SUPPLEMENTARY INFORMATION

Synthesis, characterisation, X-ray diffraction and biological evaluation of new thiourea derivatives against *Mycobacterium tuberculosis and* cervical cancer

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Table S1: Bond lengths [Å] and angles [°] for compound **TU1**.

Bond lengths [Å]		**Bond angles [°]**	
S(1)-C(2)	1.680(2)	C(2)-N(1)-C(3)	122.16(17)
O(1)-C(1)	1.216(2)	C(2)-N(1)-C(4)	120.54(16)
N(1)-C(2)	1.331(2)	C(3)-N(1)-C(4)	116.84(16)
N(1)-C(3)	1.465(3)	C(11)-C(10)-C(15)	119.88(18)
N(1)-C(4)	1.481(2)	C(11)-C(10)-C(1)	119.14(17)
C(10)-C(11)	1.393(3)	C(15)-C(10)-C(1)	120.96(17)
C(10)-C(15)	1.392(3)	N(1)-C(4)-C(5)	111.24(16)
C(10)-C(1)	1.494(3)	N(1)-C(4)-C(9)	110.87(16)
C(4)-C(5)	1.521(3)	C(5)-C(4)-C(9)	111.84(17)
C(4)-C(9)	1.522(3)	C(14)-C(15)-C(10)	119.74(19)
C(15)-C(14)	1.388(3)	C(13)-C(12)-C(11)	120.3(2)
C(12)-C(13)	1.383(3)	C(13)-C(14)-C(15)	120.2(2)
C(12)-C(11)	1.386(3)	C(12)-C(13)-C(14)	120.01(19)
C(14)-C(13)	1.385(3)	C(4)-C(5)-C(6)	110.26(18)
C(5)-C(6)	1.528(3)	C(12)-C(11)-C(10)	119.81(19)
C(9)-C(8)	1.534(3)	C(4)-C(9)-C(8)	110.17(17)
C(8)-C(7)	1.518(4)	C(7)-C(8)-C(9)	111.52(19)
C(6)-C(7)	1.519(4)	C(7)-C(6)-C(5)	111.2(2)
C(1)-N(2)	1.388(2)	C(8)-C(7)-C(6)	111.02(19)
C(2)-N(2)	1.401(2)	O(1)-C(1)-N(2)	123.78(18)

Table S2: Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$) for compound **TU1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1862(1)	3623(1)	4873(1)	28(1)
O(1)	1699(3)	4555(1)	6973(1)	31(1)
N(1)	4607(3)	3381(1)	6055(1)	26(1)
C(10)	1631(4)	6241(1)	6616(1)	23(1)
C(4)	4894(4)	2317(1)	5902(1)	25(1)
C(15)	3124(4)	6928(2)	6328(1)	28(1)
C(12)	-574(4)	7569(2)	7097(1)	33(1)
C(14)	2771(4)	7932(2)	6433(1)	33(1)
C(13)	915(4)	8252(2)	6813(1)	33(1)
C(5)	7238(4)	2124(2)	5569(1)	35(1)
C(11)	-205(4)	6564(2)	7009(1)	29(1)
C(9)	4724(4)	1692(2)	6543(1)	32(1)
C(8)	4991(5)	592(2)	6373(1)	39(1)
C(6)	7467(5)	1025(2)	5402(1)	43(1)
C(7)	7321(5)	392(2)	6038(1)	44(1)
C(1)	1999(3)	5156(1)	6524(1)	24(1)
C(2)	3135(3)	3947(1)	5649(1)	23(1)
C(3)	6232(4)	3794(2)	6613(1)	36(1)
N(2)	2704(3)	4906(1)	5882(1)	26(1)

Table S3: Selected bond lengths [Å] and angles [°] for compound **TU2**.

Bond lengths [Å]		**Bond angles [°]**	
S(1)-C(2)	1.6661(13)	C(1)-N(2)-C(2)	124.22(12)
O(1)-C(1)	1.214(18)	C(2)-N(1)-C(9)	120.30(11)
N(2)-C(1)	1.389(17)	C(4)-C(3)-C(8)	120.81(13)
N(2)-C(2)	1.395(16)	C(4)-C(3)-N(1)	120.31(13)
O(3)-N(3)	1.221(18)	C(8)-C(3)-N(1)	118.81(13)
N(1)-C(2)	1.349(17)	C(9)-C(14)-C(13)	119.18(15)
N(1)-C(9)	1.447(16)	N(1)-C(2)-N(2)	116.00(11)
N(1)-C(3)	1.448(17)	N(1)-C(2)-S(1)	123.60(10)
O(2)-N(3)	1.226(16)	N(2)-C(2)-S(1)	129.35(10)
N(3)-C(18)	1.474(17)	N(2)-C(1)-C(15)	114.92(12)
C(15)-C(20)	1.389(2)	C(17)-C(18)-C(19)	122.94(13)
C(15)-C(16)	1.397(18)	C(17)-C(18)-N(3)	118.78(12)
C(15)-C(1)	1.496(18)	C(19)-C(18)-N(3)	118.28(13)
C(20)-C(19)	1.389(19)	C(18)-C(19)-C(20)	118.43(14)
C(9)-C(10)	1.380(2)	C(18)-C(17)-C(16)	118.06(12)
C(9)-C(14)	1.387(2)	C(17)-C(16)-C(15)	120.32(14)
C(3)-C(4)	1.382(2)	C(9)-C(10)-C(11)	118.89(14)
C(3)-C(8)	1.386(2)	C(3)-C(4)-C(5)	119.29(15)
C(14)-C(13)	1.388(2)	C(12)-C(13)-C(14)	120.07(14)
C(18)-C(17)	1.380(2)	C(3)-C(8)-C(7)	119.17(16)
C(17-C(16)	1.389(19)	C(13)-C(12)-C(11)	120.30(14)
C(10)-C(11)	1.392(2)	C(6)-C(7)-C(8)	120.44(15)
C(4)-C(5)	1.389(2)	C(6)-C(5)-C(4)	120.16(16)
C(13)-C(12)	1.379(3)	C(12)-C(11)-C(10)	120.28(16)
C(8)-C(7)	1.388(2)	C(7)-C(6)-C(5)	120.06(15)

