**Supporting Information**

**Crystal structure and biological evolution of 5-bromothiophene based 3,4-dihydropyrimidin-2-(1H)-thi(ones)**

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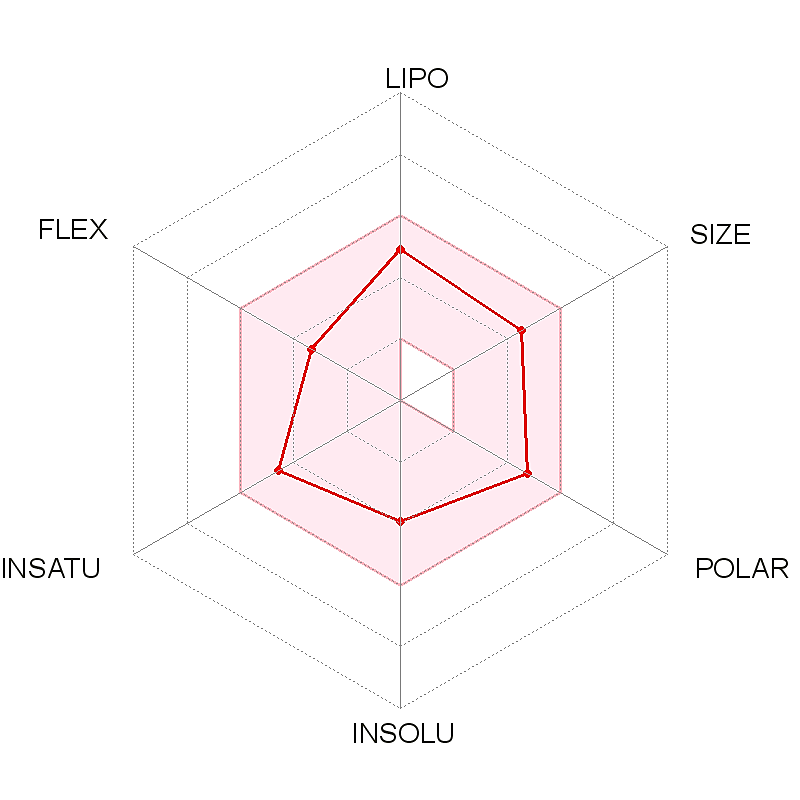
