Electronic supplementary information (ESI)

Highly Stereoselective Directed Reactions and an Efficient Synthesis of Azafuranose from a Chiral Aziridine

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Std proton

File: xp
Pulse Sequence: g2pul
Solvent: cdcl3
Ambient temperature
Operator: LKE
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions

OBSERVE H1, 399.7193723 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 30 sec
Std carbon

File: xp

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: LW
Vnmrs-400 "Varian-NMR"

Relax, delay 1.000 sec
Pulse 45.6 degrees
Acq. time 1.200 sec
Width 24599.8 Hz
360 repetitions

OBSERVE C13, 100.5150857 MHz
DECOUPLE H1, 399.7435210 MHz
Power 37 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 36 min, 21 sec
Std proton

File: xp

Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 9410.3 Hz
16 repetitions

OBSERVE H1, 399.7983368 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 85536
Total time 0 min, 55 sec
Std carbon

File: xp
Pulse Sequence: s2pu1
Solvent: cdcl3
Ambient temperature
Operator: LWK
MNR-400 “Varian-NMR”
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24500.3 Hz
192 repetitions
OBSERVE C13, 100.5039471 MHz
DECouple H1, 399.8952231 MHz
Power 37 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 83556
Total time 1 hr, 16 min, 41 sec
Std proton

File: xp
Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Operator: LWK
VNMRS-400 Varian-NMR

Relax. delay 1.000 sec
Pulse 45.0 degrees
Avg. time 2.049 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 299.7663376 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 85998
Total time 0 min, 55 sec
Std carbon

File: xp

Pulse Sequence: s2pu1
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24500.8 Hz
400 repetitions

OBSERVE C13, 100.605652 MHz
DECOUPLE H1, 399.6739265 MHz
Power 37 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 16 min, 41 sec
Std proton

File: xp
Pulse Sequence: s2pul
Solvent: cdc15
Ambient temperature
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.7923984 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 30 sec

![NMR Spectrum Image]
Std carbon

File: xp

Pulse Sequence: s2pu1
Solvent: cdc13
Ambient temperature
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acc. time 1.399 sec
Width 24598.8 Hz
172 repetitions
OBSERVE C13, 100.5085164 MHz
DECOUPLE H1, 399.7213720 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 16 min, 41 sec
Std proton

File: xp
Pulse Sequence: 2pul
Solvent: d2o
Ambient temperature
Operator: LWR
VNMRS-400 "Varian-MNR"

Relax. delay 1.000 sec
Pulse 45.8 degrees
Acq. time 2.049 sec
Width 8610.3 Hz
10 repetitions
OBSERVE HI, 399.6981999 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FF size 65536
Total time 0 min, 55 sec
Std carbon

File: xp

Pulse Sequence: s2p1
Solvent: d2o
Temp. 25.0°C / 298.1 K
Operator: LWK
VTNR-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24500.8 Hz
384 repetitions

OBSERVE C13, 100.5042054 MHz
DECOUPLE H1, 399.7002504 MHz
Power 37 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 50256
Total time 1 hr, 16 min, 41 sec
Std proton

File: xp
Pulse Sequence: s2pul
Solvent: cdc13
Ambient temperature
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.944 sec
Width 6410.3 Hz
8 repetitions

OBSERVE H1, 399.713651 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 8 min, 30 sec
Std proton

File: xp

Pulse Sequence: t2pal
Solvent: cdc13
Ambient temperature
Operator: LDH
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE  H1, 399.766370 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 8 min, 30 sec
Std carbon

File: xp
Pulse Sequence: s2pul
Solvent: cdc13
Temp. 25.0 °C / 298.1 K
Operator: H.W.
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.590 sec
Width 24589.8 Hz
460 repetitions
OBSERVE C13, 100.4986662 MHz
DECOUPLE H1, 399.6790285 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 16 min, 41 sec
Std proton

File: xp
Pulse Sequence: z2pul
Solvent: d2o
Ambient temperature
Operator: LWH
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 8410.3 Hz
10 repetitions
OBSERVE H1, 399.8819648 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 55 sec

1.054 0.21 0.53 1.00
1.000 1.00
1.11
1.10
Std carbon

file: xp

Pulse Sequence: s2pul
Solvent: d2o
Ambient temperature
Operator: LWK
VNMRS-400 "Varian-NMR"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24539.8 Hz
320 repetitions

OBSERVE C13, 100.5937747 MHz
DECOUPLE H1, 399.7223993 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 16 min, 41 sec

ppm

180 160 140 120 100 80 60 40 20

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2. X-Ray Crystal Structure of Compound 6

