKR of 1-(*m*-fluorophenyl)propan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.90 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 80 $^oC$, hold for 5 min, ramp: 4 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 21.32, $t_R$(minor) = 21.76.

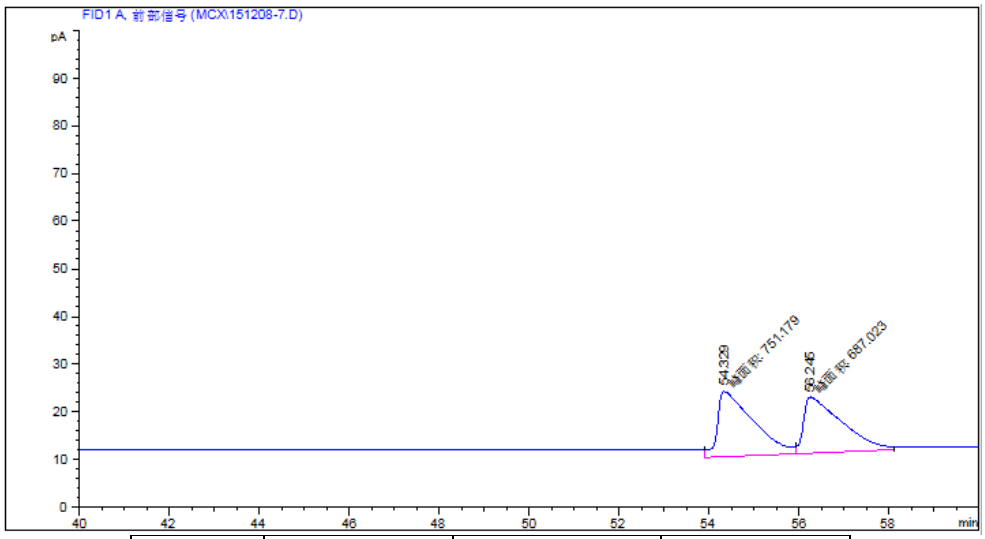



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 20.510 | 336.88757 | 50.25461 |
| 2 | 20.890 | 333.47400 | 49.74539 |

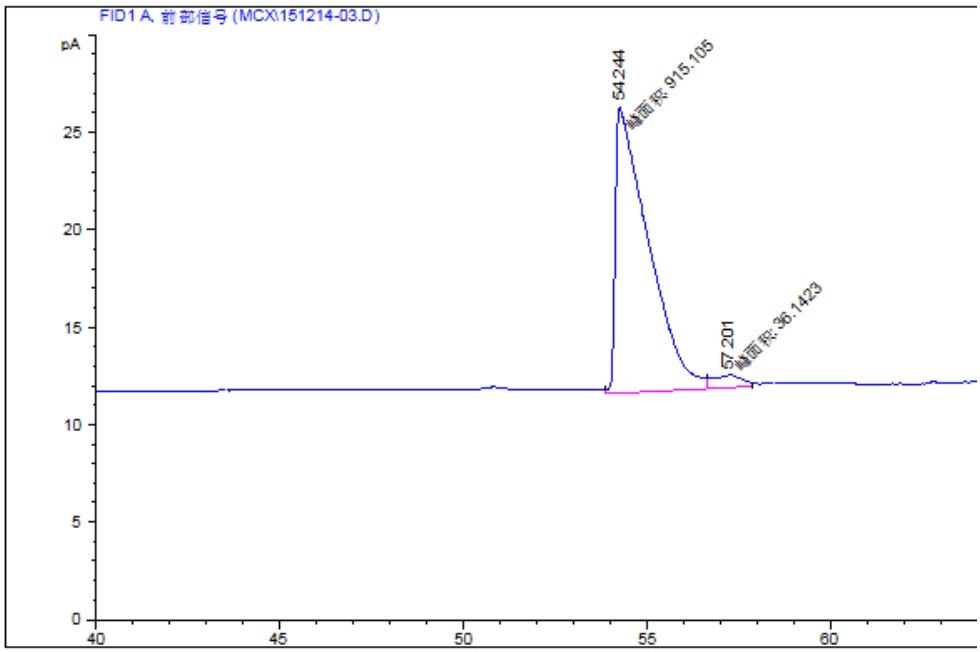



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 20.451 | 754.57745 | 96.90144 |
| 2 | 20.949 | 24.12867 | 3.09856 |

**Fig. S26** GC chromatograms of racemic 1-(*o*-fluorophenyl)propan-1-ol (top) as an authentic compound and the unreacted 1-(*o*-fluorophenyl)propan-1-ol (bottom) remained in the OKR of 1-(*o*-fluorophenyl)propan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 100 $^oC$, hold for 5 min, ramp: 2 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 20.45, $t_R$(minor) = 20.95.

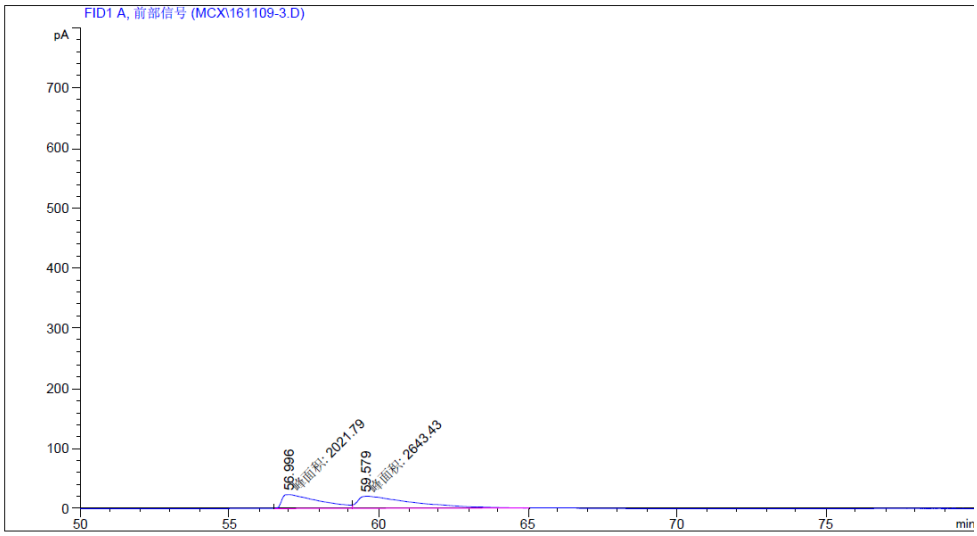



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 54.329 | 751.17865 | 52.23042 |
| 2 | 56.245 | 687.02289 | 47.76958 |

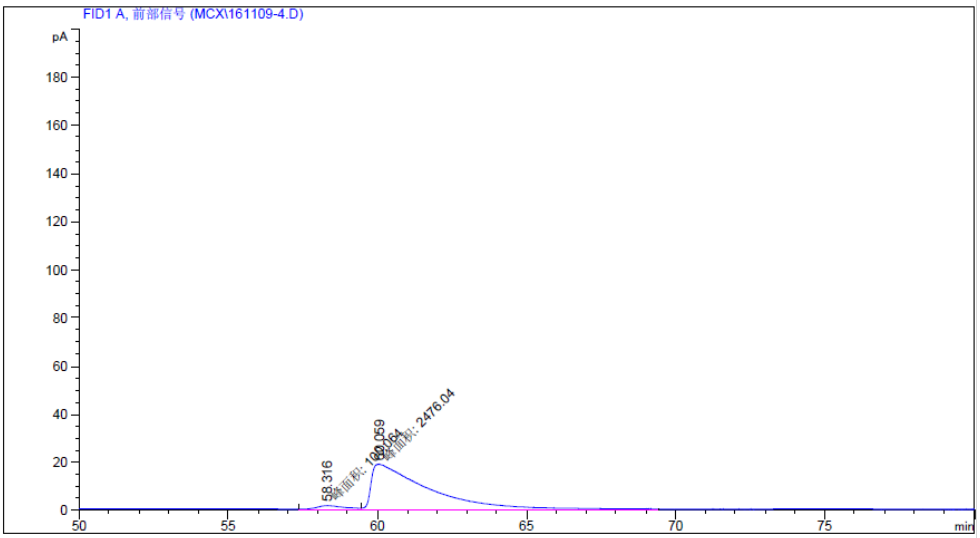



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 54.244 | 915.10461 | 96.20053 |
| 2 | 57.201 | 36.14231 | 3.79947 |

**Fig. S27** GC chromatograms of racemic 2-methyl-1-phenylpropan-1-ol (top) as an authentic compound and the unreacted 2-methyl-1-phenylpropan-1-ol (bottom) remained in the OKR of 2-methyl-1-phenylpropan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 140 $^oC$, hold for 25 min, ramp: 10 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 54.24, $t_R$(minor) = 57.20.