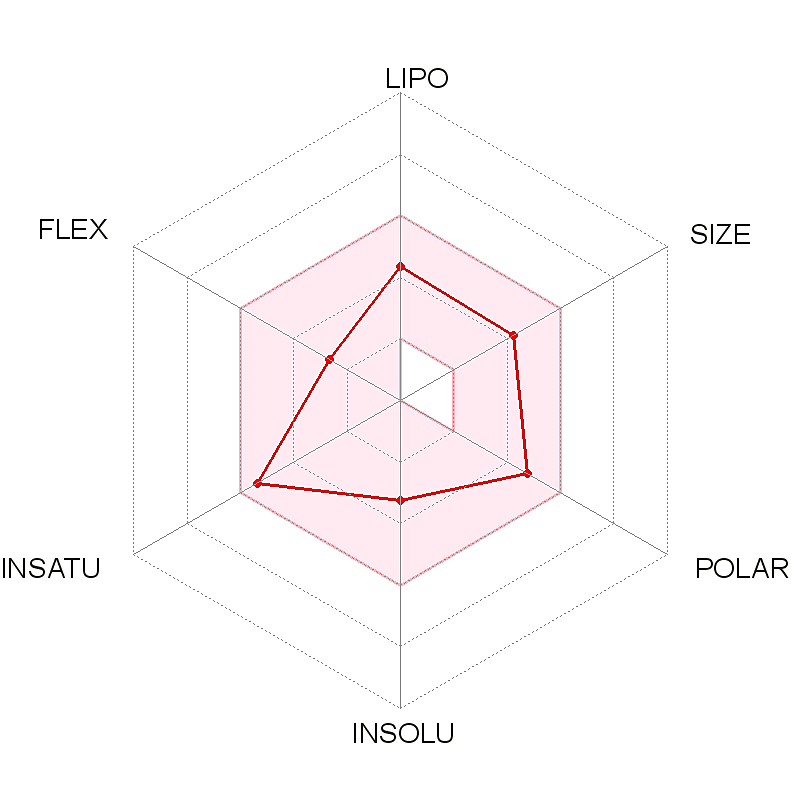
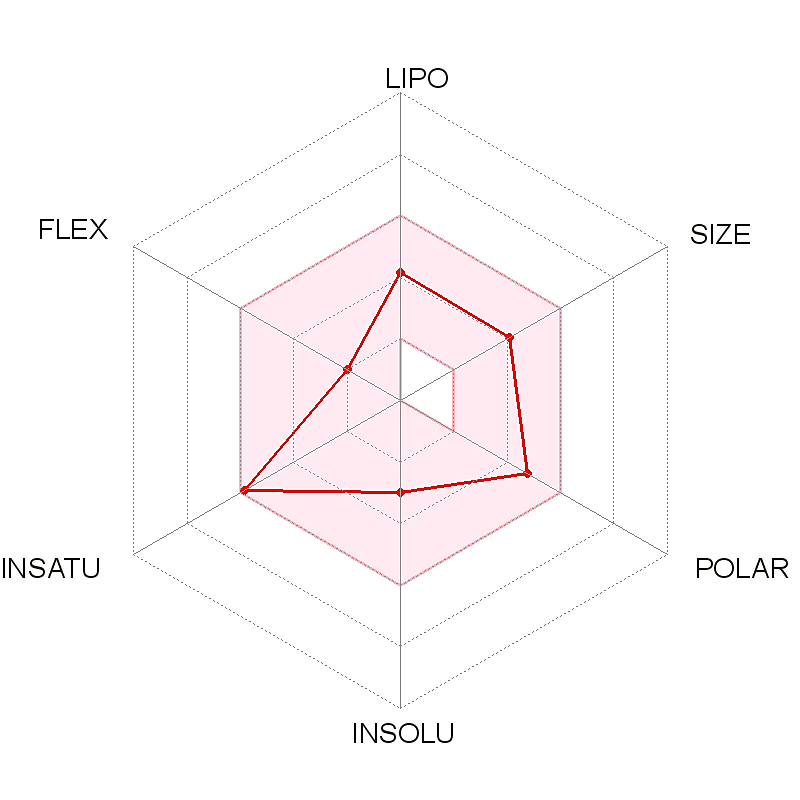
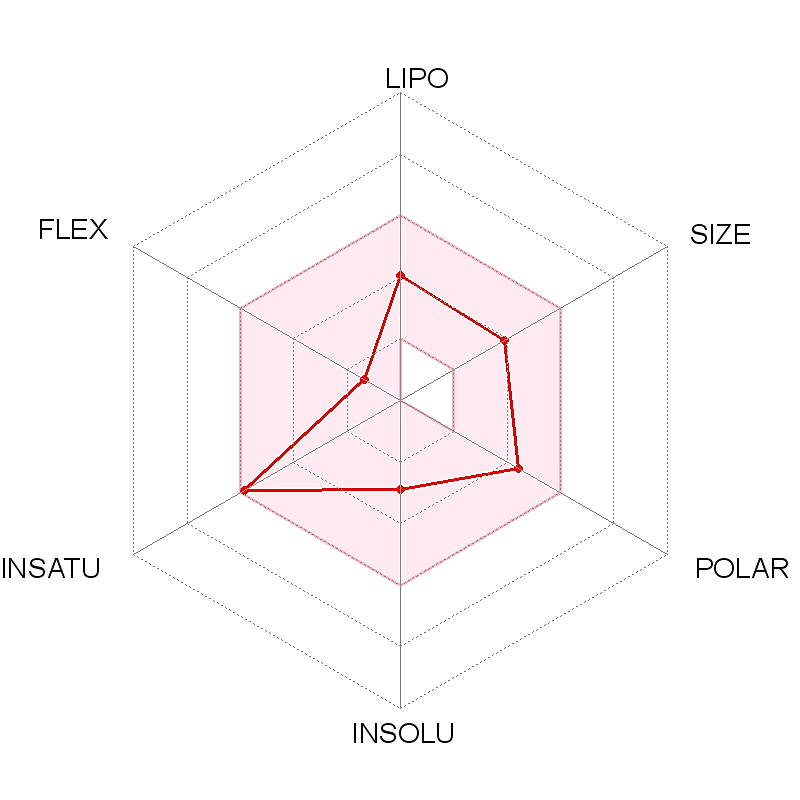
Prof. Hitendra M. Patel (Email: [hm\_patel@spuvvn.edu](mailto:hm_patel@spuvvn.edu)).

