Supplementary Material

Synthesis, Characterization, Crystal structure and Molecular docking studies of a S-methyl-dithiocarbazate derivative: Bis[2-hydroxy benzylidene hydrazono)-(methylthio)-methyl]disulphide

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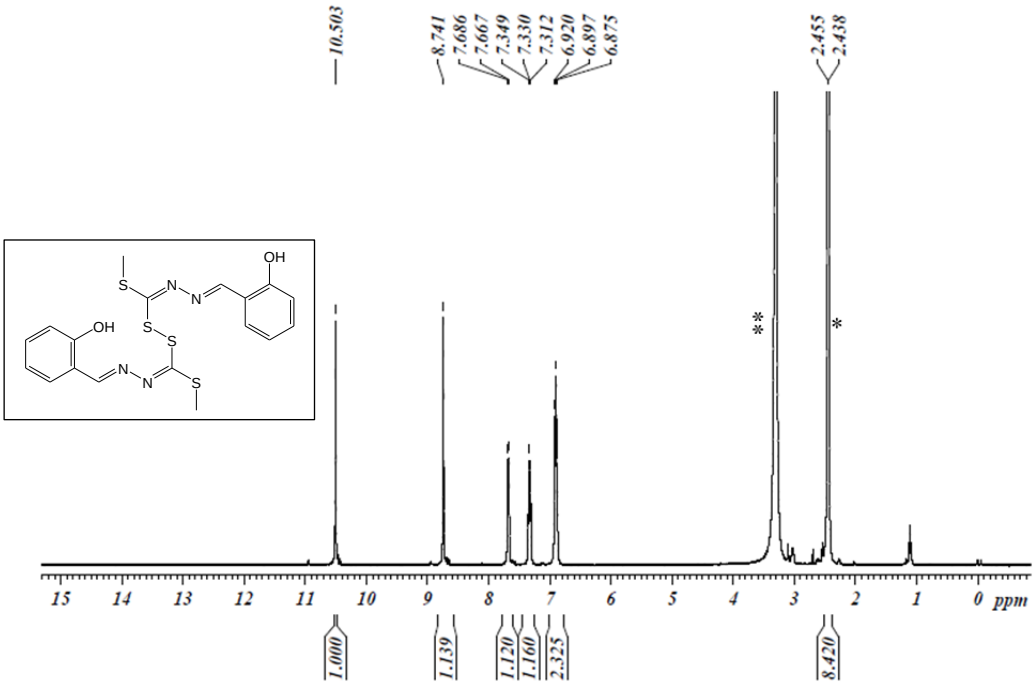

Figure S1. ^{1}H NMR of **1**, recorded in d-DMSO (∗ S-CH_3 + DMSO; ∗∗ residual water resonances)

