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Catalytic Hydrogenation of α,β -Epoxy Ketones to Form β -Hydroxy Ketones Mediated by an NADH Coenzyme Model

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General Experimental

^1H NMR and ^{13}C NMR were recorded on a Bruker AC-300 FT (^1H : 300 MHz, ^{13}C : 75.46 MHz) using TMS as internal reference. The chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz respectively. IR spectra were recorded on a Perkin-Elmer, 2000FTIR. High-resolution mass spectra (HRMS) were determined on a Micromass GCT-MS mass spectrometer. All reagents were used as supplied. BNA^+Br^- was prepared according to the literature.¹ α,β -Epoxy ketones were prepared from corresponding unsaturated ketones using alkaline hydrogen peroxide.²

The Hydrogenation of α,β -Epoxy Ketones to β -Hydroxy Ketones under Irradiation

A solution of α,β -epoxy ketones (1mmol), Na_2CO_3 (5mmol), $\text{Na}_2\text{S}_2\text{O}_4$ (3mmol) and BNA^+Br^- (0.05mmol) in 10ml of $\text{AcOEt}/\text{H}_2\text{O}$ (1:1) was irradiated with a 450w high pressure mercury lamp in a Pyrex flask ($\lambda > 320$ nm) under an argon atmosphere at room temperature for 2-6 h. The reaction mixture was extracted with chloroform and the combined extract dried with Na_2SO_4 . After evaporation of the solvent, the residue was subjected to chromatography on a silica gel column with chloroform as eluent and identified by IR, ^1H 、 ^{13}C NMR and HRMS as corresponding β -hydroxy ketones.

The Hydrogenation of α,β -Epoxy Ketones to β -Hydroxy Ketones without Irradiation

The similar procedure was adopted without irradiation. The time for the reactions was 24-30 h.

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- (1) Hasegawa, E.; Ishiyama, K.; Horaguchi, T.; Shimizu, T. *J. Org. Chem.* **1991**, *56*, 1631.
(2) Bunting, J. W.; Sindhuatmadja, S. *J. Org. Chem.* **1981**, *46*, 4211.

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3-hydroxy-1,3-diphenylpropan-1-one (2a) ^1H NMR (CDCl_3 , 300MHz) δ = 7.92 (d, J =7.4Hz, 2H), 7.55-7.27 (m, 8H), 5.34-5.30 (dd, J =4.5, 7.6Hz, 1H), 3.67 (br s, 1H), 3.42-3.29 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.3, 143.1, 136.7, 133.8, 129.1, 128.8, 128.7, 128.3, 127.8, 125.9, 70.2, 47.5. IR (film) ν = 3473, 2923, 1681, 1597, 1579, 1494, 1449, 1212, 750, 700 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{14}\text{O}_2$: 226.0994. Found: 226.0997.

3-hydroxy-1-phenyl-3-p-tolylpropan-1-one (2b) ^1H NMR (CDCl_3 , 300MHz) δ = 7.96-7.93 (m, 2H), 7.58-7.17 (m, 7H), 5.32 (t, J =6.0Hz, 1H), 3.58 (br s, 1H), 3.37-3.35 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.3, 140.2, 137.5, 136.8, 133.7, 129.4, 128.8, 128.3, 125.8, 70.1, 47.5, 21.2. IR (film) ν = 3457, 2923, 1680, 1597, 1579, 1514, 1448, 1212, 818, 758, 690 cm^{-1} . HRMS calc. $\text{C}_{16}\text{H}_{16}\text{O}_2$: 240.1150. Found: 240.1145.

3-hydroxy-3-(4-methoxy-phenyl)-1-phenylpropan-1-one (2c) ^1H NMR (CDCl_3 , 300MHz) δ = 7.95 (d, J = 7.4Hz, 2H), 7.60-7.34 (m, 5H), 6.92-6.88 (m, 2H), 5.31-5.27 (dd, J =4.7, 7.4Hz, 1H), 3.81 (s, 3H), 3.51 (br s, 1H), 3.37-3.34 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.2, 159.4, 136.8, 133.6, 132.6, 128.7, 128.6, 128.5, 128.4, 128.3, 128.1, 114.5, 114.1, 69.8, 55.5, 47.7. IR (film) ν = 3483, 2934, 1681, 1597, 1581, 1513, 1449, 1213, 832, 758, 690 cm^{-1} . HRMS calc. $\text{C}_{16}\text{H}_{16}\text{O}_3$: 256.1099. Found: 256.1103.