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1. **Bioavailability Radars of compound 4(a-j)**

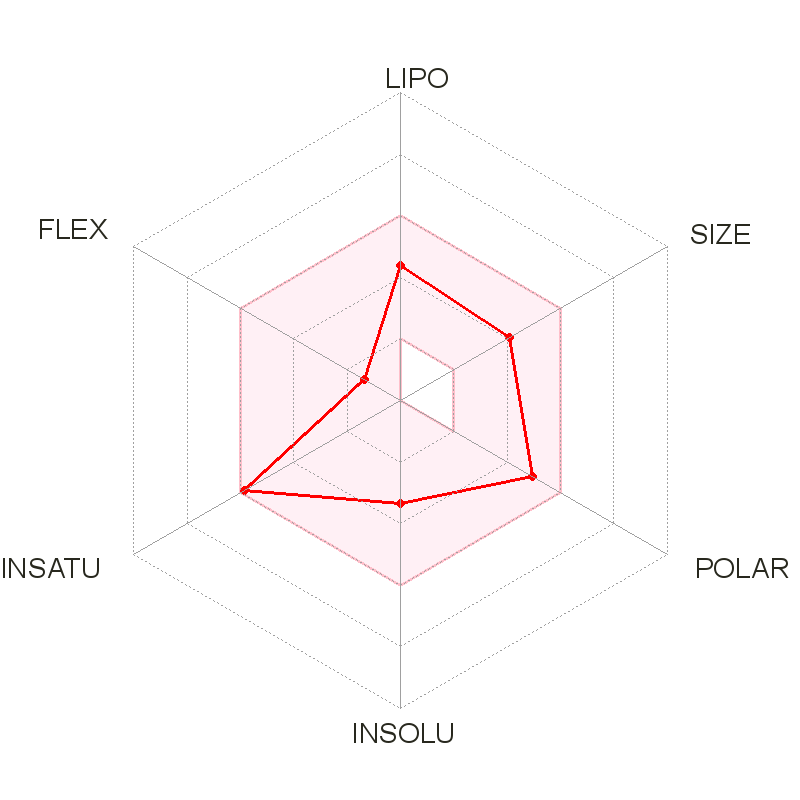
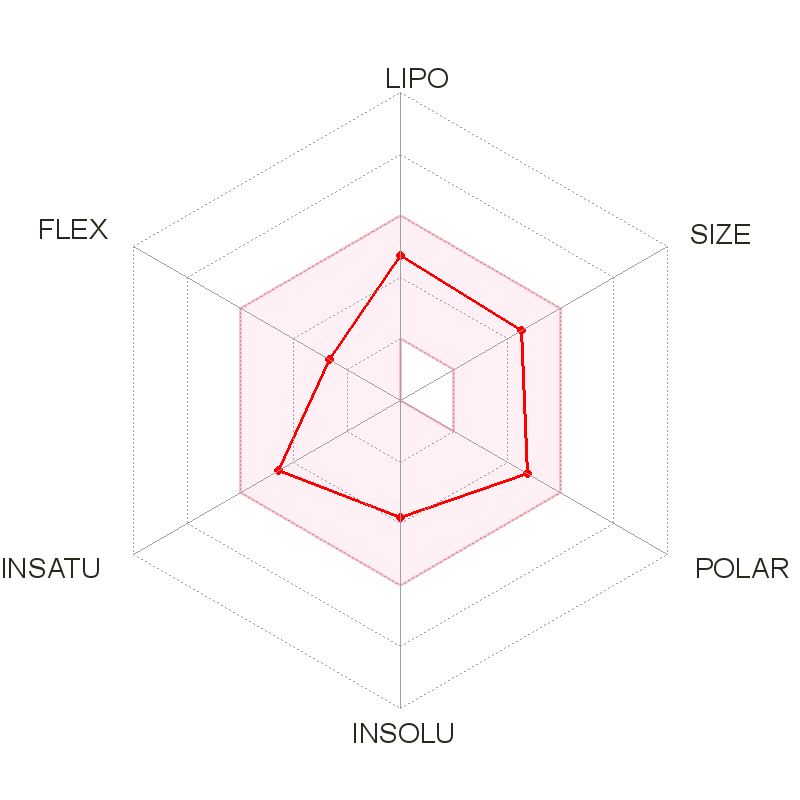