**Figure 1.** X-ray crystal structure of 6 with thermal ellipsoids drawn at the 30% probability level.

**X-ray Crystallography.** A single crystal of 6, was picked from solutions by a nylon loop (Hampton Research Co.) on a hand made cooper plate mounted inside a liquid N$_2$ Dewar vessel at ca. −40 °C and mounted on a goniometer head in a N$_2$ cryostream. Data collections were carried out on a Bruker SMART AXS diffractometer equipped with a monochromator in the Mo K$_\alpha$ ($\lambda = 0.71073$ Å) incident beam. The CCD data were integrated and scaled using the Bruker-SAINT software package, and the structure was solved and refined using SHEXTL V 6.12.$^{[1]}$ Hydrogen atoms were
located in the calculated positions. Crystal data for 6: C_{29}H_{25}N_{3}O_{10}, Monoclinic, P2(1)/c, Z = 4, a = 9.4026(2), b = 32.1434(7), c = 9.1405(2) Å, β = 110.9000(10) °, V = 2580.78(10) Å³, μ = 0.114 mm⁻¹, ρ_{calc} = 1.481 g/cm³, R₁ = 0.0357, wR₂ = 0.0912 for 6427 unique reflections, 380 variables. The crystallographic data for 6 are listed in Table 1, and Tables 2 lists the selected bond distances and angles. CCDC-902981 for 6 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

References

<table>
<thead>
<tr>
<th>Crystal data and structure refinements for 6.</th>
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<tbody>
<tr>
<td><strong>Empirical formula</strong></td>
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<tr>
<td><strong>Formula weight</strong></td>
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<tr>
<td><strong>Temperature (K)</strong></td>
</tr>
<tr>
<td><strong>Wavelength (Å)</strong></td>
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<tr>
<td><strong>Crystal system/space group</strong></td>
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<tr>
<td><strong>Unit cell dimensions</strong></td>
</tr>
<tr>
<td>a (Å)</td>
</tr>
<tr>
<td>b (Å)</td>
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<tr>
<td>c (Å)</td>
</tr>
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<td>α (°)</td>
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<tr>
<td>β (°)</td>
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<tr>
<td>γ (°)</td>
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<tr>
<td><strong>Volume (Å³)</strong></td>
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<tr>
<td><strong>Z</strong></td>
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<tr>
<td><strong>Calculated density (g/cm³)</strong></td>
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<tr>
<td><strong>Absorption coefficient (mm⁻¹)</strong></td>
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<tr>
<td><strong>Reflections collected</strong></td>
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<tr>
<td><strong>Independent reflections [R(int)]</strong></td>
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<tr>
<td><strong>Refinement method</strong></td>
</tr>
<tr>
<td><strong>Data/restraints/parameters</strong></td>
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<tr>
<td><strong>Goodness-of-fit on F²</strong></td>
</tr>
<tr>
<td><strong>Final R indices [I &gt; 2σ(I)]</strong></td>
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<tr>
<td><strong>R indices (all data)</strong></td>
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<tr>
<td><strong>Largest difference peak and hole (e/Å³)</strong></td>
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Table 2. Selected bond distances (Å) and angles (°) for 6.

<table>
<thead>
<tr>
<th>Bond Distances (Å)</th>
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<tbody>
<tr>
<td>N2-C23</td>
<td>1.4793(13)</td>
</tr>
<tr>
<td>N2-C9</td>
<td>1.4708(13)</td>
</tr>
<tr>
<td>N2-C12</td>
<td>1.4699(13)</td>
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<tr>
<td>C9-C8</td>
<td>1.5143(15)</td>
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<tr>
<td>C9-C10</td>
<td>1.5292(15)</td>
</tr>
<tr>
<td>C10-O7</td>
<td>1.4460(13)</td>
</tr>
<tr>
<td>C10-C11</td>
<td>1.5249(16)</td>
</tr>
<tr>
<td>C11-C12</td>
<td>1.5417(15)</td>
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<tr>
<td>C11-O6</td>
<td>1.4359(13)</td>
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<tr>
<td>O6-C14</td>
<td>1.3599(13)</td>
</tr>
<tr>
<td>C14-O5</td>
<td>1.2003(14)</td>
</tr>
<tr>
<td>C14-C13</td>
<td>1.5074(16)</td>
</tr>
<tr>
<td>C13-C12</td>
<td>1.5321(15)</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Bond Angles (°)</th>
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<tbody>
<tr>
<td>C12-N2-C9</td>
<td>107.84(8)</td>
</tr>
<tr>
<td>N2-C9-C10</td>
<td>102.02(8)</td>
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<td>C9-C10-C11</td>
<td>100.23(9)</td>
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<td>C10-C11-C12</td>
<td>104.87(8)</td>
</tr>
<tr>
<td>C12-C11-O6</td>
<td>107.77(9)</td>
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<tr>
<td>C11-O6-C14</td>
<td>110.86(8)</td>
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<tr>
<td>O6-C14-C13</td>
<td>110.77(9)</td>
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<tr>
<td>C14-C13-C12</td>
<td>105.31(9)</td>
</tr>
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