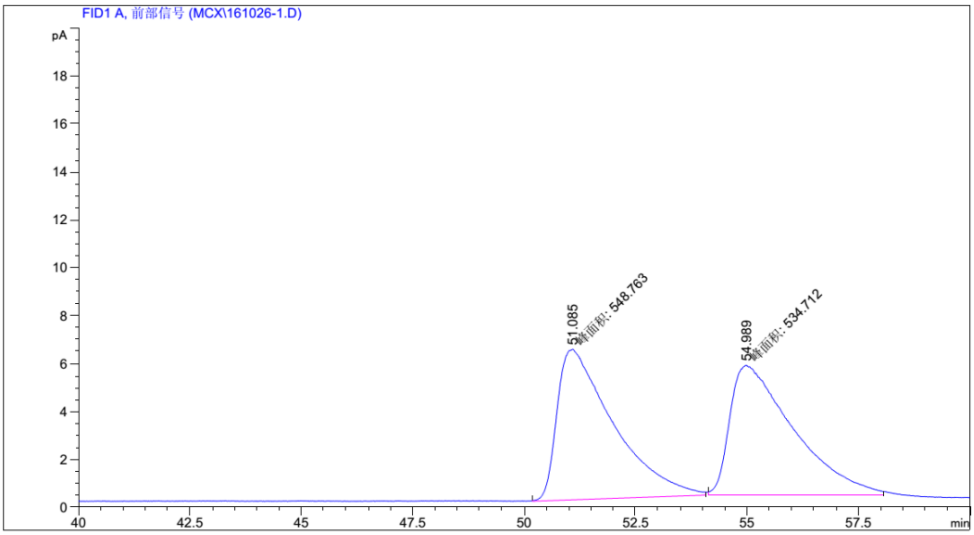



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 56.996 | 2021.78894 | 43.33752 |
| 2 | 59.579 | 2643.42749 | 56.66248 |

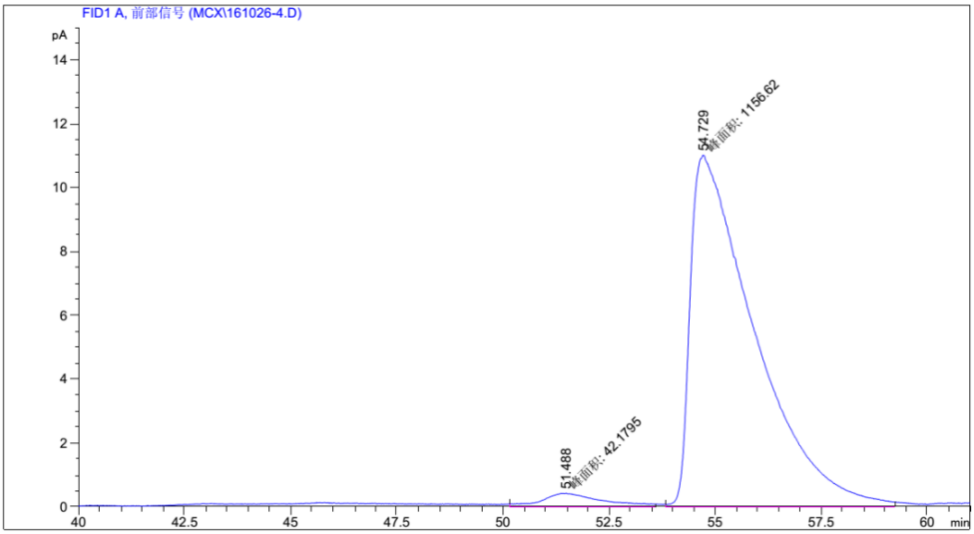



| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 58.316 | 100.06412 | 3.88432 |
| 2 | 60.059 | 2476.03882 | 96.11568 |

**Fig. S28** GC chromatograms of racemic cyclohexyl(phenyl)methanol (top) as an authentic compound and the unreacted cyclohexyl(phenyl)methanol (bottom) remained in the OKR of cyclohexyl(phenyl)methanol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 110 $^oC$, hold for 3 min, ramp: 10 $^oC$/min to 135 $^oC$, hold for 80 min, then ramp: 10 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 58.32, $t_R$(minor) = 60.06.



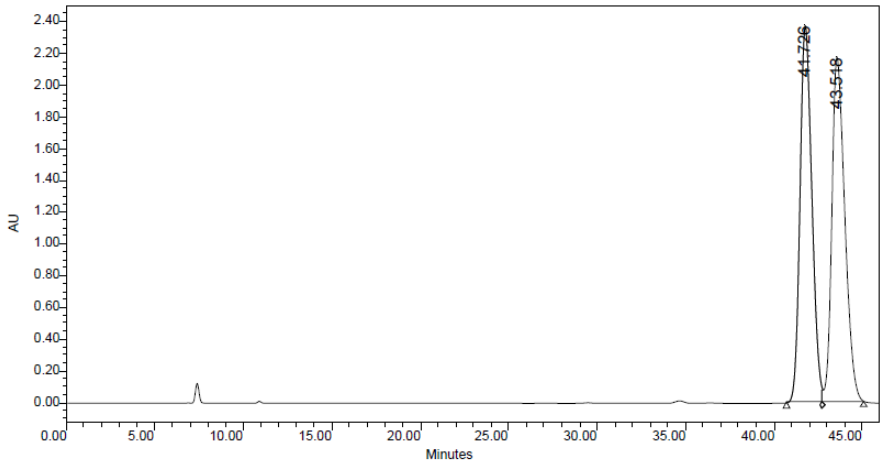

| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 51.085 | 548.76337 | 50.64846 |
| 2 | 54.989 | 534.71161 | 49.35154 |



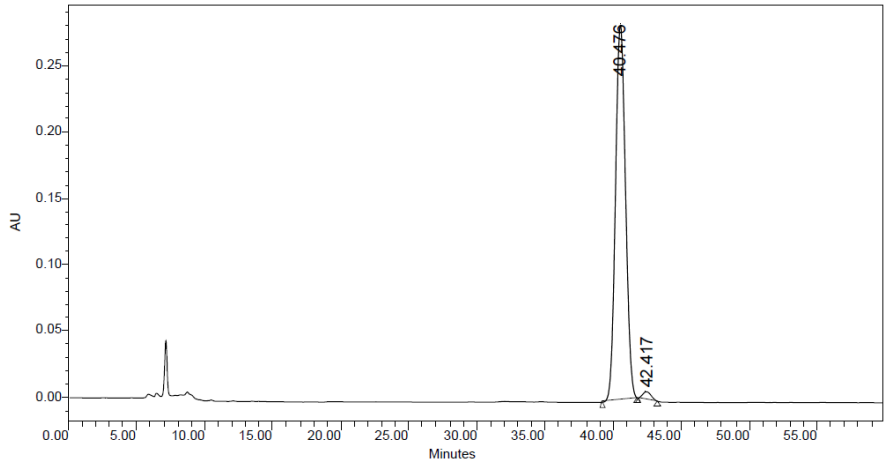

| Entry | RT(min) | Area | Area% |
|---|---|---|---|
| 1 | 51.488 | 42.17953 | 3.51848 |
| 2 | 54.729 | 1156.62170 | 96.48152 |

**Fig. S29** GC chromatograms of racemic 1-phenylheptan-1-ol (top) as an authentic compound and the unreacted 1-phenylheptan-1-ol (bottom) remained in the OKR of 1-phenylheptan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.80 equiv. based on the substrate concentration), and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. GC-7890, CP-Chirasil-Dex CB chiral column; Column temperature: 130 $^oC$, hold for 60 min, ramp: 10 $^oC$/min to 170 $^oC$, hold for 20 min. $t_R$(major) = 51.49, $t_R$(minor) = 54.73.