3-(p-chlorophenyl)-3-hydroxy-1-phenylpropan-1-one (2d) ^1H NMR (CDCl_3 , 300MHz) δ = 7.93-7.92 (m, 2H), 7.59-7.35 (m, 7H), 5.34-5.30 (t, J =6.0Hz, 1H), 3.65 (br s, 1H), 3.50-3.17 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.0, 141.7, 136.6, 133.8, 133.4, 133.0, 129.7, 129.3, 128.8, 128.8, 128.6, 128.2, 127.3, 69.5, 47.35. IR (film) ν = 3466, 2947, 1667, 1593, 1492, 1446, 1213, 830, 753, 686 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{13}^{35}\text{ClO}_2$: 260.0604. Found: 260.0607.

3-hydroxy-3-(2-methoxy-phenyl)-1-phenylpropan-1-one (2e) ^1H NMR (CDCl_3 , 300MHz) δ = 7.92-6.82 (m, 9H), 5.61-5.58 (dd, J =2.7, 9.2Hz, 1H), 3.78 (s, 3H), 3.51 (br s, 1H), 3.37-3.34 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.3, 155.7, 136.8, 133.3, 131.2, 128.5, 128.3, 128.1, 126.4, 120.8, 110.2, 65.5, 55.2, 45.8. IR (film) ν = 3509, 3010, 1679, 1598, 1518, 1492, 1449, 1243, 755, 690 cm^{-1} . HRMS calc. $\text{C}_{16}\text{H}_{16}\text{O}_3$: 256.1099. Found: 256.1095.

3-(o-chlorophenyl)-3-hydroxy-1-phenylpropan-1-one (2f) ^1H NMR (CDCl_3 , 300MHz) δ = 7.93-7.19 (m, 9H), 5.34-5.30 (d, J =9.3Hz, 1H), 3.83 (br s, 1H), 3.58-3.10 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.4, 140.5, 136.6, 133.8, 131.3, 129.5, 128.9, 128.7, 128.3, 127.4,

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70.0, 45.5. IR (film) ν = 3527, 2908, 1669, 1597, 1579, 1473, 1445, 1208, 753, 689 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{13}^{35}\text{ClO}_2$: 260.0604. Found: 260.0618.

3-hydroxy-3-phenyl-1-p-tolyl-propan-1-one (2g) ^1H NMR (CDCl_3 , 300MHz) δ = 7.85-7.82 (d, J =8.2, 2H), 7.44-7.24 (m, 7H), 5.34-5.30 (t, J =6.0Hz, 1H), 5.61 (br s, 1H), 3.34-3.32 (d, J =6.17, 2H), 2.40 (s, 3H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 199.9, 144.7, 143.2, 134.3, 129.7, 129.5, 129.1, 128.9, 128.4, 127.7, 125.9, 70.2, 47.3, 21.8. IR (film) ν = 3487, 2921, 1674, 1572, 1494, 1453, 1205, 812, 756, 700 cm^{-1} . HRMS calc. $\text{C}_{16}\text{H}_{16}\text{O}_2$: 240.1150. Found: 240.1145.

3-hydroxy-1-(4-methoxy-phenyl)-3-phenyl-propan-1-one (2h) ^1H NMR (CDCl_3 , 300MHz) δ = 7.93-7.90 (m, 2H), 7.44-7.28 (m, 5H), 6.93-6.90 (m, 2H), 5.33-5.29 (t, J =6.0Hz, 1H), 3.85 (s, 3H), 3.80 (br s, 1H), 3.31-3.29 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 198.8, 164.0, 143.3, 130.6, 129.8, 128.6, 127.7, 125.9, 114.0, 70.3, 55.6, 47.0. IR (film) ν = 3474, 2934, 1668, 1600, 1574, 1510, 1454, 1261, 1217, 832, 762, 701 cm^{-1} . HRMS calc. $\text{C}_{16}\text{H}_{16}\text{O}_3$: 256.1099. Found: 256.1103..