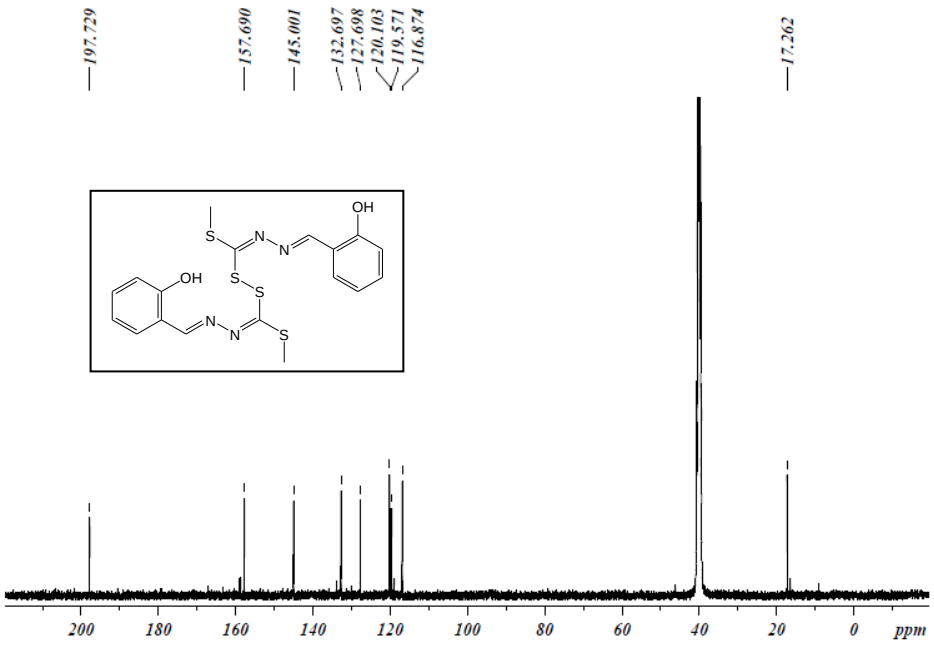

Figure S2. ^{13}C NMR of **1**, recorded in d-DMSO

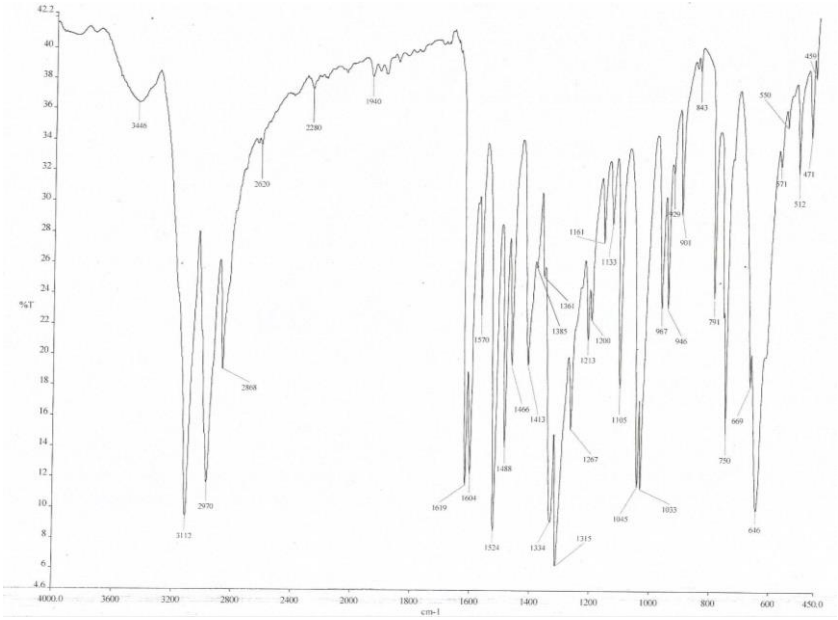

Figure S3. IR Spectra of compound **1**.

Crystallographic information:

The crystallographic information file (abbreviated CIF) loading the data sets for the compound **1** has been deposited with the Cambridge Structural Data Base, under deposit codes CCDC 1545242 (copies of these data may be obtained free of charge from The Director, CCDC,12 Union Road, Cambridge CB2 1EZ, UK, Fax: ± 44 1223 336033; Email: deposit@ccdc.cam.ac.uk or http://www.ccdc.ac.uk).

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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 = 0.0035 A          Wavelength=0.71073

Cell:            a=12.4489(8)    b=14.0742(9)       c=12.0688(8)
                 alpha=90        beta=93.403(5)     gamma=90
Temperature:     293 K

                Calculated                Reported
Volume          2110.8(2)                 2110.8(2)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H18 N4 O2 S4          ?
Sum formula     C18 H18 N4 O2 S4          C18 H18 N4 O2 S4
Mr              450.60                    450.60
Dx,g cm-3       1.418                     1.418
Z               4                         4
Mu (mm-1)       0.472                     0.472
F000            936.0                     936.0
F000'           938.26
h,k,lmax        16,19,16                  16,18,16
Nref            5611                      4803
Tmin,Tmax       0.860,0.876
Tmin'           0.860

Correction method= Not given

Data completeness= 0.856          Theta(max)= 29.007

R(reflections)= 0.0456( 3423)     wR2(reflections)= 0.1134( 4803)

S = 1.017                 Npar= 253
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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