## Additional Data: HPLC Chromatograms in the OKR of Secondary Alcohols

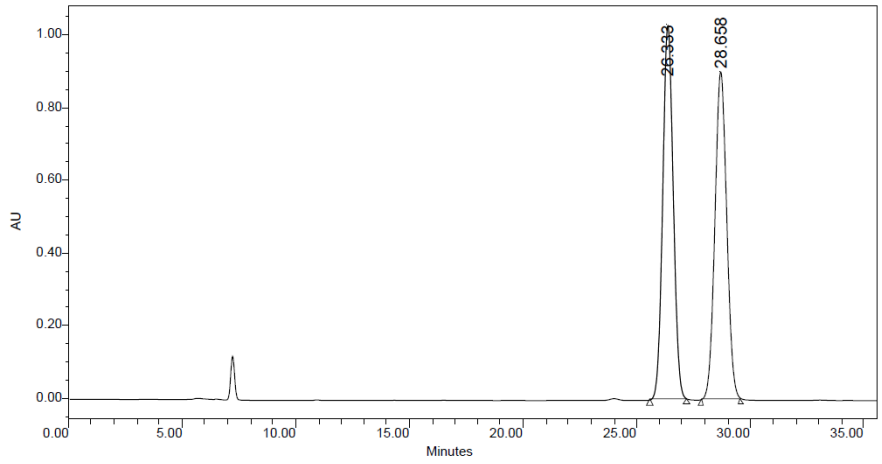



| | RT (min) | Area (μV *sec) | % Area | Height (μV) | % Height |
|---|---|---|---|---|---|
| 1 | 41.726 | 110476089 | 49.93 | 2373301 | 52.19 |
| 2 | 43.518 | 110770129 | 50.07 | 2173780 | 47.81 |

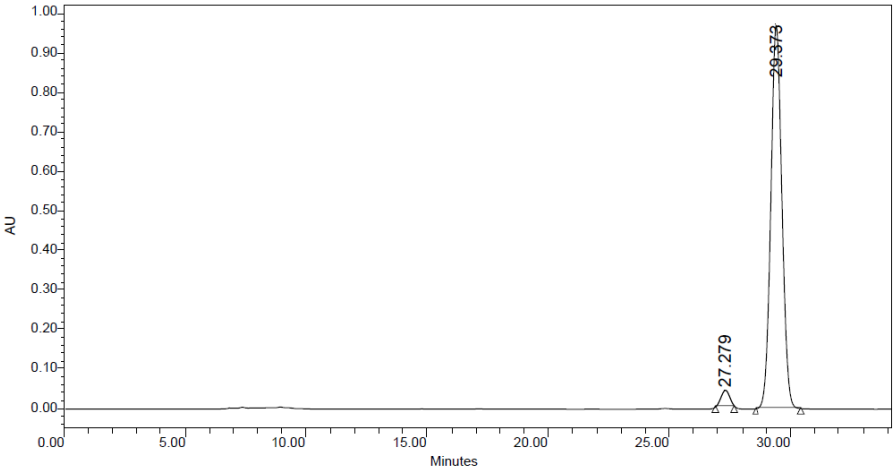



| | RT (min) | Area (μV *sec) | % Area | Height (μV) | % Height |
|---|---|---|---|---|---|
| 1 | 40.476 | 14488446 | 98.37 | 282963 | 98.04 |
| 2 | 42.417 | 240423 | 1.63 | 5663 | 1.96 |

**Fig. S30** HPLC chromatograms of racemic 1-(4-nitrophenyl)ethan-1-ol (top) as an authentic compound and the unreacted 1-(4-nitrophenyl)ethan-1-ol (bottom) remained in the oxidative kinetic resolusion (OKR) of 1-(4-nitrophenyl)ethan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.90 equiv. based on the substrate concentration) and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. HPLC-separation conditions: Chiralcel IA, 25 $^oC$, 254 nm, 90/10 hexane/i-PrOH, 1.0 mL/min; tmajor = 40.48 min, tminor = 42.42 min.




| | RT (min) | Area (𝒱 *sec) | % Area | Height (𝒱) | % Height |
|---|---|---|---|---|---|
| 1 | 26.333 | 32992598 | 50.40 | 1026155 | 53.29 |
| 2 | 28.658 | 32474123 | 49.60 | 899593 | 46.71 |




| | RT (min) | Area (𝒱 *sec) | % Area | Height (𝒱) | % Height |
|---|---|---|---|---|---|
| 1 | 27.279 | 1017066 | 3.20 | 41379 | 4.09 |
| 2 | 29.373 | 30808821 | 96.80 | 970040 | 95.91 |

**Fig. S31** HPLC chromatograms of racemic 1-([1,1'-biphenyl]-4-yl)ethan-1-ol (top) as an authentic compound and the unreacted 1-([1,1'-biphenyl]-4-yl)ethan-1-ol (bottom) remained in the OKR of 1-([1,1'-biphenyl]-4-yl)ethan-1-ol (0.50 mmol) by 30% $H_2O_2$ (0.90 equiv. based on the substrate concentration) and **2** (0.20 mol%) in the presence of $H_2SO_4$ (1.0 mol%) in $CH_3CN$ at 0 $^oC$. HPLC-separation conditions: Chiralcel IA, 25 $^oC$, 254 nm, 90/10 hexane/i-PrOH, 1.0 mL/min; tmajor = 27.28 min, tminor = 29.37 min.

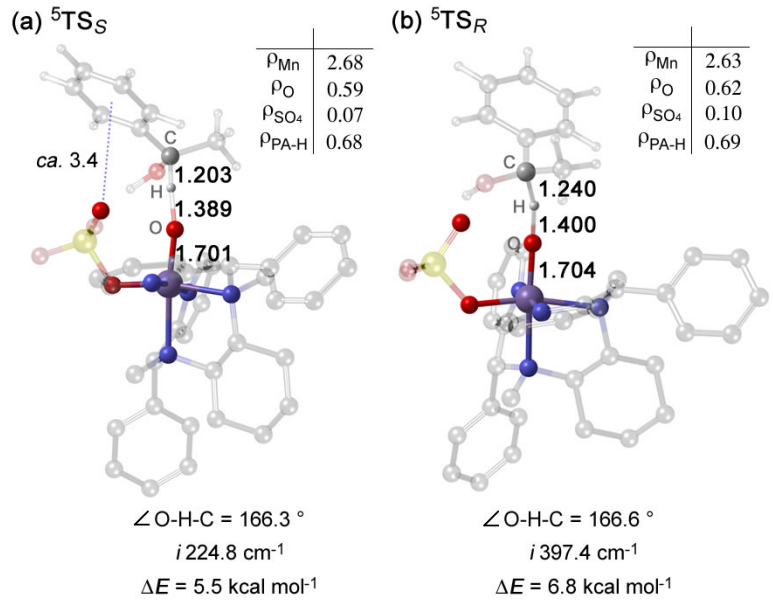
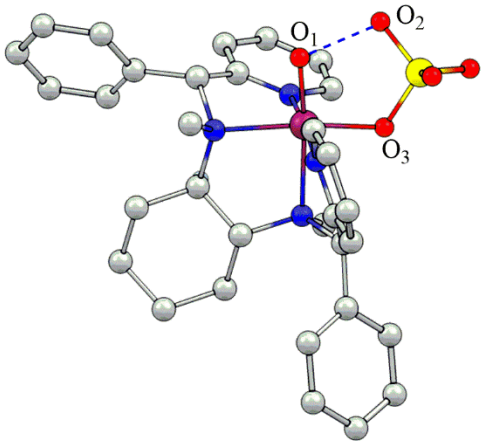