Table S4: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **TU2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	2408(1)	3652(1)	5240(1)	24(1)
O(1)	4979(2)	5989(1)	2647(1)	24(1)
N(2)	2106(2)	5091(1)	3587(1)	20(1)
O(3)	-3087(2)	9595(1)	1054(1)	37(1)
N(1)	4208(2)	3222(1)	3291(1)	20(1)
O(2)	-633(2)	10965(1)	923(1)	39(1)
N(3)	-1408(2)	9883(1)	1162(1)	26(1)
C(15)	1895(2)	7009(1)	2480(1)	18(1)
C(20)	-10(2)	6715(1)	2335(1)	20(1)
C(9)	5468(2)	2211(1)	3630(1)	20(1)
C(1)	3164(2)	6006(1)	2901(1)	19(1)
C(3)	4258(2)	3265(1)	2197(1)	21(1)
C(14)	5050(2)	880(1)	3509(1)	24(1)
C(2)	2976(2)	3991(1)	3985(1)	19(1)
C(18)	-229(2)	8874(1)	1603(1)	21(1)
C(19)	-1092(2)	7653(1)	1889(1)	22(1)
C(17)	1673(2)	9190(1)	1722(1)	23(1)
C(16)	2743(2)	8241(1)	2165(1)	22(1)
C(10)	7116(2)	2579(2)	4011(1)	28(1)
C(4)	2505(2)	3170(1)	1834(1)	26(1)
C(13)	6315(3)	-97(2)	3777(1)	29(1)
C(8)	6097(2)	3339(2)	1522(1)	28(1)

C(12)	7989(3)	260(2)	4138(1)	32(1)
C(7)	6161(3)	3349(2)	471(1)	33(1)
N				
C(11)	8387(3)	1588(2)	4262(1)	34(1)
C(6)	4418(3)	3308(2)	103(1)	33(1)

Table S5: Selected bond lengths [Å] and angles [°] for compound **TU6**.

Bond lengths [Å]		**Bond angles [°]**	
S(1)-C(2)	1.677(11)	C(2)-N(1)-C(3)	122.65(10)
O(1)-C(1)	1.218(14)	C(2)-N(1)-C(4)	120.49(9)
N(1)-C(2)	1.328(14)	C(3)-N(1)-C(4)	116.71(9)
N(1)-C(3)	1.468(14)	C(1)-N(2)-C(2)	124.91(10)
N(1)-C(4)	1.480(14)	O(1)-C(1)-N(2)	121.75(11)
N(2)-C(1)	1.385(14)	O(1)-C(1)-C(10)	123.51(10)
N(2)-C(2)	1.405(14)	N(2)-C(1)-C(10)	144.72(9)
C(1)-C(10)	1.494(16)	C(11)-C(10)-C(15)	119.96(11)
C(10)-C(11)	1.401(16)	C(11)-C(10)-C(1)	119.63(10)
C(10)-C(15)	1.410(15)	C(15)-C(10)-C(1)	120.29(10)
C(4)-C(9)	1.522(16)	N(1)-C(4)-C(1)	110.69(9)
C(4)-C(5)	1.527(15)	N(1)-C(4)-C(9)	111.27(9)
C(11)-C(12)	1.385(18)	C(9)-C(4)-C(5)	111.96(10)
C(15)-C(14)	1.393(17)	N(1)-C(2)-N(2)	116.51(10)
C(15)-C(16)	1.508(17)	N(1)-C(2)-S(1)	125.90(9)
C(9)-C(8)	1.528(16)	N(2)-C(2)-S(1)	117.58(8)
C(14)-C(13)	1.386(19)	C(12)-C(11)-C(10)	120.97(11)
C(8)-C(7)	1.522(18)	C(14)-C(15)-C(10)	117.68(11)
C(5)-C(6)	1.529(17)	C(14)-C(15)-C(16)	119.08(11)
C(7)-C(6)	1.523(19)	C(10)-C(15)-C(16)	123.24(11)
C(12)-C(13)	1.382(19)	C(4)-C(9)-C(8)	109.97(9)

Table S6: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **TU6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	7673(1)	4869(1)	5812(1)	26(1)
O(1)	6419(1)	3147(1)	6102(1)	31(1)
N(1)	6344(1)	4018(1)	3660(1)	22(1)
N(2)	5336(1)	4060(1)	5776(1)	23(1)
C(1)	5431(2)	3504(1)	6340(1)	22(1)
C(10)	4201(2)	3379(1)	7208(1)	21(1)
C(4)	7598(2)	4179(1)	2864(1)	22(1)
C(2)	6428(2)	4285(1)	5000(1)	21(1)
C(11)	2542(2)	3673(1)	6774(1)	26(1)
C(15)	4648(2)	2942(1)	8389(1)	23(1)
C(9)	8462(2)	3649(1)	2469(1)	25(1)
C(14)	3374(2)	2811(1)	9057(2)	30(1)
C(16)	6430(2)	2619(1)	8964(2)	30(1)
C(3)	4948(2)	3587(1)	2833(2)	30(1)
C(8)	9790(2)	3824(1)	1689(2)	28(1)
C(5)	6633(2)	4549(1)	1365(2)	30(1)
C(7)	8844(2)	4188(1)	183(2)	33(1)
C(6)	7966(2)	4715(1)	580(2)	33(1)

C(12)	1297(2)	3530(1)	7450(2)	32(1)
C(13)	1714(2)	3094(1)	8584(2)	33(1)