**4d**

**4c**

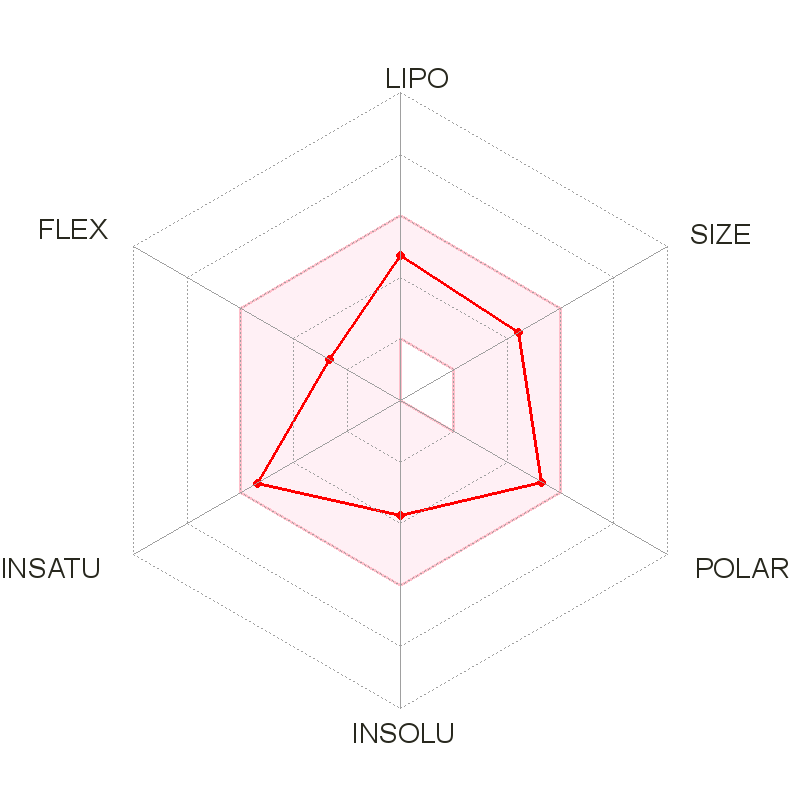
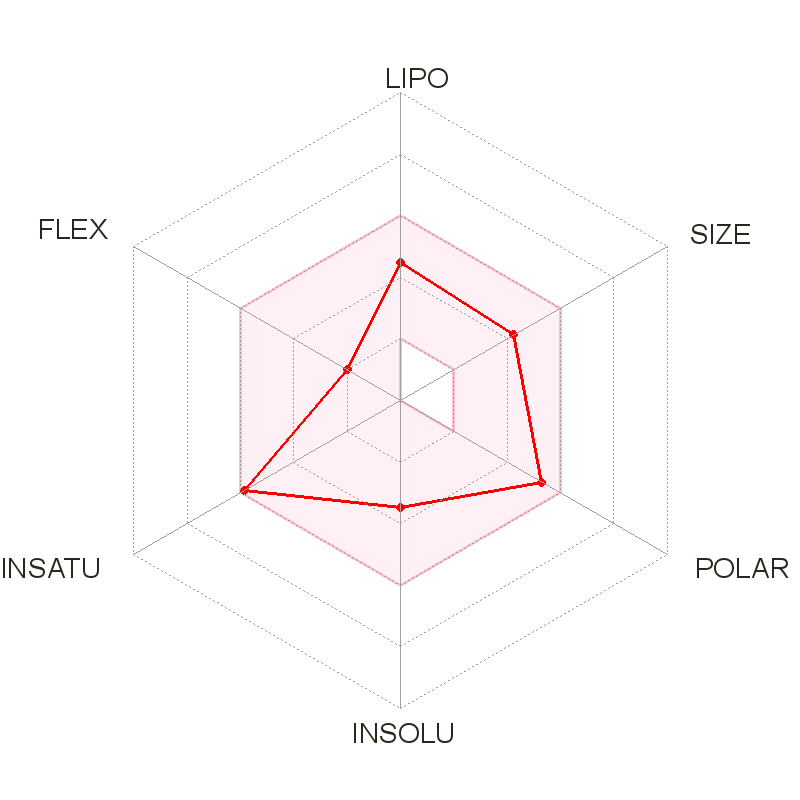
**4a**