**Fig. S32** UB3LYP/LACVP* key geometric information for transition states of $C_\alpha$-H bond activation for both *R*- and *S*-1-phenylethanol mediated by a high-valent Mn-oxo complex ($[LMnO(SO_4)]^+$). Length, angle, imaginary frequency are in Å, degree (°), and $cm^{-1}$ units. Hydrogen atoms in the ligand are omitted for clarity.

| Distance | | | spin density | | |
|---|---|---|---|---|---|
| $Mn-O_1$ | $Mn-O_3$ | $O_1-O_2$ | Mn | $O_1$ | $O_2$ |
| 1.722 | 1.885 | 2.253 | 2.79 | 0.87 | 0.42 |



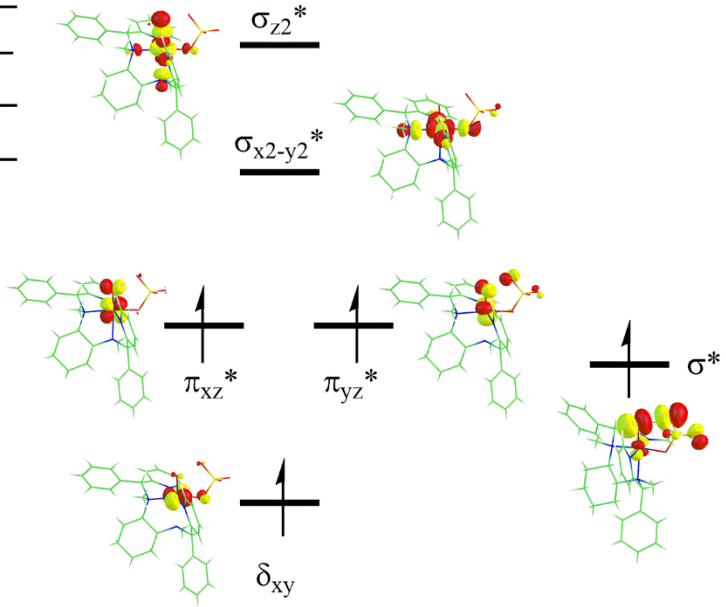




**Fig. S33** Geometric and electronic configuration of $^5$**I**.

# Cartesian Coordinates

## $^5$I

| | | | |
|---|---|---|---|
| 25 | -0.183148000 | 0.047179000 | 0.173585000 |
| 7 | -0.064449000 | 0.047505000 | 2.357328000 |
| 7 | 1.929464000 | -0.019568000 | 0.256047000 |
| 7 | -0.539721000 | -1.906971000 | 0.566986000 |
| 7 | 0.235312000 | 2.017572000 | -0.077211000 |
| 6 | -0.511303000 | 1.358655000 | 2.905268000 |
| 1 | -1.478582000 | 1.603935000 | 2.466354000 |
| 1 | 0.207784000 | 2.134382000 | 2.644997000 |
| 1 | -0.615835000 | 1.321754000 | 3.991959000 |
| 6 | 1.368095000 | -0.284593000 | 2.722839000 |
| 1 | 1.433622000 | -1.376557000 | 2.691029000 |
| 6 | 1.796602000 | 0.202265000 | 4.128412000 |
| 1 | 1.785989000 | 1.298138000 | 4.149300000 |
| 1 | 1.083305000 | -0.140437000 | 4.878548000 |
| 6 | 3.209301000 | -0.277123000 | 4.486818000 |
| 1 | 3.225465000 | -1.373558000 | 4.553012000 |
| 1 | 3.475938000 | 0.104318000 | 5.478848000 |
| 6 | 4.216826000 | 0.192929000 | 3.436294000 |
| 1 | 4.305262000 | 1.287351000 | 3.468689000 |
| 1 | 5.213605000 | -0.211912000 | 3.644202000 |
| 6 | 3.782020000 | -0.253263000 | 2.033699000 |
| 1 | 3.773406000 | -1.348878000 | 2.004902000 |
| 1 | 4.507842000 | 0.082528000 | 1.293151000 |
| 6 | 2.368212000 | 0.276327000 | 1.685452000 |
| 1 | 2.362550000 | 1.367413000 | 1.767294000 |
| 6 | 2.412843000 | -1.344471000 | -0.229574000 |
| 1 | 1.932653000 | -1.556872000 | -1.184831000 |
| 1 | 2.152226000 | -2.119849000 | 0.488832000 |
| 1 | 3.495289000 | -1.333668000 | -0.369035000 |
| 6 | 2.348902000 | 1.061405000 | -0.758649000 |
| 1 | 2.013735000 | 0.628527000 | -1.707446000 |
| 6 | 1.472619000 | 2.280283000 | -0.553577000 |
| 1 | 1.823680000 | 3.572537000 | -0.936725000 |
| 1 | 2.810918000 | 3.767906000 | -1.334018000 |
| 6 | 0.890204000 | 4.601011000 | -0.810772000 |
| 1 | 1.153537000 | 5.611650000 | -1.105136000 |
| 6 | -0.378357000 | 4.314063000 | -0.311598000 |
| 1 | -1.135195000 | 5.081749000 | -0.200291000 |
| 6 | -0.675229000 | 3.003122000 | 0.035902000 |
| 1 | -1.651828000 | 2.715572000 | 0.400737000 |
| 6 | 3.838479000 | 1.341145000 | -0.887391000 |
| 6 | 4.549244000 | 0.709677000 | -1.918850000 |
| 1 | 4.028967000 | 0.042797000 | -2.601109000 |
| 6 | 5.916727000 | 0.935728000 | -2.089050000 |
| 1 | 6.448442000 | 0.435751000 | -2.893057000 |
| 6 | 6.590973000 | 1.809316000 | -1.234883000 |
| 1 | 7.653466000 | 1.991217000 | -1.367387000 |
| 6 | 5.890653000 | 2.459785000 | -0.214802000 |
| 1 | 6.405112000 | 3.149887000 | 0.447207000 |
| 6 | 4.525757000 | 2.230032000 | -0.042965000 |
| 1 | 4.000693000 | 2.753659000 | 0.750422000 |
| 6 | -1.069471000 | -1.028569000 | 2.771003000 |
| 1 | -2.030725000 | -0.564516000 | 2.525381000 |
| 6 | -0.957415000 | -2.205292000 | 1.818608000 |
| 6 | -1.383380000 | -3.495338000 | 2.128937000 |
| 1 | -1.733083000 | -3.720588000 | 3.127709000 |
| 6 | -1.363593000 | -4.481487000 | 1.143359000 |
| 1 | -1.690601000 | -5.489206000 | 1.378197000 |
| 6 | -0.934071000 | -4.155143000 | -0.141469000 |
| 1 | -0.914191000 | -4.887277000 | -0.940324000 |
| 6 | -0.543099000 | -2.848846000 | -0.396839000 |
| 1 | -0.240679000 | -2.515193000 | -1.380778000 |
| 6 | -1.120046000 | -1.396038000 | 4.248691000 |
| 6 | -0.256246000 | -2.338264000 | 4.833145000 |
| 1 | 0.486806000 | -2.852688000 | 4.230954000 |
| 6 | -0.345524000 | -2.636304000 | 6.192854000 |
| 1 | 0.330676000 | -3.367040000 | 6.626593000 |
| 6 | -1.302736000 | -2.003256000 | 6.990921000 |
| 1 | -1.371536000 | -2.238638000 | 8.048986000 |
| 6 | -2.177090000 | -1.078051000 | 6.419251000 |
| 1 | -2.933547000 | -0.590677000 | 7.027140000 |
| 6 | -2.088404000 | -0.782523000 | 5.057095000 |
| 1 | -2.784938000 | -0.073269000 | 4.617876000 |
| 8 | -4.024853000 | 1.256345000 | -0.826267000 |
| 16 | -2.907324000 | 0.308488000 | -0.979171000 |
| 8 | -2.027232000 | 0.399043000 | 0.348189000 |
| 8 | -3.253861000 | -1.095123000 | -1.221557000 |
| 8 | -1.978344000 | 0.901192000 | -2.072833000 |
| 8 | -0.129336000 | -0.261446000 | -1.519238000 |