1-(p-fluorophenyl)-3-hydroxy-3-phenylpropan-1-one (2i) ^1H NMR (CDCl_3 , 300MHz) δ = 7.94-7.89 (m, 2H), 7.42-7.31 (m, 5H), 7.10-7.05 (m, 2H), 5.30 (d, J =8.6 Hz, 1H), 3.81 (br s, 1H), 3.40-3.19 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 197.8, 167.3, 143.2, 133.0, 133.0, 130.8, 130.6, 128.3, 127.4, 125.6, 115.6, 115.3, 69.7, 47.2. IR (film) ν = 3462, 2888, 2916, 1679, 1597, 1507, 1453, 1231, 835, 764, 700 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{13}\text{FO}_2$: 244.0900. Found: 244.0908.

1-(p-bromophenyl)-3-hydroxy-3-phenylpropan-1-one (2j) ^1H NMR (CDCl_3 , 300MHz) δ = 7.78-7.75 (m, 2H), 7.57-7.55 (m, 2H), 7.41-7.27 (m, 5H), 5.32-5.28 (dd, J =3.2, 8.7Hz, 1H), 3.53 (br s, 1H), 3.38-3.20 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 198.9, 143.0, 135.4, 132.1, 129.7, 128.9, 128.6, 127.8, 125.8, 70.0, 47.5. IR (film) ν = 3464, 2949, 1668, 1583, 1566, 1485, 1454, 1281, 1208, 821, 758, 719, 699 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{13}\text{BrO}_2$: 304.0099. Found: 304.0108.

1-(p-chlorophenyl)-3-hydroxy-3-phenylpropan-1-one (2k) ^1H NMR (CDCl_3 , 300MHz) δ = 7.89-7.86 (m, 2H), 7.44-7.25 (m, 7H), 5.35-5.31 (dd, J =3.5, 8.4Hz, 1H), 3.51 (br s, 1H), 3.41-3.25 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 198.6, 143.0, 140.0, 135.0, 129.6, 129.4, 129.0, 128.6, 127.9, 127.7, 125.8, 69.9, 47.4. IR (film) ν = 3465, 2949, 1668, 1587, 1569, 1490, 1454, 1282, 1208, 825, 760, 700 cm^{-1} . HRMS calc. $\text{C}_{15}\text{H}_{13}^{35}\text{ClO}_2$: 260.0604. Found: 260.0600.

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1-(2-furyl)-3-hydroxy-3-phenylpropan-1-one (2l) ^1H NMR (CDCl_3 , 300MHz) δ = 7.59-7.58 (m, 1H), 7.43-7.36 (m, 5H), 7.22-7.21 (m, 1H), 6.55-6.53 (m, 1H), 5.33-5.29 (dd, J =4.5, 7.8Hz, 1H), 3.31-3.17 (m, 2H), 2.96 (br s, 1H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 188.2, 152.3, 146.9, 143.0, 128.8, 128.3, 127.4, 125.6, 118.1, 112.5, 112.3, 69.8, 47.0. IR (film) ν = 3453, 2920, 1666, 1601, 1567, 1495, 1467, 1163, 764, 701 cm^{-1} . HRMS calc. $\text{C}_{13}\text{H}_{12}\text{O}_3$: 216.0786. Found: 216.0778.

1-(2-thienyl)-3-hydroxy-3-phenylpropan-1-one (2m) ^1H NMR (CDCl_3 , 300MHz) δ = 7.71-7.67 (m, 2H), 7.45-7.30 (m, 5H), 7.14-7.11 (m, 1H), 5.35-5.31 (dd, J =5.0, 7.2Hz, 1H), 3.33-3.26 (m, 2H), 2.82 (br s, 1H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 192.8, 144.0, 143.0, 134.6, 132.8, 129.1, 128.7, 128.6, 128.4, 127.9, 125.9, 70.4, 48.1. IR (film) ν = 3462, 2904, 1654, 1603, 1517, 1493, 1452, 1414, 1219, 857, 728, 700 cm^{-1} . HRMS calc. $\text{C}_{13}\text{H}_{12}\text{O}_2\text{S}$: 232.0558. Found: 232.0554.