**4b**



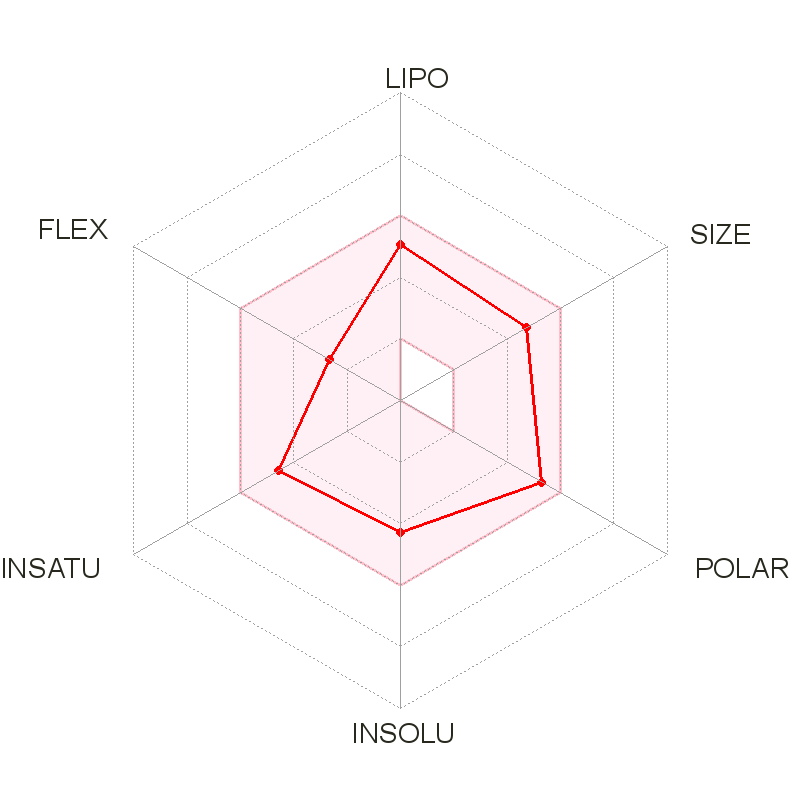
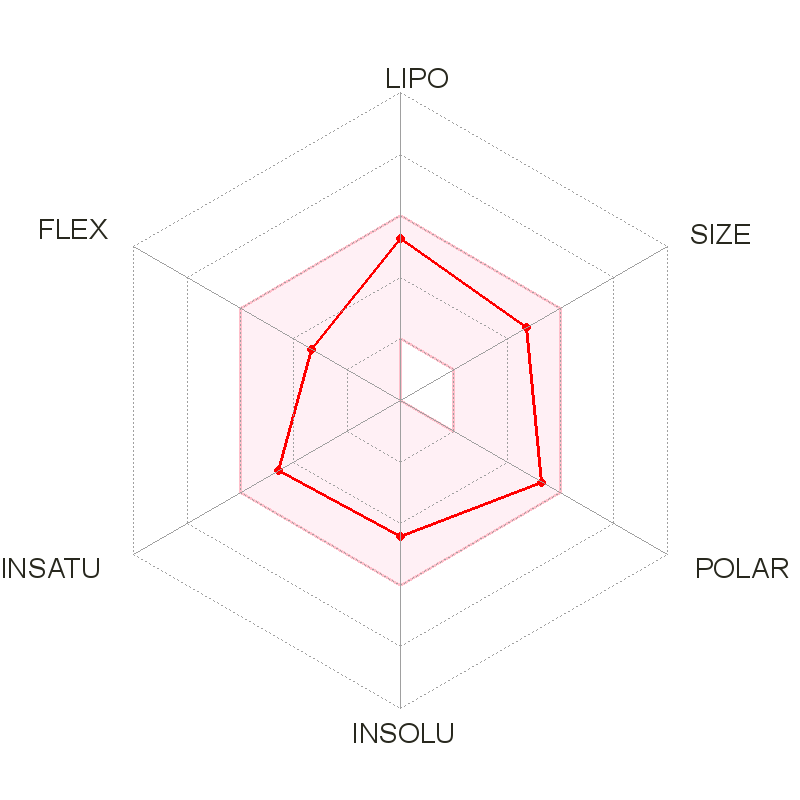
**4e**

