

Supplementary Information

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Supplement: Synthesis, characterization, thermal degradation and urease inhibitory studies of the new hydrazide based Schiff base ligand 2-(2-hydroxyphenyl)-3-{[(*E*)-(2-hydroxyphenyl)methylidene]amino}-2,3-dihydroquinazolin-4(1*H*)-one

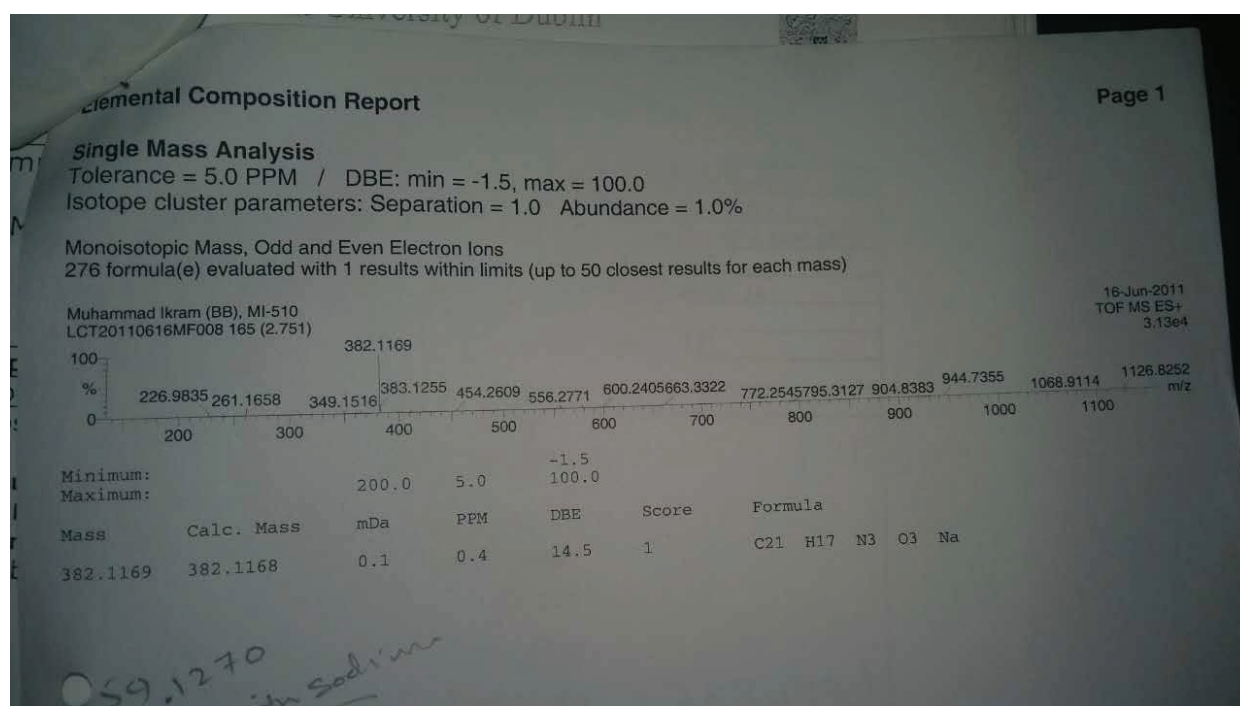


Figure S1: Mass spectrum of H-HHAQ ligand.

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checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

Bond precision: C-C = 0.0112 Å Wavelength=0.71073

Cell: a=10.2571(9) b=14.4341(12) c=23.706(2)

 alpha=90 beta=90 gamma=90

Temperature: 295 K

	Calculated	Reported
Volume	3509.7(5)	3509.7(5)
Space group	C 2 2 21	C 2 2 21
Hall group	C 2c 2	C 2c 2
Moiety formula	C21 H17 N3 O3	?
Sum formula	C21 H17 N3 O3	C21 H17 N3 O3
Mr	359.38	359.38
Dx, g cm ⁻³	1.360	1.360
Z	8	8
Mu (mm ⁻¹)	0.093	0.093
F000	1504.0	1504.0
F000'	1504.67	
h,k,lmax	13,18,30	12,17,29
Nref	3837[2146]	3037
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 1.42/0.79 Theta(max)= 26.956

R(reflections)= 0.0820(1435) wR2(reflections)= 0.0886(3037)

S = 0.998 Npar= 255

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 A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
 Crystal habit description.
 The following tests will not be performed.
 CRYSR_01
 PLAT222_ALERT_3_A Large Non-Solvent H Uiso(max)/Uiso(min) .. 10.0 Ratio

 Alert level B

PLAT035_ALERT_1_B No _chemical_absolute_configuration info given . Please Do !
 PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.0112 Ang.

 Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: _refine_ls_abs_structure_Flack 0.500
 From the CIF: _refine_ls_abs_structure_Flack_su 1.000
 PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low 47 %
 PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given . Please Do !
 PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
 PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
 PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
 PLAT245_ALERT_2_C U(iso) H19 Smaller than U(eq) N19 by ... 0.031 AngSq
 PLAT352_ALERT_3_C Short N-H (X0.87,N1.01A) N19 - H19 ... 0.72 Ang.
 PLAT410_ALERT_2_C Short Intra H...H Contact H8 .. H20 .. 1.98 Ang.

 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
 PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
 PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
 PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT301_ALERT_3_G Main Residue Disorder Percentage = 26 Note
 PLAT791_ALERT_4_G The Model has Chirality at C20 R Verify
 PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 55 Note

- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 11 **ALERT level G** = General information/check it is not something unexpected

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 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
 6 ALERT type 4 Improvement, methodology, query or suggestion
 2 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 20/08/2014; check.def file version of 18/08/2014

Datablock shelx - ellipsoid plot