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H9A    ..  H10B    ..       2.12 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.374 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)          7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        15 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  S4     ..  C14     ..      3.28 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       776 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.        2 Note
```

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 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 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 24/11/2016; check.def file version of 23/11/2016

Datablock shelx - ellipsoid plot

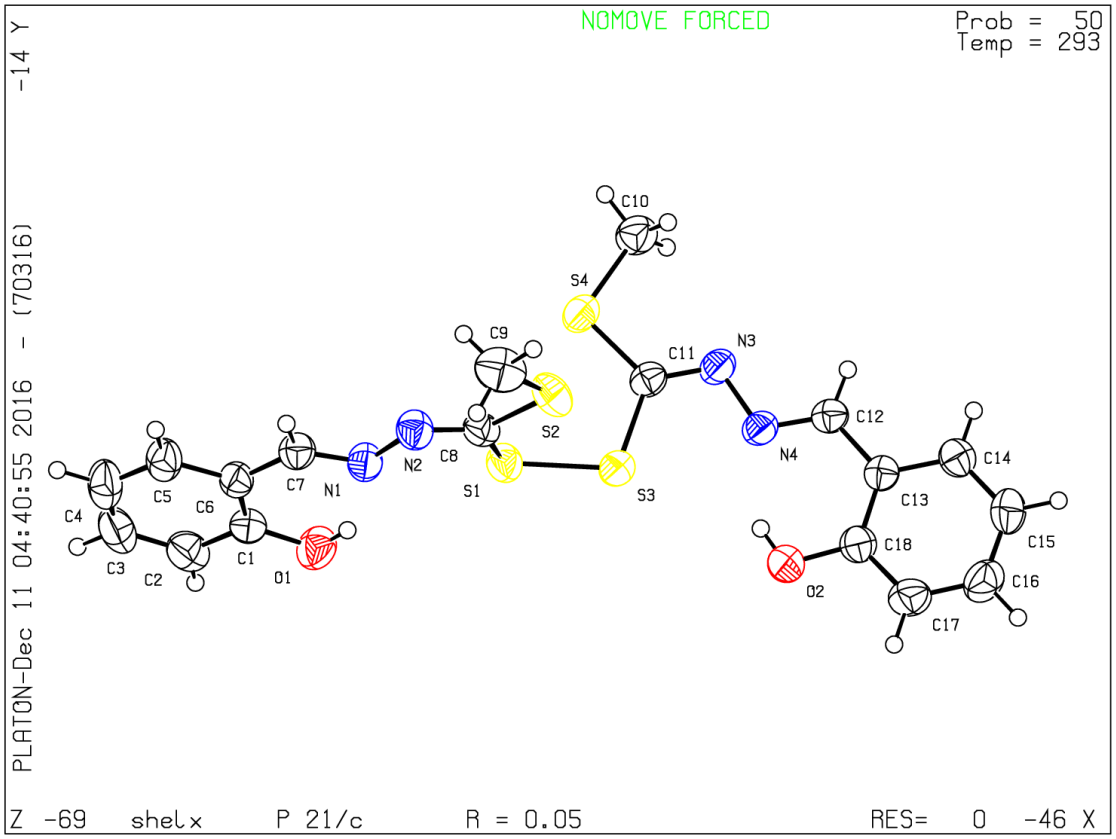

Table S1 Selected bond lengths (Å) and bond angles (°) for compound **1**.

Bond length		**Bond angles**	
S1-C8	1.786(2)	C8-S1-S3	104.63(8)
S1-S3	2.039(9)	C11-S4-C10	101.44(12)
S4-C11	1.737(8)	C11-S3-S1	105.80(8)
S4-C10	1.793(3)	C8-S2-C9	99.84(13)
S3-C11	1.793(2)	C12-N4-N3	114.59(18)
S2-C8	1.737(2)	C11-N3-N4	111.83(18)
S2-C9	1.789(3)	C14-C13-C12	119.8(2)
N4-C12	1.281(3)	C18-C13-C12	121.9(2)
N4-N3	1.408(2)	N4-C12-C13	121.8(2)
N3-C11	1.278(3)	N2-C8-S2	121.11(19)
O1-C1	1.355(3)	N2-C8-S1	120.80(17)
O2-C18	1.351(3)	S2-C8-S1	118.07(14)
C13-C12	1.451(3)	C8-N2-N1	113.6(2)
C8-N2	1.273(3)	C5-C6-C7	119.1(2)
N2-N1	1.406(3)	C1-C6-C7	122.0(2)
C6-C7	1.449(3)	C7-N1-N2	113.2(2)
N1-C7	1.280(3)	O2-C18-C17	117.9(2)
		O2-C18-C13	122.2(2)
		N1-C7-C6	122.7(2)
		N3-C11-S4	123.25(18)
		N3-C11-S3	119.65(17)
		S4-C11-S3	117.07(13)
		O1-C1-C2	118.1(2)
		O1-C1-C6	122.1(2)
		Torsion angles (°)	
		N2-C8-S1-S3	−169.5 (2)
		C8-S1-S3-C11	−89.0 (1)
		S1-S3-C11-S4	1.4 (1)
		S1-S3-C11-N3	179.9 (2)
		S2-C8-S1-S3	11.9 (1)