**4f**



**4h**

**4g**



**4j**

**4i**

1. 1H-NMR data of compounds **4(a-j)**

**Compound 4a**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide1.TIF**

**Compound 4b**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide3.TIF**

**Compound 4c**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide5.TIF**

**Compound 4d**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide7.TIF**

**Compound 4e**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide9.TIF**

**Compound 4f**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide13.TIF**

**Compound 4g**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide15.TIF**

**Compound 4h**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide17.TIF**

**Compound 4i**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide19.TIF**

**Compound 4j**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide21.TIF**

1. Selected 13C-APT data of compounds **4(a-j)**

**Compound 4a**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide2.TIF**

**Compound 4bE:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide4.TIF**

**Compound 4c**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide6.TIF**

**Compound 4d**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide8.TIF**

**Compound 4e**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide10.TIF**

**Compound 4f**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide14.TIF**

**Compound 4g**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide16.TIF**

**Compound 4h**

**E:\Ph.D\Thesis\FIGURES\C5\Spectra\Spectra\Slide18.TIF**

1. ATR-FTIR spectra of compounds **4(a-j)**

**Compound 4a**



**Compound 4b**



**Compound 4c**



**Compound 4d**



**Compound 4e**



**Compound 4f**



**Compound 4g**



**Compound 4h**



**Compound 4i**



**Compound 4j**



# **Single crystal X-ray diffraction analysis of compound 4c**

**checkCIF (basic structural check) running**

*Checking for embedded fcf data in CIF ...*   
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait* **. .**

**checkCIF/PLATON (basic structural check)**

Structure factors have been supplied for datablock(s) MB1

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](http://www.iucr.org/iucr-top/cif/cif_core/definitions/index.html)  
Please wait while processing .... [Interpreting this report](http://journals.iucr.org/services/cif/checking/checkcifreport.html)

[Structure factor report](http://checkcif.iucr.org/M6MImYCLT4lrO/010620104816162747000/ckf.html)  
  
**Datablock: MB1**

|  |  |  |
| --- | --- | --- |
| Bond precision: | C-C = 0.0123 A | Wavelength=0.71073 |

|  |  |  |  |
| --- | --- | --- | --- |
| Cell: | a=7.3244(3) | b=13.5742(6) | c=14.8486(7) |
|  | alpha=94.044(2) | beta=103.959(2) | gamma=99.511(2) |
| Temperature: | 296 K |  |  |

|  |  |  |
| --- | --- | --- |
|  | Calculated | Reported |
| Volume | 1403.57(11) | 1403.57(11) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C12 H13 Br N2 O3 S | C12 H13 Br N2 O3 S |
| Sum formula | C12 H13 Br N2 O3 S | C12 H13 Br N2 O3 S |
| Mr | 345.20 | 345.20 |
| Dx,g cm-3 | 1.634 | 1.634 |
| Z | 4 | 4 |
| Mu (mm-1) | 3.082 | 3.082 |
| F000 | 696.0 | 696.0 |
| F000' | 695.63 |  |
| h,k,lmax | 8,16,17 | 8,16,17 |
| Nref | 4937 | 4920 |
| Tmin,Tmax | 0.467,0.735 | 0.513,0.748 |
| Tmin' | 0.458 |  |

|  |  |
| --- | --- |
| Correction method= # Reported T Limits: Tmin=0.513 Tmax=0.748 AbsCorr = MULTI-SCAN |  |

|  |  |
| --- | --- |
| Data completeness= 0.997 | Theta(max)= 24.994 |

|  |  |
| --- | --- |
| R(reflections)= 0.0802( 2720) | wR2(reflections)= 0.2405( 4920) |

|  |  |
| --- | --- |
| S = 1.062 | Npar= 374 |

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.

http://www.iucr.org/iucr-top/logos/orange.gif**Alert level B**

[PLAT234\_ALERT\_4\_B](javascript:makeHelpWindow(%22PLAT234.html%22)) Large Hirshfeld Difference C19 --C20 . 0.26 Ang.

