Stereoselective syntheses of racemic quercitols and bromoquercitols starting from cyclohexa-1,4-diene: *gala-*, *epi-*, *muco-* and *neo-*quercitol†

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Experimental Section

**General:** Melting points are uncorrected. Infrared spectra were obtained from solution in 0.1 mm cells or KBr pellets on a regular instrument. The $^1$H and $^{13}$C NMR spectra were recorded on 300 (75) MHz spectrometers. Apparent splitting is given in all cases. Column chromatography was performed on silica gel (60-mesh, Merck), TLC was carried out on Merck 0.2 mm silica gel 60 F$_{254}$ analytical aluminum plates.
$^1$H-NMR in CDCl$_3$

\[ \text{Diagram of } \text{H-NMR spectrum} \]

$^{13}$C-NMR in CDCl$_3$

\[ \text{Diagram of } \text{C-NMR spectrum} \]
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
DEPT

CH₃ and CH up
CH₂ down

CH only

all protonated carbons

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$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
$^1$H-NMR in CDCl$_3$

![NMR spectrum for 18]

$^{13}$C-NMR in CDCl$_3$

![NMR spectrum for 18]
$^{1}$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
DEPT

CH₃ and CH up
CH₂ down

CH only

all protonated carbons

APT

170.16
169.96
70.94
69.06
67.36
31.79
21.01
20.85

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COSY
HETCOR
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
DEPT

CH$_3$ and CH up
CH$_2$ down

CH only

all protonated carbons
HETCOR
**DEPT**

CH$_3$ and CH up
CH$_2$ down

CH only

all protonated carbons

**APT**

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HETCOR

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**1H-NMR in CDCl₃**

![H-NMR spectrum](image)

**13C-NMR in CDCl₃**

![C-NMR spectrum](image)
DEPT

CH$_3$ and CH up
CH$_2$ down

CH only

all protonated carbons
COSY

COSY (expanded)
HETCOR
**$^1$H-NMR in CDCl$_3$**

![H-NMR spectrum](image)

**$^{13}$C-NMR in CDCl$_3$**

![C-NMR spectrum](image)
DEPT

\[
\begin{array}{c}
\text{AcO} \\
\text{OAc} \\
\text{OAc} \\
\text{AcO} \\
\end{array}
\]

CH₂ and CH up
CH₂ down

CH only

all protonated carbons

---

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$^1$H-NMR in D$_2$O

$^{13}$C-NMR in D$_2$O
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
\(^1\text{H-NMR in CDCl}_3\)

\[ \text{O}_x \text{OAc} \]
\[ \text{MeO} \text{OAc} \]

28

\[ 5.50 \]
\[ 4.86 \]
\[ 3.7 \]
\[ 3.6 \]
\[ 3.5 \]
\[ 3.4 \]
\[ 3.3 \]
\[ 3.2 \]

\[ 1.09 \]
\[ 1.02 \]
\[ 0.99 \]
\[ 2.20 \]
\[ 6.78 \]
\[ 2.89 \]

\[^{13}\text{C-NMR in CDCl}_3\]

\[ \text{O}_x \text{OAc} \]
\[ \text{MeO} \text{OAc} \]

28

\[ 170.5 \]
\[ 169.5 \]

\[ 55.0 \]
\[ 54.5 \]
\[ 54.0 \]
\[ 53.5 \]

\[ 27.89 \]

\[ 21.5 \]
\[ 21.0 \]
\[ 20.5 \]
DEPT

CH\textsubscript{3} and CH up
CH\textsubscript{2} down

CH only

all protonated carbons
HETCOR

![HETCOR diagram](image_url)

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$^1\text{H-NMR in CDCl}_3$

$^{13}\text{C-NMR in CDCl}_3$
DEPT

CH<sub>2</sub> and CH up
CH<sub>2</sub> down

CH only

all protonated carbons

APT

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HETCOR

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**1H-NMR in CDCl₃**

![1H-NMR spectrum](image)

**13C-NMR in CDCl₃**

![13C-NMR spectrum](image)
DEPT

CH₂ and CH up
CH₂ down

CH only

all protonated carbons

APT

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COSY

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$^{13}$C-NMR in CDCl$_3$
COSY in CDCl₃
HETCOR in CDCl$_3$
$^1$H-NMR in D$_2$O

$^{13}$C-NMR in D$_2$O
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
DEPT

CH₃ and CH up
CH₂ down

CH only

all protonated carbons
HETCOR
$^1$H-NMR in D$_2$O

$^{13}$C-NMR in D$_2$O
$^1$H-NMR in CDCl$_3$

$^{13}$C-NMR in CDCl$_3$
$^1$H-NMR in CDCl₃

$^{13}$C-NMR in CDCl₃
COSY

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HMBC (expanded 1)
HMBC (expanded 2)

