

Supplementary Information

When Serendipity Knocks on the Door: Synthesis and Physicochemical Characterization of 7-Chloro-2,3-dihydro-5H-thiazolo[3,2-a]pyrimidin-5-one

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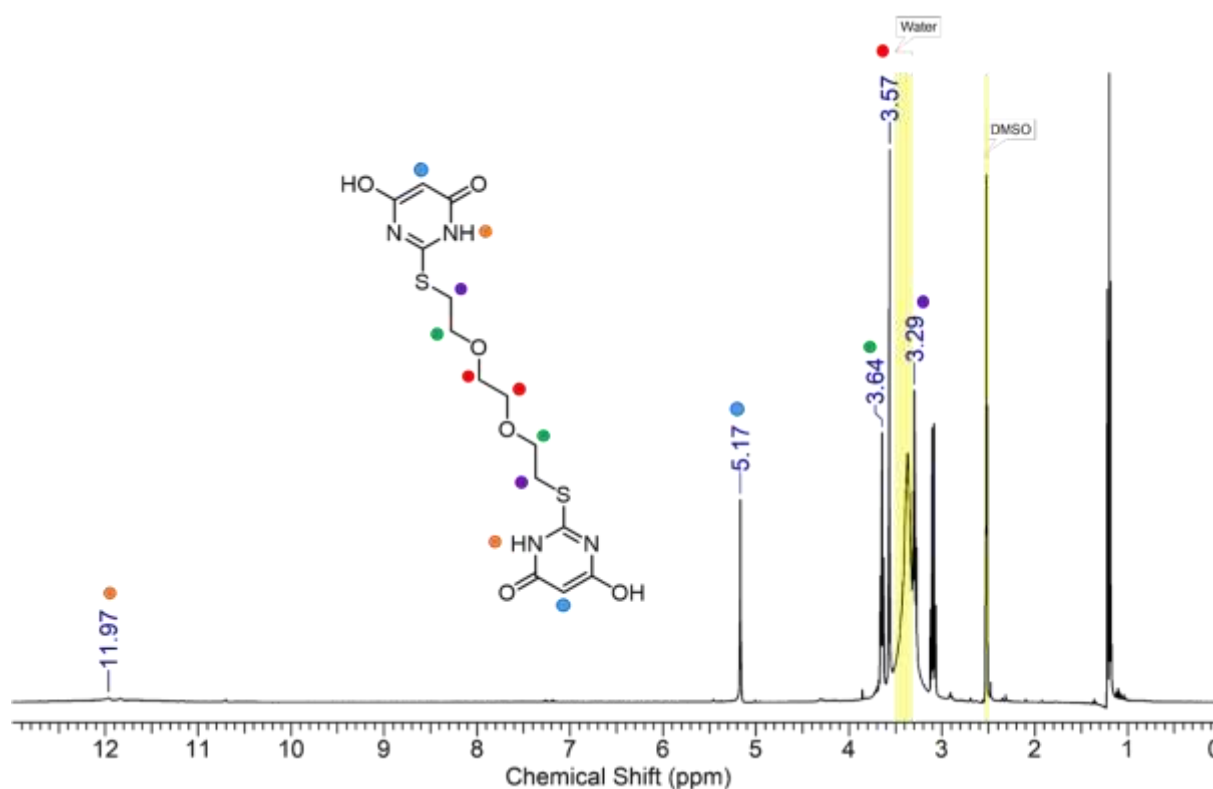


Figure S1. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 3.