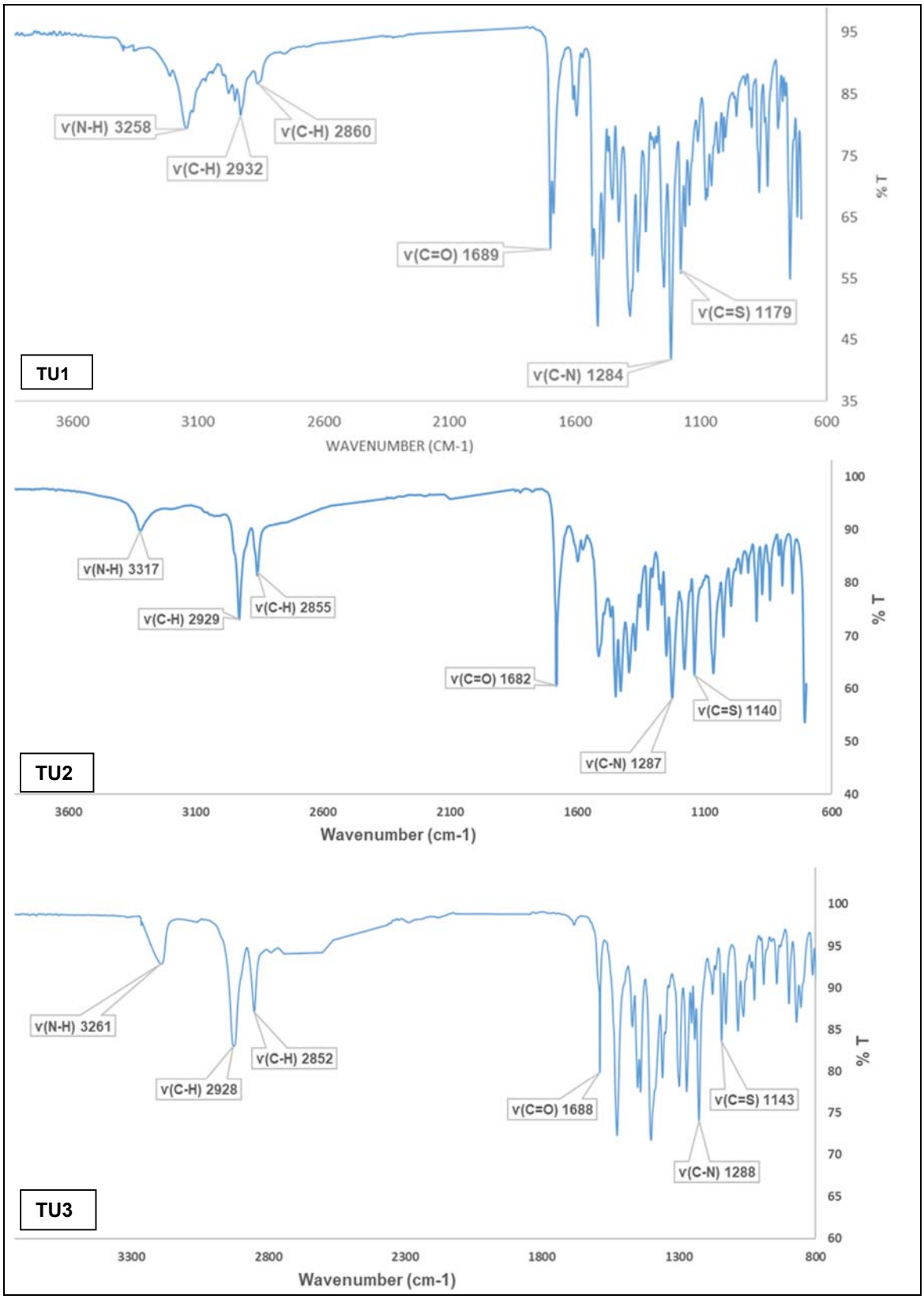

Figure S1: IR spectra for compound **TU1** - **TU3**

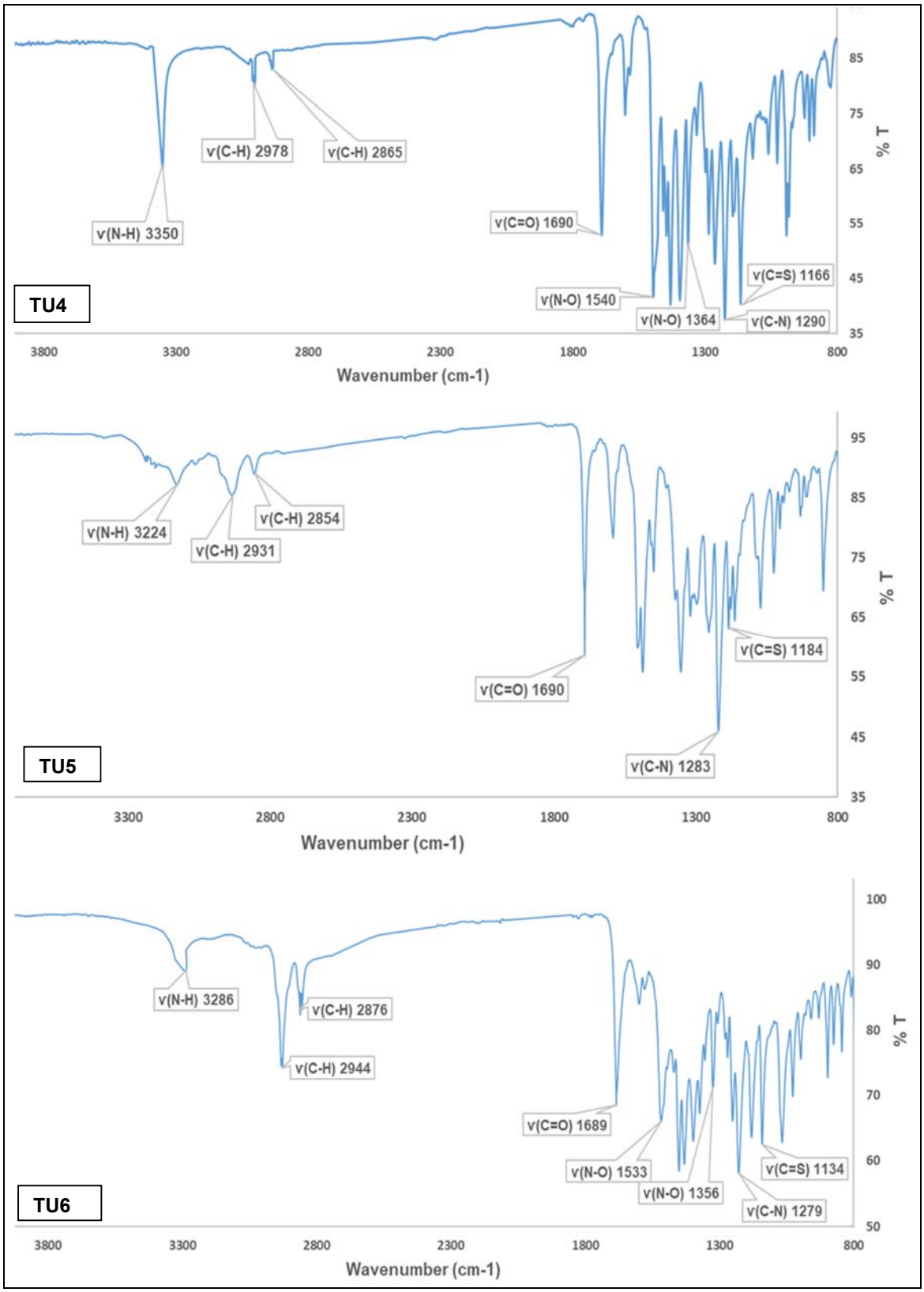

Figure S2: IR spectra for compound **TU4** - **TU6**

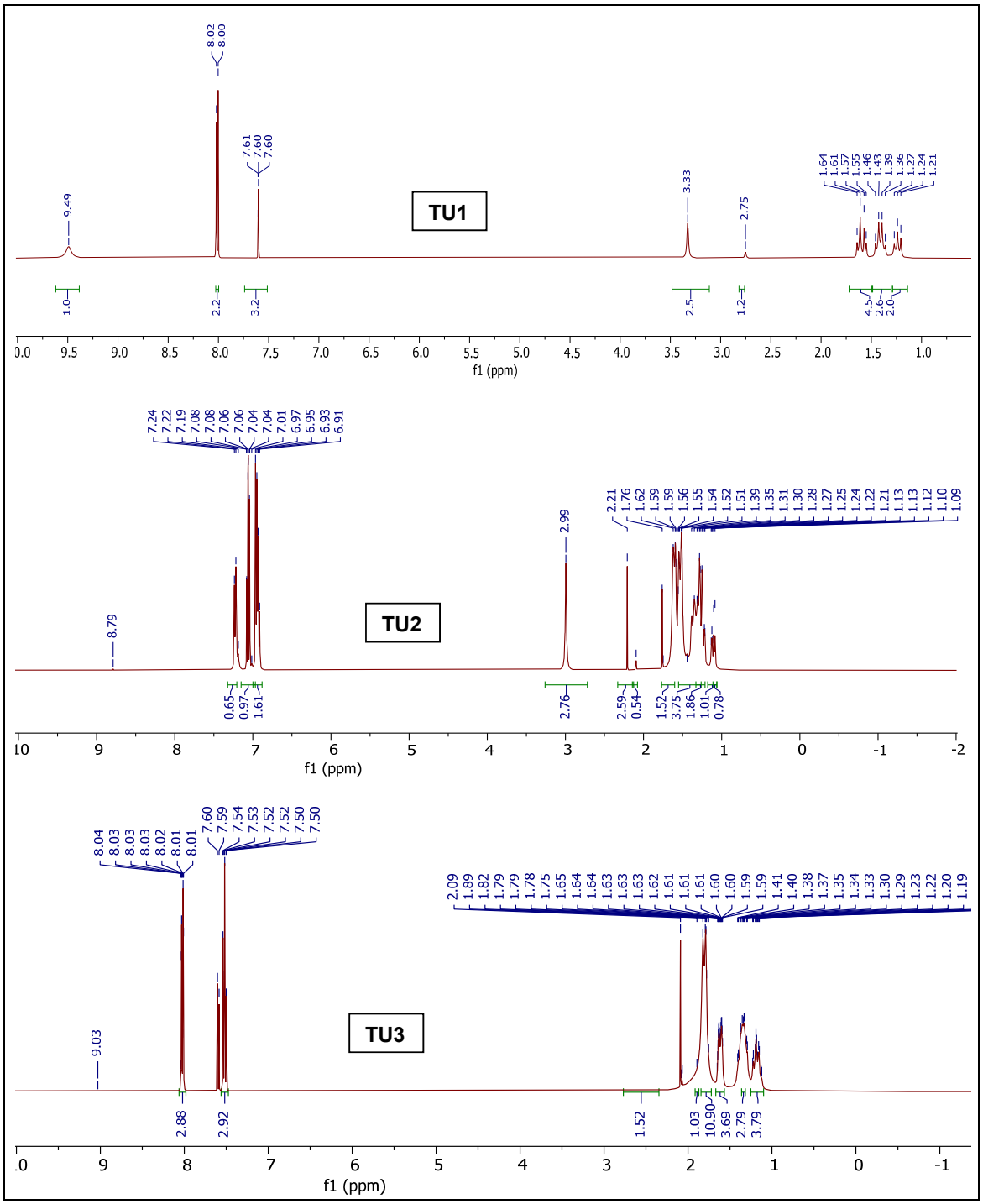

Figure S3: ^{1}H NMR for compounds **TU1** - **TU3**

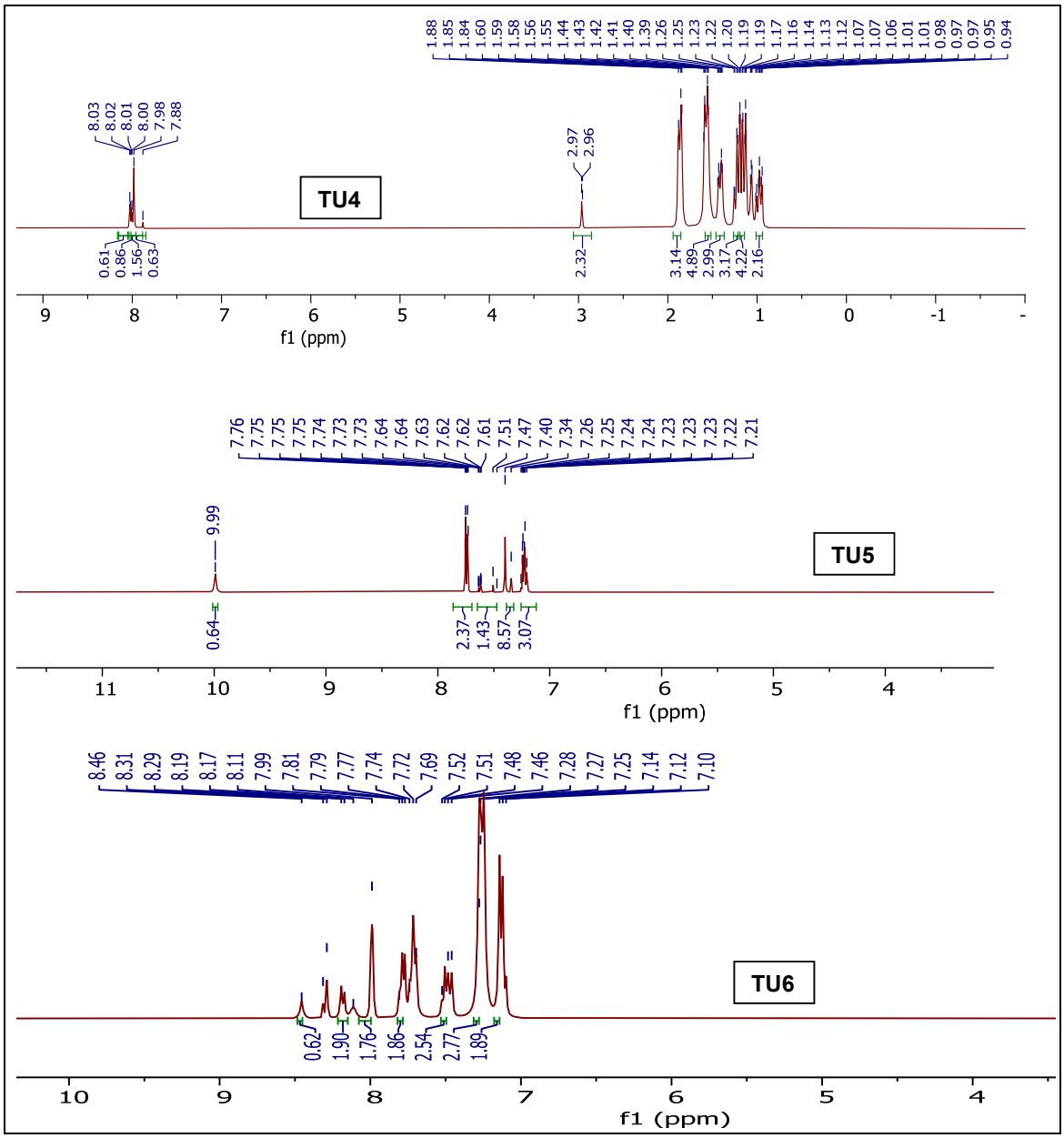

Figure S4: ^{1}H NMR for compounds **TU4** - **TU6**

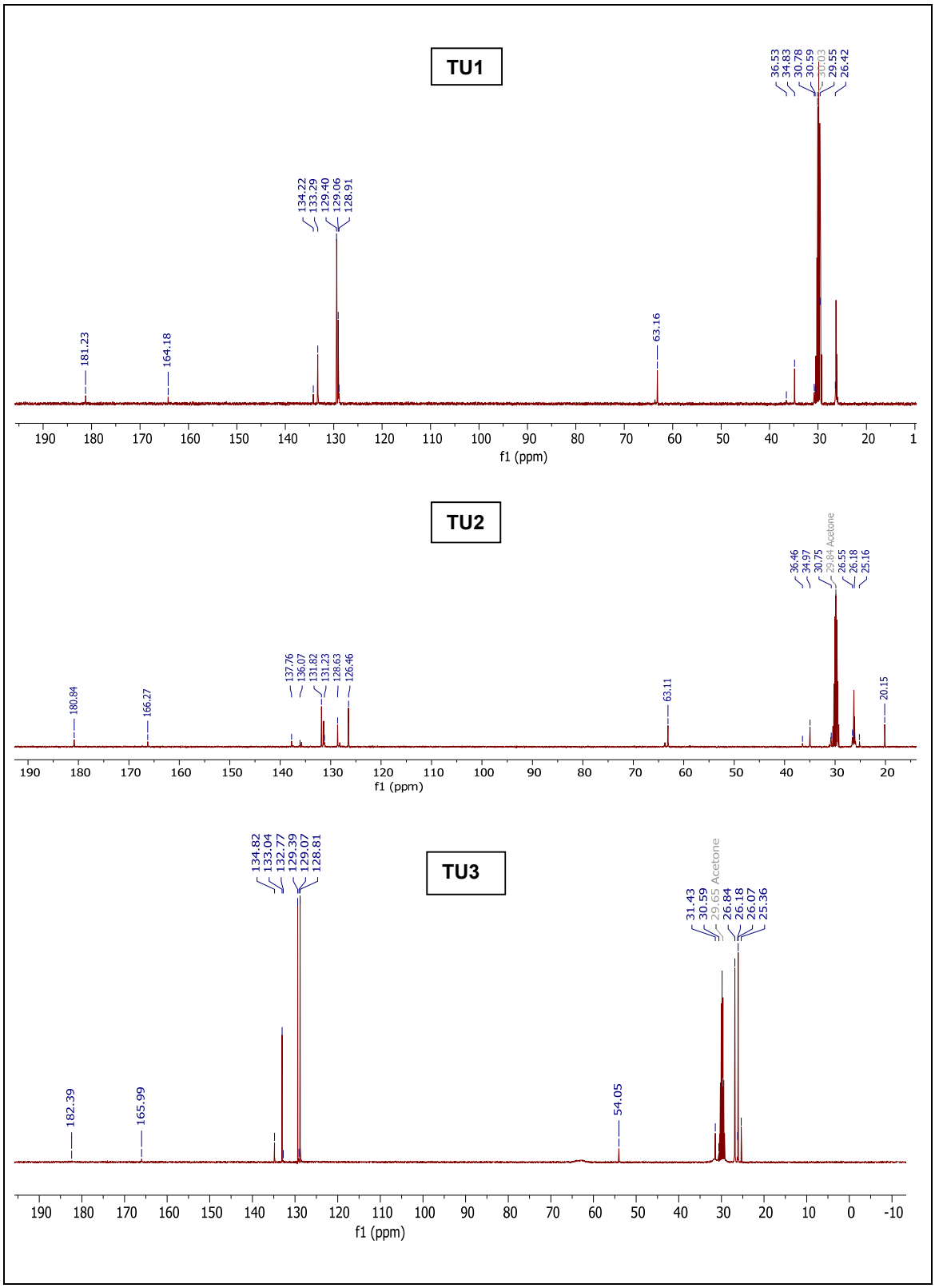

Figure S5: ^{13}C NMR for compound **TU1** - **TU3**