## $^3$I

| | | | |
|---|---|---|---|
| 25 | -0.197543000 | 0.065017000 | 0.175066000 |
| 7 | -0.052832000 | 0.052517000 | 2.352296000 |
| 7 | 1.936511000 | -0.013870000 | 0.248605000 |
| 7 | -0.543156000 | -1.890902000 | 0.558537000 |
| 7 | 0.242923000 | 2.035232000 | -0.071620000 |
| 6 | -0.489810000 | 1.365769000 | 2.904814000 |
| 1 | -1.456135000 | 1.619245000 | 2.468520000 |
| 1 | 0.234394000 | 2.137227000 | 2.646480000 |
| 1 | -0.592891000 | 1.324436000 | 3.991309000 |
| 6 | 1.377678000 | -0.290874000 | 2.713999000 |
| 1 | 1.436492000 | -1.383012000 | 2.675936000 |
| 6 | 1.810351000 | 0.185946000 | 4.121523000 |
| 1 | 1.806092000 | 1.281689000 | 4.148480000 |
| 1 | 1.096177000 | -0.156805000 | 4.870789000 |
| 6 | 3.220788000 | -0.303388000 | 4.475453000 |
| 1 | 3.231207000 | -1.400236000 | 4.535538000 |
| 1 | 3.490453000 | 0.071109000 | 5.469264000 |
| 6 | 4.229459000 | 0.167501000 | 3.426415000 |
| 1 | 4.323923000 | 1.261177000 | 3.465282000 |
| 1 | 5.224247000 | -0.244033000 | 3.630492000 |
| 6 | 3.790760000 | -0.267896000 | 2.021729000 |
| 1 | 3.776949000 | -1.363251000 | 1.985918000 |
| 1 | 4.517249000 | 0.069297000 | 1.282384000 |
| 6 | 2.379286000 | 0.270851000 | 1.677947000 |
| 1 | 2.379470000 | 1.361292000 | 1.767230000 |
| 6 | 2.415991000 | -1.337058000 | -0.245977000 |
| 1 | 1.945048000 | -1.542337000 | -1.207833000 |
| 1 | 2.144774000 | -2.117903000 | 0.462479000 |
| 1 | 3.499461000 | -1.333398000 | -0.377225000 |
| 6 | 2.357372000 | 1.073169000 | -0.757316000 |
| 1 | 2.030751000 | 0.648258000 | -1.713139000 |
| 6 | 1.480888000 | 2.292556000 | -0.549373000 |
| 6 | 1.833662000 | 3.583344000 | -0.935882000 |
| 1 | 2.821239000 | 3.775906000 | -1.333700000 |
| 6 | 0.901348000 | 4.613378000 | -0.814552000 |
| 1 | 1.166538000 | 5.622482000 | -1.112402000 |
| 6 | -0.369446000 | 4.329815000 | -0.318843000 |
| 1 | -1.126333000 | 5.098399000 | -0.214632000 |
| 6 | -0.669075000 | 3.020756000 | 0.033150000 |
| 1 | -1.648550000 | 2.731675000 | 0.389767000 |
| 6 | 3.847342000 | 1.354909000 | -0.878738000 |
| 6 | 4.563626000 | 0.727063000 | -1.908609000 |
| 1 | 4.047345000 | 0.063380000 | -2.596982000 |
| 6 | 5.932124000 | 0.953275000 | -2.069743000 |
| 1 | 6.468313000 | 0.456438000 | -2.872682000 |
| 6 | 6.601657000 | 1.822941000 | -1.207888000 |
| 1 | 7.665017000 | 2.004702000 | -1.333247000 |
| 6 | 5.895685000 | 2.469741000 | -0.189365000 |
| 1 | 6.406540000 | 3.156920000 | 0.478398000 |
| 6 | 4.529715000 | 2.240262000 | -0.026603000 |
| 1 | 4.000396000 | 2.761282000 | 0.765618000 |
| 6 | -1.067526000 | -1.017080000 | 2.762680000 |
| 1 | -2.024306000 | -0.546299000 | 2.511385000 |
| 6 | -0.956879000 | -2.193276000 | 1.810327000 |
| 6 | -1.375233000 | -3.485913000 | 2.118386000 |
| 1 | -1.720923000 | -3.715284000 | 3.117578000 |
| 6 | -1.352704000 | -4.469336000 | 1.130066000 |
| 1 | -1.673792000 | -5.479306000 | 1.363141000 |
| 6 | -0.928546000 | -4.137793000 | -0.155189000 |
| 1 | -0.906880000 | -4.867759000 | -0.955893000 |
| 6 | -0.545751000 | -2.828977000 | -0.408909000 |
| 1 | -0.249042000 | -2.495288000 | -1.394400000 |
| 6 | -1.127464000 | -1.382649000 | 4.239990000 |
| 6 | -0.269009000 | -2.325639000 | 4.831080000 |
| 1 | 0.478285000 | -2.840863000 | 4.234868000 |
| 6 | -0.369123000 | -2.623040000 | 6.190142000 |
| 1 | 0.302809000 | -3.354418000 | 6.629317000 |
| 6 | -1.331601000 | -1.988373000 | 6.980588000 |
| 1 | -1.408757000 | -2.223329000 | 8.038154000 |
| 6 | -2.200218000 | -1.061968000 | 6.402188000 |
| 1 | -2.960383000 | -0.573167000 | 7.004223000 |
| 6 | -2.100859000 | -0.767024000 | 5.040715000 |
| 1 | -2.792816000 | -0.056773000 | 4.595938000 |
| 8 | -4.038342000 | 1.222114000 | -0.763540000 |
| 16 | -2.978014000 | 0.218615000 | -0.957385000 |
| 8 | -1.972654000 | 0.443721000 | 0.321451000 |
| 8 | -3.391767000 | -1.191932000 | -0.919502000 |
| 8 | -2.107483000 | 0.567120000 | -2.159408000 |
| 8 | -0.186257000 | -0.198427000 | -1.478889000 |

## *S*-Sub

| | | | |
|---|---|---|---|
| 6 | 0.100985000 | 0.063842000 | 1.537241000 |
| 8 | 0.336959000 | 1.355326000 | 2.108133000 |
| 1 | 0.893970000 | -0.631492000 | 1.854371000 |
| 1 | 1.172871000 | 1.686920000 | 1.741190000 |
| 6 | -1.228051000 | -0.422615000 | 2.117367000 |
| 1 | -1.455444000 | -1.432785000 | 1.763194000 |
| 1 | -1.177779000 | -0.437671000 | 3.211418000 |
| 1 | -2.042053000 | 0.244445000 | 1.812924000 |
| 6 | 0.080821000 | 0.100338000 | 0.014942000 |
| 6 | 0.503212000 | -1.011606000 | -0.725227000 |
| 6 | -0.388038000 | 1.229008000 | -0.670142000 |
| 6 | 0.449326000 | -1.002278000 | -2.120506000 |
| 1 | 0.879773000 | -1.890302000 | -0.205322000 |
| 6 | -0.437979000 | 1.243449000 | -2.065594000 |
| 1 | -0.703211000 | 2.099035000 | -0.101573000 |
| 6 | -0.021806000 | 0.126980000 | -2.795434000 |
| 1 | 0.782535000 | -1.872532000 | -2.679973000 |
| 1 | -0.800661000 | 2.127817000 | -2.583263000 |
| 1 | -0.059064000 | 0.138566000 | -3.881440000 |