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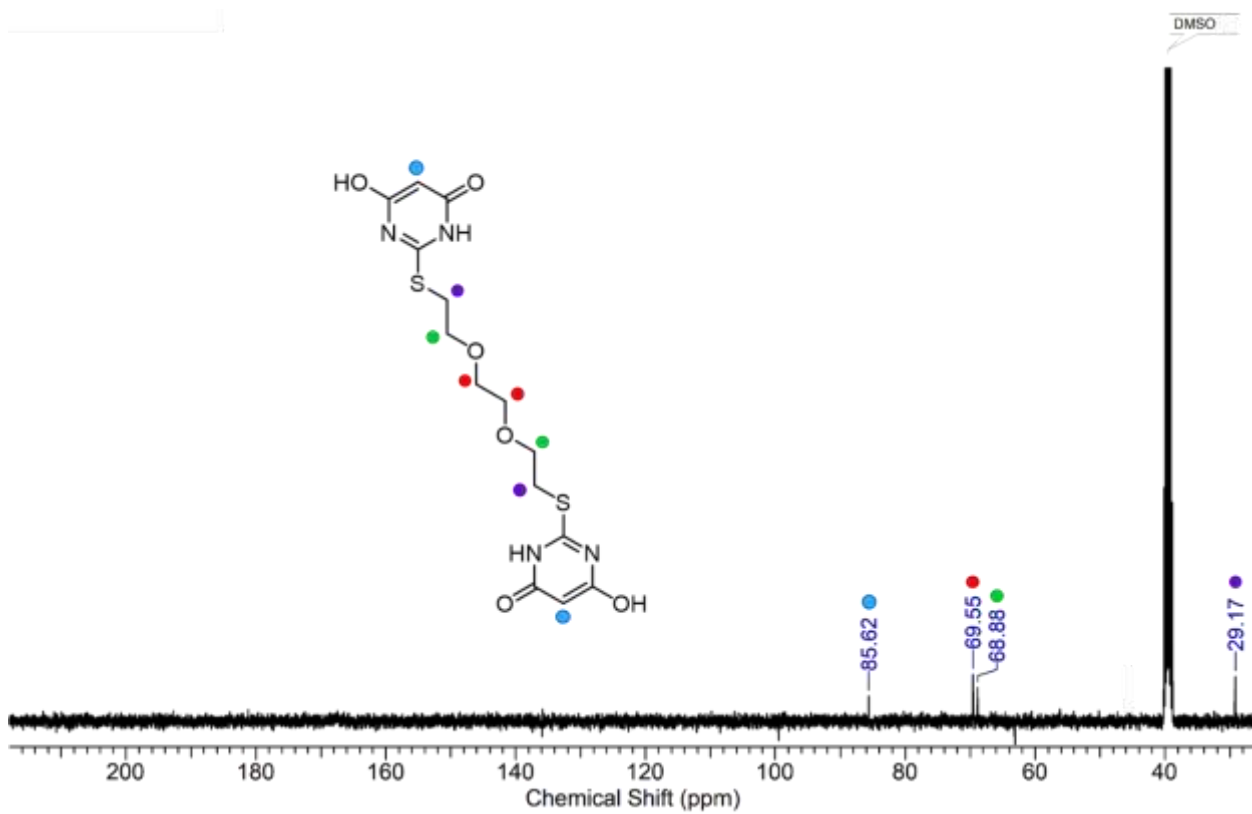


Figure S2. ^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of compound 3.

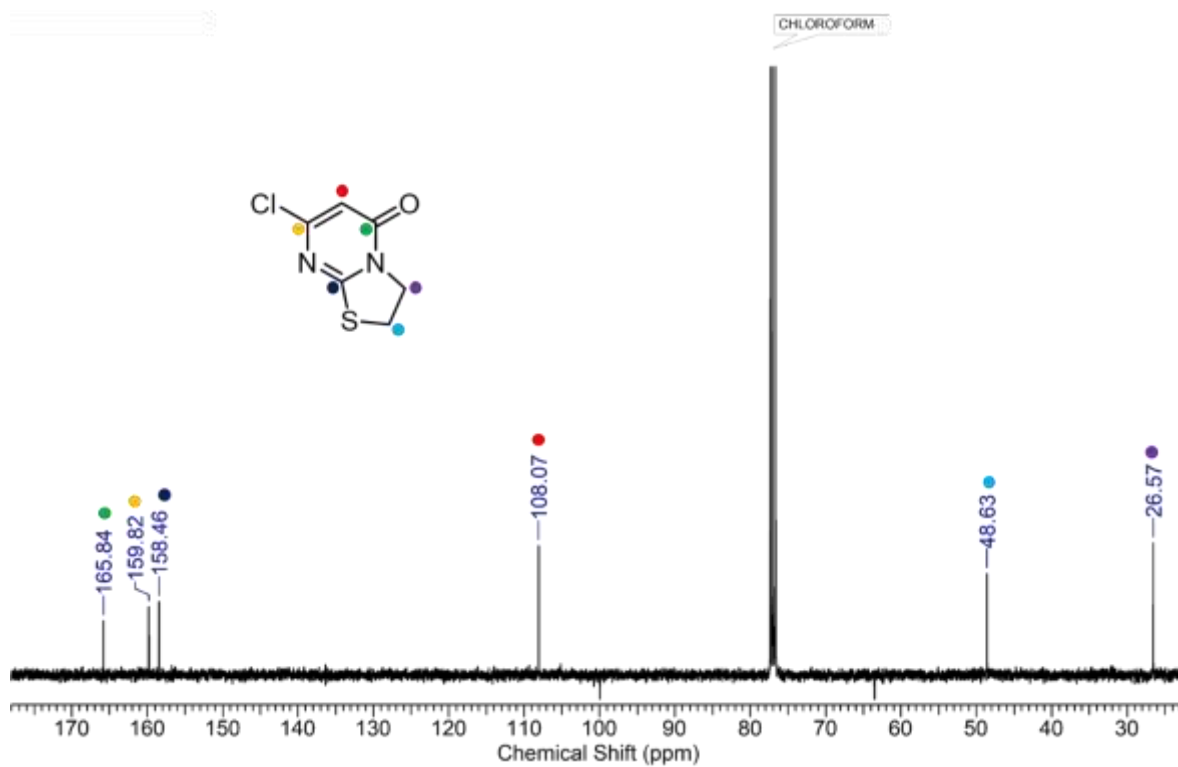


Figure S3. ^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$) of compound 4.

