# Synthesis of 2,3-Dihydro-4(1H)-quinolones and the Corresponding 4(1H)-Quinolones via Low-temperature Fries Rearrangement of 

## $N$-Arylazetidin-2-ones*

Jens Lange, ${ }^{\mathrm{A}}$ Alex C. Bissember, ${ }^{\mathrm{A}}$ Martin G. Banwell, ${ }^{\mathrm{A}, \mathrm{B}}$ and Ian A. Cade ${ }^{\mathrm{A}}$<br>${ }^{\text {A }}$ Research School of Chemistry, Institute of Advanced Studies, The Australian National University, Canberra, ACT 0200, Australia.<br>${ }^{\text {B }}$ Corresponding author. Email: mgb@rsc.anu.edu.au

Contents Page

1. ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR Spectra for Compounds $\mathbf{1 i}, \mathbf{1 0}, \mathbf{1 s}, \mathbf{1 t}, \mathbf{1 u}, \mathbf{2 0}, \mathbf{2 p}, \mathbf{2 q}, \mathbf{2 r}, \mathbf{2 s}, \mathbf{2 t}, \mathbf{2 u}$, $\mathbf{8 a}, \mathbf{8 b}, 8 \mathrm{dd}, \mathbf{8 e}, 8 \mathrm{ff}$ and $\mathbf{8 g}$
2. ORTEPs for Compounds $\mathbf{1 j}, \mathbf{1 u}, \mathbf{2 n}(\mathbf{b})$ and $\mathbf{2 q}$ ..... S38-S39

[^0]$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 1 i Recorded in DMSO- $\mathrm{d}_{6}$

$1 i$

$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound $\mathbf{1 i}$ Recorded in DMSO- $\mathrm{d}_{6}$



$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 10 Recorded in $\mathrm{CDCl}_{3}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 1s Recorded in $\mathrm{CDCl}_{3}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 1t Recorded in $\mathrm{CDCl}_{3}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 1t Recorded in $\mathrm{CDCl}_{3}$



$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound $\mathbf{1 u}$ Recorded in $\mathrm{CDCl}_{3}$



|  |  |
| :--- | :--- |
|  |  |
|  |  |
|  |  |
|  |  |


$\mathrm{F} / \mathrm{y}$

220
200
180
160
140
120
100
80
60
40
20
0 ppm
$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 20 Recorded in DMSO-d $\mathrm{d}_{6}$

$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 20 Recorded in DMSO-d $\mathrm{d}_{6}$

$\longrightarrow 193.564$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound $\mathbf{2 p}$ Recorded in $\mathrm{CDCl}_{3}$


## $75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 2 p Recorded in $\mathrm{CDCl}_{3}$






$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 2 q Recorded in $\mathrm{CDCl}_{3}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 2 r Recorded in $\mathrm{CDCl}_{3}$



$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 2s Recorded in DMSO-d ${ }_{6}$

$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 2 t Recorded in DMSO- $\mathrm{d}_{6}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 2t Recorded in DMSO- $\mathrm{d}_{6}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound $\mathbf{2 u}$ Recorded in DMSO-d $\mathbf{d}_{6}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound $\mathbf{2 u}$ Recorded in DMSO- $\mathrm{d}_{6}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 8a Recorded in DMSO- $\mathrm{d}_{6}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound $\mathbf{8 b}$ Recorded in DMSO-d ${ }_{6}$

$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound $\mathbf{8 b}$ Recorded in DMSO- $\mathrm{d}_{6}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 8d Recorded in DMSO-d $\mathrm{d}_{6}$


$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 8d Recorded in DMSO-d $\mathrm{d}_{6}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 8 e Recorded in DMSO-d $\mathrm{d}_{6}$

$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 8 e Recorded in DMSO- $\mathrm{d}_{6}$


$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 8 ff Recorded in DMSO- $\mathrm{d}_{6}$





$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound $8 f$ Recorded in DMSO-d ${ }_{6}$



$300 \mathrm{MHz}{ }^{1} \mathrm{H}$ NMR Spectrum of Compound 8 g Recorded in DMSO- $\mathrm{d}_{6}$

$75 \mathrm{MHz}{ }^{13} \mathrm{C}$ NMR Spectrum of Compound 8 g Recorded in DMSO-d $\mathrm{d}_{6}$




Figure S1. Compound 1j (CCDC 801993) with displacement ellipsoids drawn at the 50\% probability level. H atoms are shown as spheres of arbitrary radius.


Figure S2. Compound 1u (CCDC 801994) with displacement ellipsoids drawn at the 50\% probability level. H atoms are shown as spheres of arbitrary radius.


Figure S3. Compound 2n(b) (CCDC 801995) with displacement ellipsoids drawn at the 50\% probability level. H atoms are shown as spheres of arbitrary radius.


Figure S4. Compound 2q (CCDC 801996) with displacement ellipsoids drawn at the 50\% probability level. H atoms are shown as spheres of arbitrary radius.


[^0]:    * Dedicated to the memory of Athel L. J. Beckwith FAA, FRS, an inspirational chemist and a wonderful friend and colleague, who died tragically on May $15^{\text {th }}, 2010$.