## *R*-Sub

| | | | |
|---|---|---|---|
| 6 | 0.167368000 | 0.012791000 | 1.572992000 |
| 8 | 1.079800000 | 0.972109000 | 2.117642000 |
| 1 | -0.843286000 | 0.196056000 | 1.970251000 |
| 1 | 0.805492000 | 1.847456000 | 1.798383000 |
| 6 | 0.639862000 | -1.355346000 | 2.067936000 |
| 1 | 0.676662000 | -1.367350000 | 3.162542000 |
| 1 | -0.042339000 | -2.142470000 | 1.731976000 |
| 1 | 1.641082000 | -1.573622000 | 1.680565000 |
| 6 | 0.100822000 | 0.078221000 | 0.053239000 |
| 6 | -1.088850000 | -0.233958000 | -0.617504000 |
| 6 | 1.231104000 | 0.420516000 | -0.700644000 |
| 6 | -1.147695000 | -0.215267000 | -2.012429000 |
| 1 | -1.976808000 | -0.490125000 | -0.042954000 |
| 6 | 1.174123000 | 0.444879000 | -2.095800000 |
| 1 | 2.152104000 | 0.678300000 | -0.185892000 |
| 6 | -0.014653000 | 0.124740000 | -2.756445000 |
| 1 | -2.079064000 | -0.457650000 | -2.517545000 |
| 1 | 2.058531000 | 0.715430000 | -2.666996000 |
| 1 | -0.059750000 | 0.145187000 | -3.842025000 |

## $^5$TS$_S$

| | | | |
|---|---|---|---|
| 25 | -0.029283000 | -0.309958000 | 0.133531000 |
| 7 | 2.098415000 | -0.448459000 | 0.695626000 |
| 7 | 0.539161000 | 1.598949000 | -0.660212000 |
| 7 | 0.720653000 | -1.440302000 | -1.395305000 |
| 7 | -0.547904000 | 0.902480000 | 1.685081000 |
| 6 | 2.255935000 | -0.386815000 | 2.173312000 |
| 1 | 1.576689000 | -1.112976000 | 2.620040000 |
| 1 | 2.002553000 | 0.609537000 | 2.533736000 |
| 1 | 3.278368000 | -0.624060000 | 2.477011000 |
| 6 | 2.822932000 | 0.671557000 | -0.022023000 |
| 1 | 3.030040000 | 0.290576000 | -1.027255000 |
| 6 | 4.158342000 | 1.094233000 | 0.639811000 |
| 1 | 3.947809000 | 1.527317000 | 1.624659000 |
| 1 | 4.790339000 | 0.220694000 | 0.802749000 |
| 6 | 4.908860000 | 2.137199000 | -0.198943000 |
| 1 | 5.206493000 | 1.698244000 | -1.161057000 |
| 1 | 5.832917000 | 2.416046000 | 0.320255000 |
| 6 | 4.030474000 | 3.366118000 | -0.441251000 |
| 1 | 3.856809000 | 3.892395000 | 0.507393000 |
| 1 | 4.530675000 | 4.075915000 | -1.109871000 |
| 6 | 2.689311000 | 2.953092000 | -1.061584000 |
| 1 | 2.885533000 | 2.500212000 | -2.040491000 |
| 1 | 2.070149000 | 3.833784000 | -1.233754000 |
| 6 | 1.938127000 | 1.933323000 | -0.171272000 |
| 1 | 1.801877000 | 2.364158000 | 0.825625000 |
| 6 | 0.438394000 | 1.577620000 | -2.145793000 |
| 1 | -0.540500000 | 1.182293000 | -2.415104000 |
| 1 | 1.213034000 | 0.934506000 | -2.560770000 |
| 1 | 0.545038000 | 2.580664000 | -2.563881000 |
| 6 | -0.546390000 | 2.530786000 | -0.106501000 |
| 1 | -1.443552000 | 2.176906000 | -0.625893000 |
| 6 | -0.783933000 | 2.190242000 | 1.352511000 |
| 6 | -1.331986000 | 3.072891000 | 2.281263000 |
| 1 | -1.534155000 | 4.097402000 | 1.997986000 |
| 6 | -1.620797000 | 2.620079000 | 3.568088000 |
| 1 | -2.045640000 | 3.299442000 | 4.299913000 |
| 6 | -1.363765000 | 1.290833000 | 3.896510000 |
| 1 | -1.576322000 | 0.895848000 | 4.883243000 |
| 6 | -0.837286000 | 0.454625000 | 2.920560000 |
| 1 | -0.648397000 | -0.593479000 | 3.106069000 |
| 6 | -0.399106000 | 4.015261000 | -0.412064000 |
| 6 | -1.094092000 | 4.545341000 | -1.509176000 |
| 1 | -1.725142000 | 3.896237000 | -2.110564000 |
| 6 | -0.994164000 | 5.899623000 | -1.835457000 |
| 1 | -1.539747000 | 6.288597000 | -2.690108000 |
| 6 | -0.204391000 | 6.748388000 | -1.058727000 |
| 1 | -0.128264000 | 7.803077000 | -1.306736000 |
| 6 | 0.479625000 | 6.237119000 | 0.047914000 |
| 1 | 1.088175000 | 6.891897000 | 0.664631000 |
| 6 | 0.382037000 | 4.883396000 | 0.369898000 |
| 1 | 0.914732000 | 4.510514000 | 1.239790000 |
| 6 | 2.491221000 | -1.843358000 | 0.219272000 |
| 1 | 1.923540000 | -2.492528000 | 0.894434000 |
| 6 | 1.880680000 | -2.090975000 | -1.147885000 |
| 6 | 2.378462000 | -3.021908000 | -2.058408000 |
| 1 | 3.297894000 | -3.548858000 | -1.840423000 |
| 6 | 1.680956000 | -3.270640000 | -3.239579000 |
| 1 | 2.063021000 | -3.992231000 | -3.954409000 |
| 6 | 0.490202000 | -2.590029000 | -3.481830000 |

| | | | |
|---|---|---|---|
| 1 | -0.090726000 | -2.756028000 | -4.381643000 |
| 6 | 0.036858000 | -1.690503000 | -2.526894000 |
| 1 | -0.896837000 | -1.162813000 | -2.639474000 |
| 6 | 3.958208000 | -2.234969000 | 0.352957000 |
| 6 | 4.931835000 | -1.897481000 | -0.602649000 |
| 1 | 4.657590000 | -1.335946000 | -1.491095000 |
| 6 | 6.261031000 | -2.284775000 | -0.431700000 |
| 1 | 6.998735000 | -2.014693000 | -1.181596000 |
| 6 | 6.640523000 | -3.020116000 | 0.695043000 |
| 1 | 7.675608000 | -3.322521000 | 0.825056000 |
| 6 | 5.681116000 | -3.373162000 | 1.644755000 |
| 1 | 5.962334000 | -3.954663000 | 2.517838000 |
| 6 | 4.350102000 | -2.987536000 | 1.469809000 |
| 1 | 3.607549000 | -3.281783000 | 2.207138000 |
| 8 | -1.673579000 | -3.263641000 | 2.543872000 |
| 16 | -1.767114000 | -2.535469000 | 1.259997000 |
| 8 | -0.289857000 | -1.843447000 | 1.123118000 |
| 8 | -1.904772000 | -3.460781000 | 0.077907000 |
| 8 | -2.730798000 | -1.419635000 | 1.208801000 |
| 8 | -1.600643000 | -0.212930000 | -0.511007000 |
| 1 | -2.793632000 | -0.645330000 | -1.076635000 |
| 1 | -2.768731000 | -2.840955000 | -1.187939000 |
| 6 | -3.650860000 | -1.166578000 | -1.740995000 |
| 8 | -3.094724000 | -2.384681000 | -2.027973000 |
| 6 | -3.755196000 | -0.310016000 | -2.998481000 |
| 1 | -4.077223000 | 0.707887000 | -2.770020000 |
| 1 | -2.793737000 | -0.267672000 | -3.516600000 |
| 1 | -4.491074000 | -0.758612000 | -3.676786000 |
| 6 | -4.819027000 | -1.145858000 | -0.819521000 |
| 6 | -5.359944000 | 0.086821000 | -0.390966000 |
| 6 | -5.410770000 | -2.345962000 | -0.371530000 |
| 6 | -6.479343000 | 0.115979000 | 0.431798000 |
| 1 | -4.893341000 | 1.018508000 | -0.695607000 |
| 6 | -6.535107000 | -2.310827000 | 0.443543000 |
| 1 | -5.002026000 | -3.295588000 | -0.698110000 |
| 6 | -7.072182000 | -1.082033000 | 0.851603000 |
| 1 | -6.891178000 | 1.068489000 | 0.751112000 |
| 1 | -7.001739000 | -3.239121000 | 0.759402000 |
| 1 | -7.948257000 | -1.058519000 | 1.492937000 |