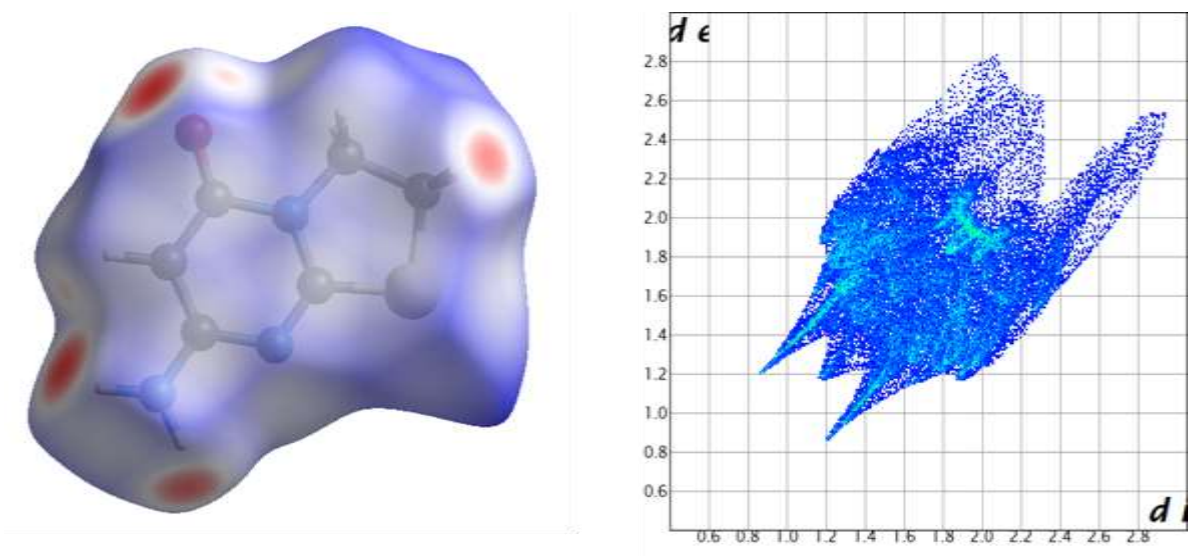


Figure S4. Hirshfeld surface and 2D fingerprint plot for the compound HIXRUB.¹

Reference

1. Low, J. N.; Ferguson, G.; Melguizo, M.; Sánchez, A.; *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **1999**, *55*, IUC9900048.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CITHiPy

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: CITHiPy

Bond precision: C-C = 0.0045 Å Wavelength=1.54184

Cell: a=8.977(4) b=9.276(5) c=9.512(3)
 alpha=88.12(2) beta=87.98(2) gamma=80.53(3)
Temperature: 293 K

	Calculated	Reported
Volume	780.5(6)	780.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C6 H5 Cl N2 O S	2(C6 H5 Cl N2 O S)
Sum formula	C6 H5 Cl N2 O S	C12 H10 Cl2 N4 O2 S2
Mr	188.63	377.26
Dx, g cm-3	1.605	1.605
Z	4	2
Mu (mm-1)	6.356	6.357
F000	384.0	384.0
F000'	387.64	
h,k,lmax	10,11,11	10,11,11
Nref	2756	2644
Tmin,Tmax	0.881,0.909	0.586,0.754
Tmin'	0.881	

Correction method= # Reported T Limits: Tmin=0.586 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.959 Theta(max)= 66.500

R(reflections)= 0.0383(2157) wR2(reflections)= 0.1023(2644)

S = 1.062 Npar= 200

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 B

[PLAT029_ALERT_3_B](#) _diffn_measured_fraction_theta_full value Low . 0.959 Why?

Author Response: This alert is due to low ratio caused by very weak data beyond $\sin(\theta)/\lambda > 0.66$ (i.e. low resolution). this problem is common in small crystals and twinned crystals and in this case the data were restricted to theta max 66.5 with intensities values above 3 sigma line.

Alert level C

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C7	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0045	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.060	Check
PLAT911_ALERT_3_C	Missing PCF Refl Between Thmin & STh/L= 0.595	112	Report

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	22	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	174	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	71%	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

4 **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
7 **ALERT type 3** Indicator that the structure quality may be low
1 **ALERT type 4** Improvement, methodology, query or suggestion
0 **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* or *IUCrData*, 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.

