Supplementary Material

Synthesis of 2-aryl-(4 or 5)-aryl-1H-imidazoles and 2-hydroxy-3,6-diaryl-pyrazines via a cascade process

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**Note for NMR spectra:** The NMR signals of some compounds (like 3p) are very weak. The reason is that their solubility in DMSO-$d_6$ is extremely low, and even lower in other deuterated reagents. The signals of deuterated solvent DMSO-$d_6$ at $\delta$ 2.45-2.55 (ppm) in respective $^1$H-NMR spectrum and at $\delta$ 39.4-39.6 (ppm) for DMSO-$d_6$ in respective $^{13}$C-NMR spectrum were observed. The signals of water (DMSO-$d_6$ absorbs water easily) around $\delta$ 3.33 (ppm) in respective $^1$H-NMR spectrum were observed. The signals of residual acetone around 2.09 (ppm) in $^1$H-NMR spectrum and around 30.6 (ppm) in $^{13}$C-NMR spectrum were observed in some compounds like 2n and 2n'.

Single-crystal data for compounds 2j (CCDC 920522), 2k (CCDC 873930) and 3p (CCDC 920523) have been deposited in the Cambridge Crystallographic Data Centre. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/data_request/cif.
**checkCIF/PLATON report**

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

### Datablock: 2j

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<td>-P 2ybc</td>
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**Correction method:** MULTI-SCANS

Data completeness = 0.973  Theta(max) = 29.140

R(reflections) = 0.0545  (3024)  wR2(reflections) = 0.1272 (3290)

S = 0.999  Npar = 193

---

The following ALERTS were generated. Each ALERT has the format:

test-name ALERT alert-type alert-level.

Click on the hyperlinks for more details of the test.

- **Alert level C**
  
  ABSTY02_ALERT_1_C: An _exptl_absorpt_correction_type has been without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
  
  Absorption correction given as Multi-scans
Alert level G
ADGTV01_ALERT_1_G Extra text has been found in the _exptl_absorp_correction_type field, which should be only a single keyword. A literature citation should be included in the _exptl_absorp_process_details field.

PLAT005_ALERT_5_G No _lucr_refine_instructions_details in the CIF
PLAT079_ALERT_4_G Centre of Gravity not Within Unit Cell: Resid. H 2 NE 0

0 ALERT level A = Most likely a serious problem - resolve or explain
1 ALERT level B = A potentially serious problem, consider carefully
2 ALERT level C = Check, ensure it is not caused by an omission or oversight
3 ALERT level D = General information/check it is not something unexpected
4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
8 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the “special_details” fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation), however, if you intend to submit to Acta Crystallographica Section C or E, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals
Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 24/04/2013; check.def file version of 23/04/2013
**checkCIF/PLATON report**

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: 2k**

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<td>Sum formula:</td>
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Correction method: Not given

Data completeness= 1.55/0.78  Theta(max)= 29.160

R(reflections)= 0.0353( 2051)  wR2(reflections)= 0.0840( 2435)

\( S = 1.001 \)  \( \text{Npar} = 176 \)

The following ALERTS were generated. Each ALERT has the format ‘test-name ALERT alert-type alert-level’. Click on the hyperlinks for more details of the test.

![Alert level C](image)

*Alert level C*  
**STRESS_ALERT_4_C**  
From the CIF: _refine_ls_abs_structure_Pack -1.800  
From the CIF: _refine_ls_abs_structure_Pack_su 1.400
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<td>Most likely a serious problem - resolve or explain</td>
</tr>
<tr>
<td>F</td>
<td>A potentially serious problem, consider carefully</td>
</tr>
<tr>
<td>C</td>
<td>Check. Ensure it is not caused by an omission or oversight</td>
</tr>
<tr>
<td>G</td>
<td>General information, check it is not something unexpected</td>
</tr>
</tbody>
</table>

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems, it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. 

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checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3p

Bond precision: C-C = 0.0035 Å  Wavelength=0.71073 Å

Cell:  
\[a=19.908(8)\]  \[b=10.770(4)\]  \[c=13.126(5)\]  
\[\alpha=90^\circ\]  \[\beta=130.374(4)\]  \[\gamma=90^\circ\]

Temperature: 153 K

Volume: 2144.1(14) Å³  
Space group: C 2/c  
Halo group: ?

Moloty formula: C10 H6 N4 O S2  
Sum formula: C10 H6 N4 O S2  
Mr: 262.33  
Dx.g cm⁻³: 1.625

\(Z\)  
\(Z\) (mm⁻¹) 0.493  
P000 1072.0  
P000' 1074.29  
h,k,lmax 27,14,17  
Dref 2850  
 Tmin, Tmax 0.956, 0.976  
 Tmin' 0.786

Correction method: MULTI-SCANS

Data completeness: 0.999  
Theta(max): 28.990°

R(reflections): 0.0474(2388)  
wR2(reflections): 0.1267(2847)

S = 1.002  
Npar = 172

The following ALERTS were generated. Each ALERT has the format:
test-name ALERT alert-type alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

ABST00_ALERT_1_C  An _scale_absorption_correction_type has been given without a literature citation. This should be contained in the _scale_absorption_process_details field.
Absorption correction given as Multi-scans
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.01

Alert level G

ABCT001_ALERT_1_G Extra text has been found in the _exp1_absorp_correction_type field, which should be only a single keyword. A literature citation should be included in the _exp1_absorp_process_details field.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6
PLAT005_ALERT_5_G No _lucr_refine_instructions_details in the CIF 7
PLAT003_ALERT_3_G Note: Main Residue Disorder ................. 10 %
PLAT010_ALERT_4_G Number of Unusual/Non-Standard Labels .......... 1
PLAT011_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... 1
PLAT000_ALERT_2_G Note: Number of Least-Squares Restraints ....... 5

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PLATON version of 24/04/2013; check.def file version of 23/04/2013

NOMOVE FORCED

z = 0.68 3p 2.7%  R = 0.05  RES = 0 -3 X