3-hydroxy-1-naphthalen-2-yl-3-phenylpropan-1-one (2n) ^1H NMR (CDCl_3 , 300MHz) δ = 8.46 (s, 1H), 8.02-7.87 (m, 4H), 7.50-7.38 (m, 7H), 5.44-5.39 (t, J =6.0Hz, 1H), 3.65 (br s, 1H), 3.58-3.51 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 200.0, 143.2, 135.8, 134.0, 132.5, 130.2, 129.7, 128.8, 128.6, 127.8, 127.7, 127.0, 125.9, 123.6, 70.2, 47.6. IR (film) ν = 3522, 2886, 1672, 1592, 1493, 1467, 1453, 1414, 1197, 822, 753, 702 cm^{-1} . HRMS calc. $\text{C}_{19}\text{H}_{14}\text{O}$: 258.1045 ($\text{M}^+ - \text{H}_2\text{O}$). Found: 258.1053 ($\text{M}^+ - \text{H}_2\text{O}$).

1-biphenyl-4-yl-3-hydroxy-3-phenylpropan-1-one (2o) ^1H NMR (CDCl_3 , 300MHz) δ = 8.02 (d, J =8.5 Hz, 2H), 7.69-7.60 (m, 4H), 7.46-7.38 (m, 8H), 5.38-5.35 (t, J =6.0Hz, 1H), 3.62 (br s, 1H), 3.48-3.35 (m, 2H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 199.8, 146.4, 143.2, 139.8, 135.4, 129.1, 128.9, 128.7, 128.5, 127.8, 127.4, 127.3, 125.9, 70.2, 47.5. IR (film) ν = 3530, 2924, 1665, 1603, 1560, 1495, 1450, 1199, 836, 767, 701. HRMS calc. $\text{C}_{21}\text{H}_{16}\text{O}$: 284.1201 ($\text{M}^+ - \text{H}_2\text{O}$). Found: 284.1209 ($\text{M}^+ - \text{H}_2\text{O}$).

4-hydroxy-4-phenylbutan-2-one (2p) ^1H NMR (CDCl_3 , 300MHz) δ = 7.34-7.24 (m, 5H), 5.14-5.10 (m, 1H), 3.32 (br s, 1H), 2.91-2.74 (m, 2H), 2.16 (s, 3H). ^{13}C NMR (CDCl_3 , 75MHz) δ = 209.2, 142.9, 128.6, 127.7, 125.7, 69.9, 52.0, 30.8. IR (film) ν = 3424, 3030, 1710, 1603, 1494, 1453, 1306, 1062, 756, 701 cm^{-1} . HRMS calc. $\text{C}_{10}\text{H}_{12}\text{O}_2$: 164.0837. Found: 164.0844.

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Current Data Parameters
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EXPNO 1
PROCNO 1

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Current Data Parameters
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 EXPNO 4
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 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 49
 DS 4
 SWH 22675.735 Hz
 FIDRES 0.346004 Hz
 AQ 1.4451188 sec
 RG 1625.5
 DM 22.050 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 3.00 usec
 PL1 -1.00 dB
 SF01 75.4768051 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 16.00 dB
 SF02 300.1315007 MHz

F2 - Processing parameters
 S1 131072
 SF 75.4677528 MHz
 KW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 211.788 ppm
 F1 15983.14 Hz
 F2P -2.833 ppm
 F2 -213.82 Hz
 PPKCM 9.75549 ppm/cm
 HZCM 736.22522 Hz/cm

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Current Data Parameters
NAME          an10207
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20051020
Time          14 30
INSTRUM       av300
PROBHD        5 mm BBO BH-1H
PULPRG        zgpg
TD            65536
SOLVENT       CDCl3
NS            57
DS            4
SWH           25675.736 Hz
FIDRES        0.346004 Hz
AQ            1.4451188 sec
RG            1625.5
DM            22.050 usec
DE            6.00 usec
TE            300.0 K
D1            2.00000000 sec
d11           0.0300000 sec
NDCST         0.0000000 sec
NUCRRK        0.0150000 sec

***** CHANNEL f1 13C *****
MUC1          13C
P1            -3.00 usec
PL1           -1.00 dB
SF01          75.4768951 MHz

***** CHANNEL f2 *****
CPDPRG2       waltz16
MUC2          1H
PCPD2         60.00 usec
PL2           -3.00 dB
PL12          15.00 dB
SF02          300.1315007 MHz

F2 - Processing parameters
SI            131072
SF            75.4677488 MHz
EM            EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

1D NMR plot parameters
CX            22.00 cm
CY            0.00 cm
F1P           212.340 ppm
F1            16024.79 Hz
F2P           -1.762 ppm
F2            -134.50 Hz
NUC1PM        9.73281 ppb/cm
NUC2PM        734.51300 ppb/cm
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