[Chemical structure image]

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HMBC (expanded 3)

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NOESY

AcO

Br

Br

OAc

OAc

35
\( ^1\text{H-NMR in D}_2\text{O} \)

\( ^{13}\text{C-NMR in D}_2\text{O} \)
**$^1$H-NMR in CDCl$_3$**

![H-NMR spectrum](image)

**$^{13}$C-NMR in CDCl$_3$**

![C-NMR spectrum](image)
DEPT

CH\textsubscript{3} and CH up
CH\textsubscript{2} down

CH only

all protonated carbons
COSY

[Chemical structure image]

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HETCOR
\(^1\text{H-NMR in D}_2\text{O}\)

\[\text{HO} \quad \text{HO} \quad \text{OH} \quad \text{Br}^+ \quad 40\]

\(^{13}\text{C-NMR in D}_2\text{O}\)

\[\text{HO} \quad \text{OH} \quad \text{OH} \quad \text{Br}^+ \quad 40\]
$^1$H-NMR in CDCl$_3$
$^1$H-NMR in benzene-d$_6$

$^{13}$C-NMR in benzene-d$_6$
DEPT in benzene-d6

CH₃ and CH up
CH₂ down

CH only

All protonated carbons

APT in benzene-d6

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COSY in benzene-d6
HETCOR
$^1$H-NMR in D$_2$O

$^{13}$C-NMR in D$_2$O
COSY in D$_2$O
COSY

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[Chemical structure diagram]

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$^{1}H$-NMR in D$_2$O

$^{13}$C-NMR in D$_2$O
COSY in D$_2$O

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$^1$H-NMR in CD$_3$OD

$^{13}$C-NMR in CD$_3$OD
$^{1}H$-NMR in CD$_3$OD

$^{13}$C-NMR in CD$_3$OD
$^1$H-NMR in CD$_3$OD

$^{13}$C-NMR in CD$_3$OD

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**Epoxide 20**

Job type: Geometry optimization.  
Method: RB3LYP  
Basis set: 6-31G**

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Epoxide 21

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G**

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H        -5.629757   0.322849  -0.859789
H        -4.349639   1.557236  -0.889951
C        -0.517520  -1.786098   0.171148
H        -0.177915  -2.781834  -0.108967
C        -1.944102  -1.561137   0.465051
H        -2.640252  -2.396142   0.387392
O         -0.984198  -1.661866   1.526608
C         2.548074  -1.570874  -0.412371
C         1.508725   2.463961   0.051985
O         2.174083   3.207764  -0.624989
O         2.232759  -2.268441  -1.349422
C         3.918513  -1.493202   0.210880
H         4.312333  -0.476786   0.118917
H         4.583014  -2.195048  -0.291254
H         3.860463  -1.729424   1.277308
C         1.687360   2.320344   1.550415
H         0.770219   2.579673   2.089267
H         2.480734   3.003568   1.850592
H         1.960696   1.297444   1.820326
Epoxide 28

Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G**
Job type: Geometry optimization.
Method: RB3LYP
Basis set: 6-31G**

C        0.520473  -1.136445  0.600540
C       -1.426439  0.538988  0.370534
C       -2.469140 -0.589530  0.292326
C       -0.241370  0.052951  1.214610
H       -1.139790  0.790193  -0.650047
H       -2.844134 -0.817179  1.307176
H       -0.667693  0.333822  2.148759
H       -1.860500  1.424814  0.843926
O        0.680980  1.038554  1.702611
O       -3.563268 -0.272078  -0.552260
C       -4.508466  0.617902  0.013314
H       -4.900128  0.238831  0.969968
H       -5.332354  0.696218 -0.699023
H       -4.095923  1.622711  0.180827
C       -0.401497  2.123153  -0.100920
H       -0.052697  3.154419  -0.105925
C       -1.044645  1.852882  -0.262455
H       -2.597888  2.694342  -0.367633
O       -0.938127  1.679234  -1.354844
C        2.611419 -1.377527  -0.521782
C        1.453512  1.894815  0.953687
O        2.507901  2.244978  1.423660
O        2.754955 -2.476456  -0.037659
C        0.911124  2.453296  -0.344680
H        0.814484  1.672054  -1.100153
H        1.612507  3.210873  -0.693701
H       -0.069898  2.909754  -0.191194
C        3.604746 -0.643379  -1.383836
H        3.151738 -0.386545  -2.345705
H        4.482374 -1.269224  -1.540030
H        3.891417  0.290667  -0.891056
H        1.065069 -1.658903  1.391069
O        1.492967 -0.620358  -0.331366