**$^3TS_S$**

| | | | |
|---|---|---|---|
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| 7 | 2.196412000 | 0.134130000 | 0.693476000 |
| 7 | -0.066684000 | 1.417985000 | -0.587704000 |
| 7 | 1.168929000 | -1.379767000 | -1.300603000 |
| 7 | -0.764052000 | 0.409057000 | 1.791453000 |
| 6 | 2.377382000 | 0.269648000 | 2.164948000 |
| 1 | 2.035325000 | -0.649942000 | 2.640075000 |
| 1 | 1.786005000 | 1.106084000 | 2.535755000 |
| 1 | 3.425629000 | 0.433714000 | 2.425199000 |
| 6 | 2.424693000 | 1.430971000 | -0.051950000 |
| 1 | 2.723851000 | 1.140349000 | -1.063581000 |
| 6 | 3.528492000 | 2.330814000 | 0.556464000 |
| 1 | 3.209369000 | 2.669110000 | 1.549126000 |
| 1 | 4.445535000 | 1.757163000 | 0.692388000 |
| 6 | 3.802836000 | 3.564257000 | -0.313835000 |
| 1 | 4.211253000 | 3.252760000 | -1.284767000 |
| 1 | 4.570007000 | 4.179481000 | 0.169591000 |
| 6 | 2.518577000 | 4.367196000 | -0.526311000 |
| 1 | 2.190728000 | 4.805746000 | 0.425952000 |
| 1 | 2.690174000 | 5.200719000 | -1.216554000 |
| 6 | 1.410197000 | 3.470759000 | -1.095581000 |
| 1 | 1.731602000 | 3.102362000 | -2.076678000 |
| 1 | 0.503367000 | 4.054166000 | -1.251925000 |
| 6 | 1.128788000 | 2.264054000 | -0.164696000 |
| 1 | 0.878294000 | 2.632947000 | 0.834405000 |
| 6 | -0.195411000 | 1.323388000 | -2.071683000 |
| 1 | -0.968645000 | 0.595434000 | -2.313477000 |
| 1 | 0.749000000 | 0.996138000 | -2.503062000 |
| 1 | -0.471725000 | 2.287701000 | -2.501558000 |
| 6 | -1.395968000 | 1.921526000 | 0.004836000 |
| 1 | -2.138178000 | 1.294867000 | -0.499656000 |
| 6 | -1.461232000 | 1.519803000 | 1.466812000 |
| 6 | -2.277957000 | 2.140240000 | 2.409497000 |
| 1 | -2.847900000 | 3.018314000 | 2.135797000 |
| 6 | -2.358316000 | 1.612870000 | 3.698194000 |
| 1 | -2.991056000 | 2.088899000 | 4.440004000 |
| 6 | -1.629616000 | 0.468326000 | 4.015252000 |
| 1 | -1.670052000 | 0.021241000 | 5.001667000 |
| 6 | -0.848150000 | -0.117272000 | 3.028370000 |
| 1 | -0.292563000 | -1.030595000 | 3.195496000 |
| 6 | -1.770229000 | 3.367487000 | -0.288681000 |
| 6 | -2.603815000 | 3.633407000 | -1.385354000 |
| 1 | -2.971901000 | 2.813069000 | -1.995556000 |
| 6 | -2.975102000 | 4.941835000 | -1.701316000 |
| 1 | -3.620430000 | 5.126060000 | -2.554908000 |
| 6 | -2.525514000 | 6.003752000 | -0.915552000 |
| 1 | -2.815998000 | 7.022195000 | -1.156014000 |
| 6 | -1.708834000 | 5.750623000 | 0.190412000 |
| 1 | -1.363367000 | 6.570016000 | 0.813544000 |
| 6 | -1.335518000 | 4.443897000 | 0.503568000 |
| 1 | -0.707487000 | 4.270550000 | 1.372171000 |
| 6 | 3.058804000 | -1.019641000 | 0.188825000 |
| 1 | 2.822539000 | -1.822028000 | 0.896102000 |
| 6 | 2.505928000 | -1.513628000 | -1.136074000 |
| 6 | 3.264757000 | -2.200415000 | -2.081577000 |
| 1 | 4.330395000 | -2.315154000 | -1.934396000 |
| 6 | 2.640488000 | -2.745522000 | -3.202476000 |
| 1 | 3.226375000 | -3.278045000 | -3.944567000 |
| 6 | 1.261048000 | -2.615334000 | -3.344489000 |
| 1 | 0.730644000 | -3.042101000 | -4.187853000 |
| 6 | 0.552694000 | -1.938885000 | -2.361665000 |
| 1 | -0.526726000 | -1.865643000 | -2.389229000 |
| 6 | 4.569055000 | -0.820018000 | 0.227750000 |
| 6 | 5.281128000 | -0.161794000 | -0.789603000 |
| 1 | 4.762921000 | 0.224825000 | -1.662210000 |
| 6 | 6.664260000 | -0.004267000 | -0.702032000 |
| 1 | 7.196785000 | 0.506942000 | -1.498559000 |
| 6 | 7.361125000 | -0.505840000 | 0.400996000 |
| 1 | 8.438355000 | -0.383591000 | 0.466310000 |
| 6 | 6.667868000 | -1.174729000 | 1.410625000 |
| 1 | 7.200986000 | -1.580001000 | 2.265532000 |
| 6 | 5.283286000 | -1.334733000 | 1.319744000 |
| 1 | 4.755138000 | -1.871924000 | 2.103131000 |
| 8 | -0.258867000 | -3.975687000 | 2.500353000 |
| 16 | -0.207368000 | -3.470300000 | 1.116275000 |
| 8 | 0.496005000 | -1.985071000 | 1.288432000 |
| 8 | 0.666126000 | -4.212827000 | 0.189247000 |
| 8 | -1.570591000 | -3.167376000 | 0.548586000 |
| 8 | -1.337776000 | -1.135224000 | -0.319536000 |
| 6 | -3.410582000 | -1.470124000 | -1.817528000 |
| 8 | -2.808611000 | -2.724451000 | -2.030388000 |
| 1 | -2.545334000 | -0.852726000 | -1.241741000 |
| 1 | -2.411395000 | -3.011450000 | -1.178111000 |
| 6 | -3.723807000 | -0.840399000 | -3.169473000 |
| 1 | -4.142479000 | 0.162641000 | -3.050543000 |
| 1 | -2.820006000 | -0.774511000 | -3.783497000 |
| 1 | -4.457972000 | -1.456255000 | -3.703107000 |
| 6 | -4.585001000 | -1.508892000 | -0.860235000 |
| 6 | -5.168300000 | -0.313740000 | -0.403667000 |
| 6 | -5.111558000 | -2.729456000 | -0.410872000 |
| 6 | -6.252535000 | -0.339371000 | 0.471773000 |
| 1 | -4.773726000 | 0.643990000 | -0.734373000 |
| 6 | -6.198419000 | -2.755391000 | 0.465491000 |
| 1 | -4.675345000 | -3.657288000 | -0.765463000 |
| 6 | -6.771690000 | -1.562287000 | 0.911414000 |
| 1 | -6.692129000 | 0.593735000 | 0.813305000 |
| 1 | -6.598945000 | -3.709624000 | 0.796955000 |
| 1 | -7.615745000 | -1.582585000 | 1.595092000 |