[PLAT360\_ALERT\_2\_B](javascript:makeHelpWindow(%22PLAT360.html%22)) Short C(sp3)-C(sp3) Bond C19 - C20 . 1.25 Ang.

http://www.iucr.org/iucr-top/logos/yellow.gif**Alert level C**

[PLAT220\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT220.html%22)) NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 5.7 Ratio

[PLAT222\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT222.html%22)) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.6 Ratio

[PLAT234\_ALERT\_4\_C](javascript:makeHelpWindow(%22PLAT234.html%22)) Large Hirshfeld Difference C23 --C24 . 0.18 Ang.

[PLAT241\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT241.html%22)) High MainMol Ueq as Compared to Neighbors of C22 Check

**And 3 other PLAT241 Alerts**

[PLAT241\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT241.html%22)) High MainMol Ueq as Compared to Neighbors of C23 Check

[PLAT241\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT241.html%22)) High MainMol Ueq as Compared to Neighbors of C11 Check

[PLAT241\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT241.html%22)) High MainMol Ueq as Compared to Neighbors of C12 Check

[PLAT242\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT242.html%22)) Low MainMol Ueq as Compared to Neighbors of C21 Check

**And 3 other PLAT242 Alerts**

[PLAT242\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT242.html%22)) Low MainMol Ueq as Compared to Neighbors of C24 Check

[PLAT242\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT242.html%22)) Low MainMol Ueq as Compared to Neighbors of C9 Check

[PLAT242\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT242.html%22)) Low MainMol Ueq as Compared to Neighbors of C10 Check

[PLAT341\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT341.html%22)) Low Bond Precision on C-C Bonds ............... 0.01233 Ang.

[PLAT352\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT352.html%22)) Short N-H (X0.87,N1.01A) N4 - H4N . 0.74 Ang.

[PLAT431\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT431.html%22)) Short Inter HL..A Contact Br2 ..S2A . 3.35 Ang.

-x,1-y,1-z = 2\_566 Check

[PLAT906\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT906.html%22)) Large K Value in the Analysis of Variance ...... 3.468 Check

[PLAT911\_ALERT\_3\_C](javascript:makeHelpWindow(%22PLAT911.html%22)) Missing FCF Refl Between Thmin & STh/L= 0.595 17 Report

[PLAT978\_ALERT\_2\_C](javascript:makeHelpWindow(%22PLAT978.html%22)) Number C-C Bonds with Positive Residual Density. 0 Info

http://www.iucr.org/iucr-top/logos/gray.gif**Alert level G**

[PLAT154\_ALERT\_1\_G](javascript:makeHelpWindow(%22PLAT154.html%22)) The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree

[PLAT301\_ALERT\_3\_G](javascript:makeHelpWindow(%22PLAT301.html%22)) Main Residue Disorder ..............(Resd 1 ) 5% Note

[PLAT793\_ALERT\_4\_G](javascript:makeHelpWindow(%22PLAT793.html%22)) Model has Chirality at C3 (Centro SPGR) R Verify

[PLAT793\_ALERT\_4\_G](javascript:makeHelpWindow(%22PLAT793.html%22)) Model has Chirality at C15 (Centro SPGR) R Verify

[PLAT860\_ALERT\_3\_G](javascript:makeHelpWindow(%22PLAT860.html%22)) Number of Least-Squares Restraints ............. 1 Note

[PLAT883\_ALERT\_1\_G](javascript:makeHelpWindow(%22PLAT883.html%22)) No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

[PLAT910\_ALERT\_3\_G](javascript:makeHelpWindow(%22PLAT910.html%22)) Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

[PLAT992\_ALERT\_5\_G](javascript:makeHelpWindow(%22PLAT992.html%22)) Repd & Actual \_reflns\_number\_gt Values Differ by 1 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

12 ALERT type 2 Indicator that the structure model may be wrong or deficient

8 ALERT type 3 Indicator that the structure quality may be low

4 ALERT type 4 Improvement, methodology, query or suggestion

1 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](http://journals.iucr.org/services/cif/checking/checkform.html) 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 22/12/2019; check.def file version of 13/12/2019**

|  |
| --- |
| **Datablock MB1** - ellipsoid plot |
| http://checkcif.iucr.org/M6MImYCLT4lrO/010620104816162747000/platon_MB1te.gif |