**$^5TS_R$**

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| 7 | 0.330839000 | 1.345687000 | -0.895765000 |
| 7 | 0.401896000 | -1.784966000 | -1.049744000 |
| 7 | -0.283270000 | 1.108130000 | 1.709063000 |
| 6 | 2.633687000 | -0.094925000 | 1.838140000 |
| 1 | 2.081628000 | -0.717947000 | 2.542236000 |
| 1 | 2.428052000 | 0.953991000 | 2.051276000 |
| 1 | 3.703521000 | -0.279023000 | 1.963092000 |
| 6 | 2.718771000 | 0.520189000 | -0.585404000 |
| 1 | 2.726142000 | -0.047230000 | -1.521831000 |
| 6 | 4.151377000 | 1.036459000 | -0.303893000 |
| 1 | 4.138502000 | 1.657394000 | 0.599707000 |
| 1 | 4.821200000 | 0.198904000 | -0.106840000 |
| 6 | 4.690886000 | 1.879045000 | -1.467120000 |
| 1 | 4.792257000 | 1.253241000 | -2.364373000 |
| 1 | 5.695867000 | 2.236941000 | -1.215923000 |
| 6 | 3.754749000 | 3.053407000 | -1.759747000 |
| 1 | 3.769826000 | 3.759396000 | -0.918173000 |
| 1 | 4.090845000 | 3.607781000 | -2.643396000 |
| 6 | 2.322292000 | 2.555746000 | -1.996244000 |
| 1 | 2.319109000 | 1.916915000 | -2.887001000 |
| 1 | 1.664087000 | 3.399303000 | -2.205027000 |
| 6 | 1.794322000 | 1.743804000 | -0.788182000 |
| 1 | 1.858586000 | 2.362551000 | 0.112445000 |
| 6 | -0.080185000 | 1.042916000 | -2.295571000 |
| 1 | -1.088453000 | 0.629660000 | -2.274248000 |
| 1 | 0.599091000 | 0.309274000 | -2.727917000 |
| 1 | -0.073658000 | 1.943478000 | -2.913157000 |
| 6 | -0.623626000 | 2.394056000 | -0.314823000 |
| 1 | -1.605214000 | 1.985152000 | -0.575356000 |
| 6 | -0.563099000 | 2.329002000 | 1.200781000 |
| 6 | -0.908375000 | 3.382767000 | 2.044764000 |
| 1 | -1.147623000 | 4.352341000 | 1.628403000 |
| 6 | -0.952961000 | 3.170493000 | 3.423096000 |
| 1 | -1.219173000 | 3.985191000 | 4.088616000 |
| 6 | -0.665960000 | 1.904382000 | 3.928232000 |
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| 1 | -2.158668000 | 5.649740000 | -3.284435000 |
| 6 | -0.518920000 | 6.357545000 | -2.073267000 |
| 1 | -0.503836000 | 7.346782000 | -2.521412000 |
| 6 | 0.382722000 | 6.035374000 | -1.054888000 |
| 1 | 1.100119000 | 6.772697000 | -0.706962000 |
| 6 | 0.364670000 | 4.766504000 | -0.475927000 |
| 1 | 1.069633000 | 4.542461000 | 0.319234000 |
| 6 | 2.495952000 | -1.896226000 | 0.176096000 |
| 1 | 2.107561000 | -2.401780000 | 1.066611000 |
| 6 | 1.606407000 | -2.390637000 | -0.951741000 |
| 6 | 1.909312000 | -3.485446000 | -1.760278000 |
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| 6 | 0.964324000 | -3.944226000 | -2.677117000 |
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| 1 | 4.205938000 | -1.783220000 | -2.047221000 |
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| 1 | 6.583275000 | -2.394823000 | -2.137489000 |
| 6 | 6.690468000 | -2.979708000 | -0.062254000 |
| 1 | 7.740780000 | -3.252667000 | -0.107960000 |
| 6 | 5.979557000 | -3.120426000 | 1.130320000 |
| 1 | 6.470708000 | -3.506514000 | 2.018690000 |
| 6 | 4.627671000 | -2.773302000 | 1.182755000 |
| 1 | 4.078654000 | -2.901297000 | 2.112076000 |
| 8 | -1.544826000 | -2.530689000 | 3.376132000 |
| 16 | -1.205910000 | -2.726318000 | 1.947956000 |
| 8 | -0.010839000 | -1.648086000 | 1.665191000 |
| 8 | -0.611641000 | -4.039308000 | 1.615249000 |
| 8 | -2.313983000 | -2.331015000 | 1.014937000 |
| 8 | -1.682884000 | -0.419330000 | -0.005888000 |
| 1 | -3.009847000 | -0.079985000 | 0.283963000 |
| 1 | -3.518529000 | -1.485973000 | 1.733729000 |
| 6 | -4.183403000 | -0.031645000 | 0.680162000 |
| 8 | -4.068189000 | -0.654904000 | 1.891125000 |
| 6 | -4.540929000 | 1.436374000 | 0.839067000 |
| 1 | -3.856740000 | 1.917063000 | 1.543080000 |
| 1 | -4.509540000 | 1.969293000 | -0.113675000 |
| 1 | -5.560227000 | 1.515236000 | 1.237787000 |
| 6 | -4.836758000 | -0.801078000 | -0.419075000 |
| 6 | -4.842011000 | -0.291270000 | -1.736039000 |
| 6 | -5.432098000 | -2.054738000 | -0.168420000 |
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**$^3TS_R$**

| | | | |
|---|---|---|---|
| 25 | -0.021413000 | -0.256242000 | 0.536613000 |
| 7 | 2.164031000 | -0.482713000 | 0.541090000 |
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| 7 | 0.228470000 | -1.652308000 | -0.925446000 |
| 7 | -0.111180000 | 1.192795000 | 1.955971000 |
| 6 | 2.688831000 | -0.229659000 | 1.912598000 |
| 1 | 2.122932000 | -0.837711000 | 2.618421000 |
| 1 | 2.567439000 | 0.822319000 | 2.167093000 |
| 1 | 3.745808000 | -0.494480000 | 1.987565000 |
| 6 | 2.733517000 | 0.467527000 | -0.490101000 |
| 1 | 2.662449000 | -0.058134000 | -1.447312000 |
| 6 | 4.210338000 | 0.863694000 | -0.246109000 |
| 1 | 4.279693000 | 1.443348000 | 0.681449000 |
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| 6 | 4.765246000 | 1.713757000 | -1.396119000 |
| 1 | 4.786158000 | 1.121070000 | -2.320796000 |
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| 1 | 4.011231000 | 3.633570000 | -0.735975000 |
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| 1 | 1.835022000 | 3.485430000 | -1.940187000 |
| 6 | 1.897432000 | 1.763848000 | -0.599353000 |
| 1 | 2.040571000 | 2.336232000 | 0.321879000 |
| 6 | -0.074876000 | 1.254013000 | -2.058290000 |

| | | | |
|---|---|---|---|
| 1 | -1.112743000 | 0.922764000 | -2.025143000 |
| 1 | 0.530815000 | 0.487628000 | -2.538890000 |
| 1 | -0.017468000 | 2.175600000 | -2.640012000 |
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| 6 | -0.357236000 | 2.441003000 | 1.497341000 |
| 6 | -0.627702000 | 3.477135000 | 2.388062000 |
| 1 | -0.841204000 | 4.468690000 | 2.011324000 |
| 6 | -0.629021000 | 3.220398000 | 3.758758000 |
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| 6 | -0.368133000 | 1.929096000 | 4.212745000 |
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| 6 | 4.472131000 | -2.310569000 | -1.242063000 |
| 1 | 3.974064000 | -1.880460000 | -2.105993000 |
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