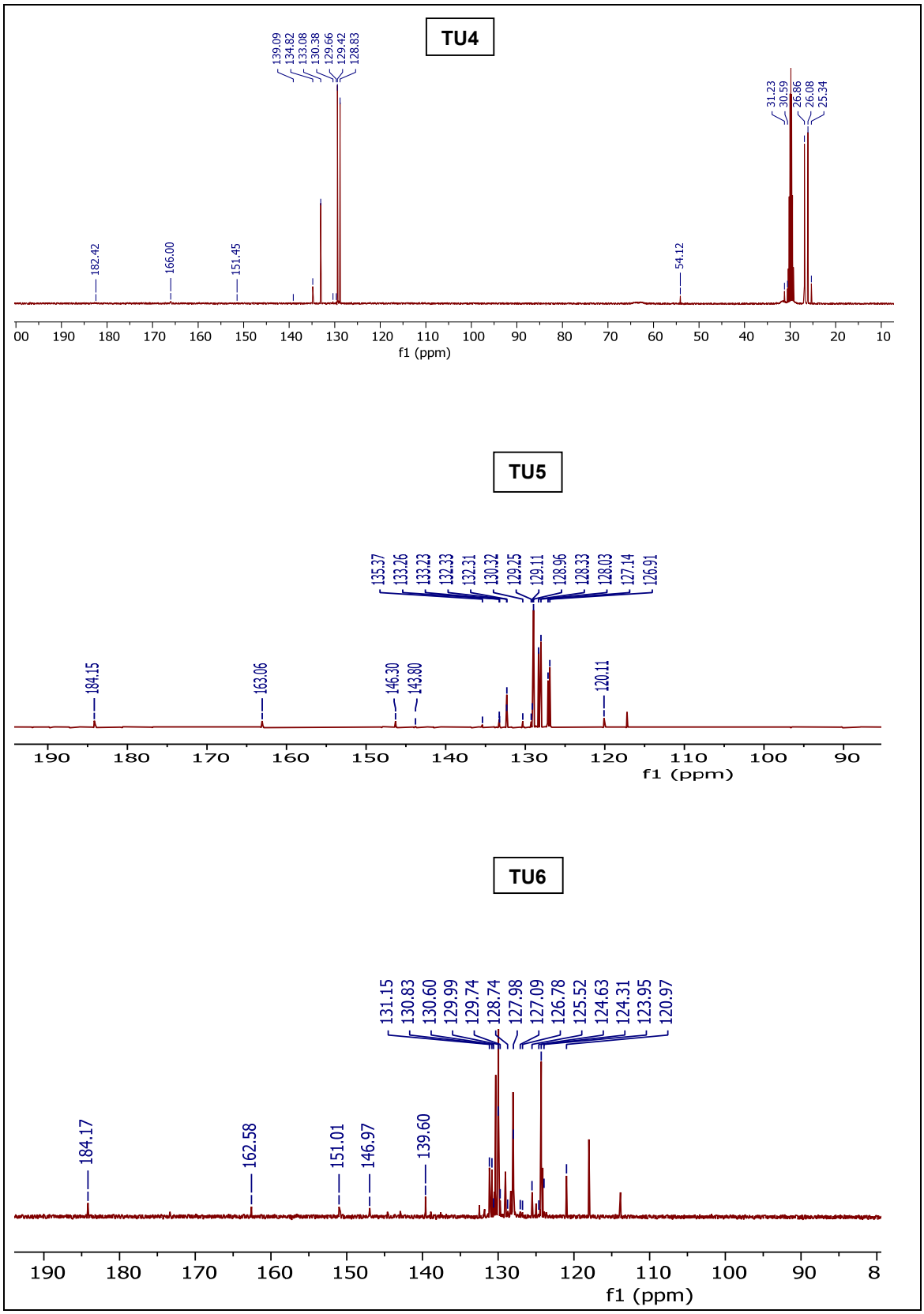

Figure S6: ^{13}C NMR for compound **TU4** - **TU6**

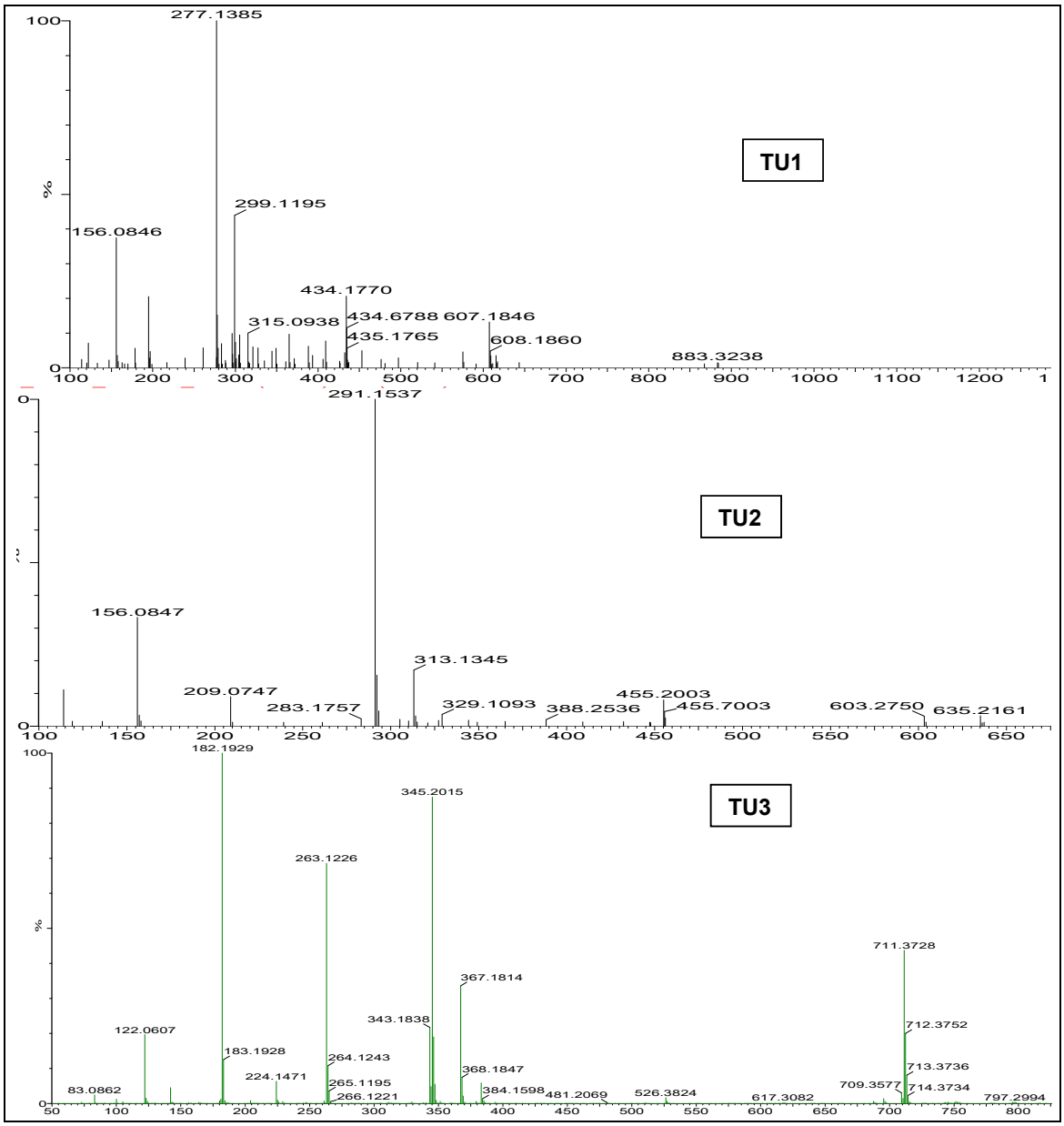

Figure S7: MS for compound **TU1** - **TU3.**

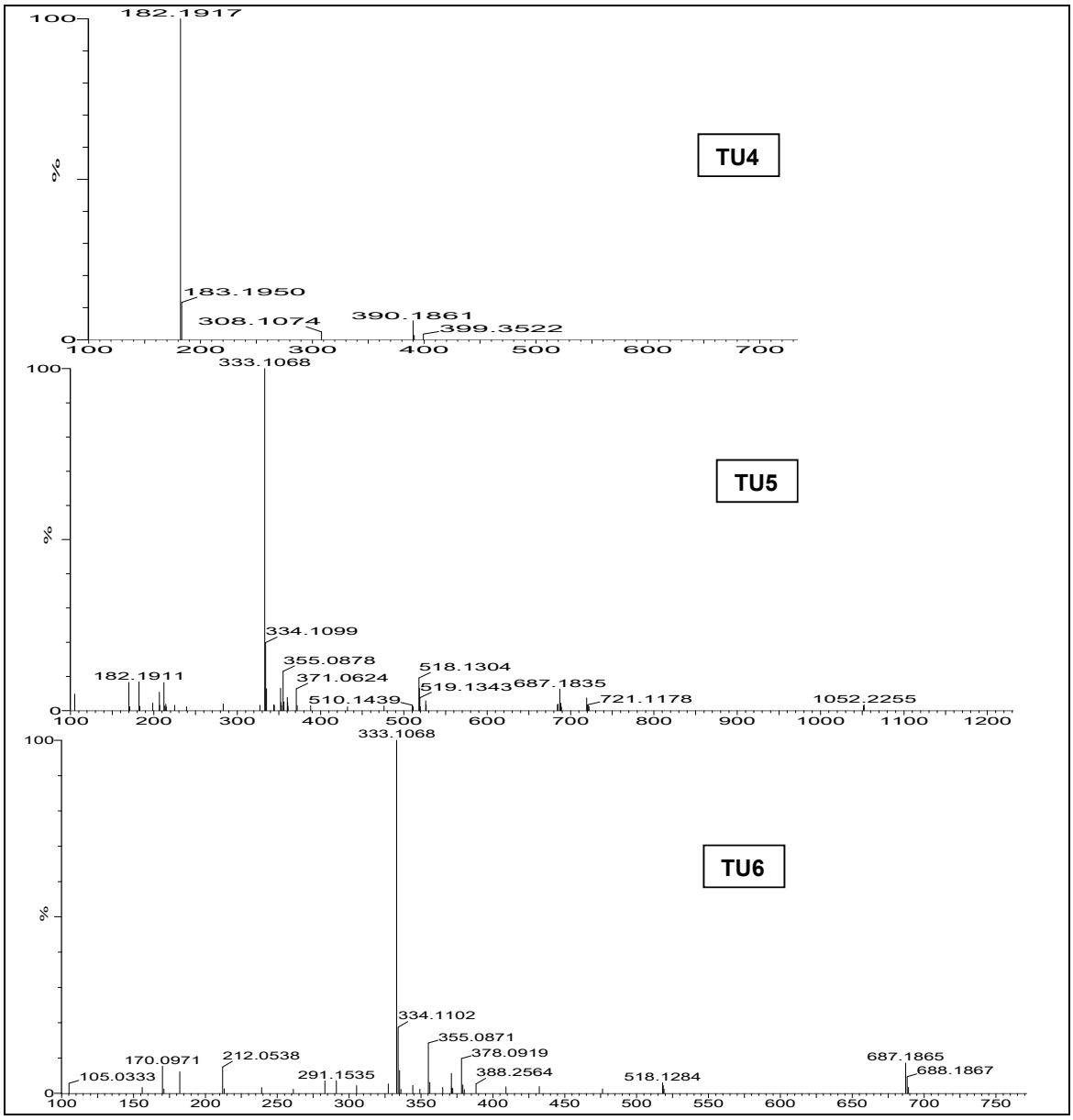

Figure S8: MS for compound **TU4 - TU6.**

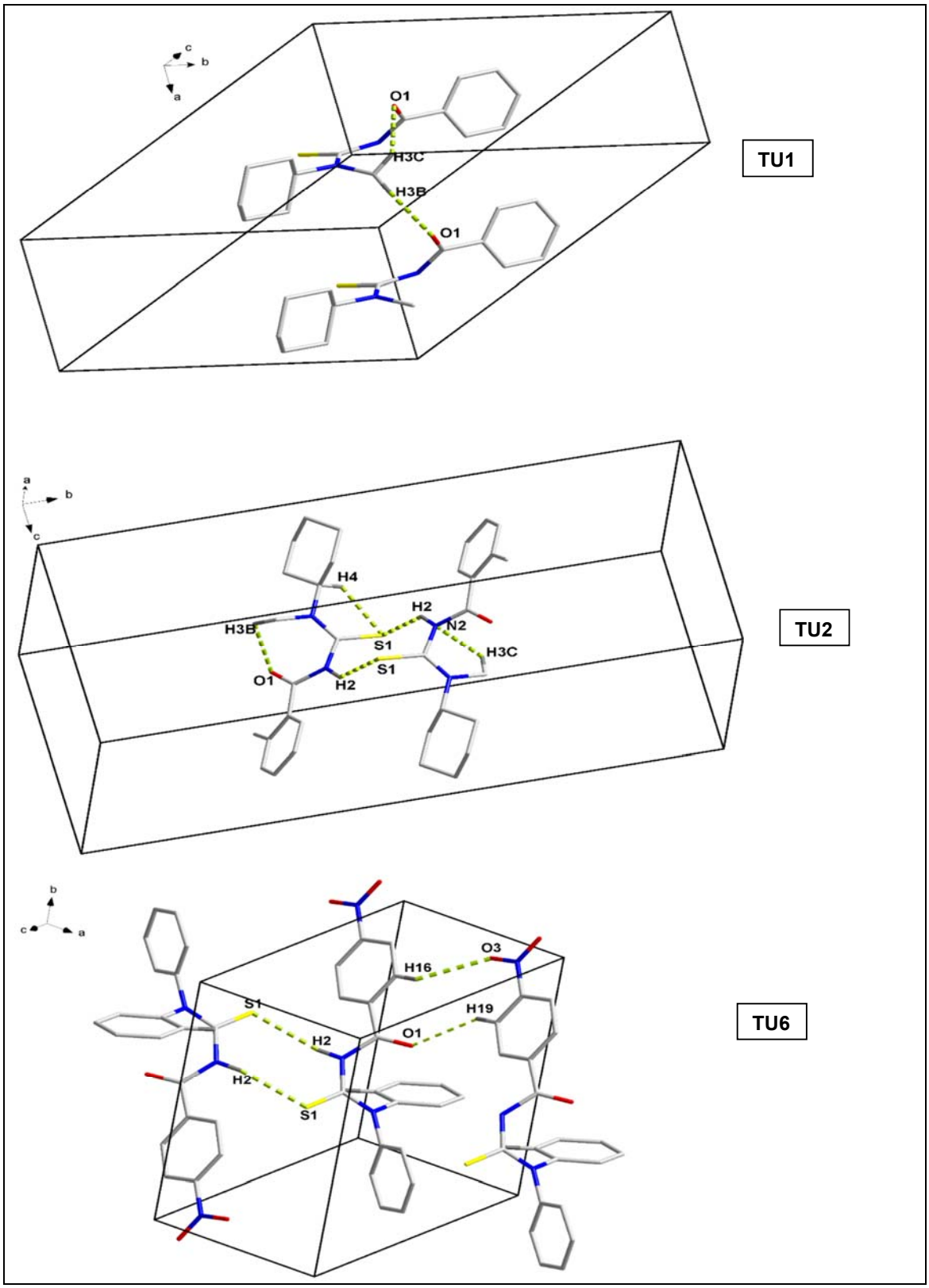

Figure S9: Hydrogen bond interactions (indicated in green dashed lines) for compound **TU1, TU2** and **TU6**.

N-(cyclohexyl(methyl)carbomothioyl) benzamide for (**TU1**)

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Structure factors have been supplied for datablock(s) am105_lt_auto

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Temperature:      150 K

                 Calculated                Reported
Volume           1457.86(4)                1457.86(4)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C15 H20 N2 O S            C15 H20 N2 O S
Sum formula      C15 H20 N2 O S            C15 H20 N2 O S
Mr               276.39                    276.39
Dx,g cm-3        1.259                     1.255
Z                4                         4
Mu (mm-1)        1.916                     1.915
F000             592.0                     588.0
F000'            594.77
h,k,lmax         7,17,24                   7,16,24
Nref             3136                      3043
Tmin,Tmax        0.672,0.713               0.387,1.000
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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

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    S1       --C2       .        6.0 s.u.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2       --H2       .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.152 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          4 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From N2      .      -0.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2        .      -0.38 eA-3
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         76 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          5 Note
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by .          1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         10 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 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
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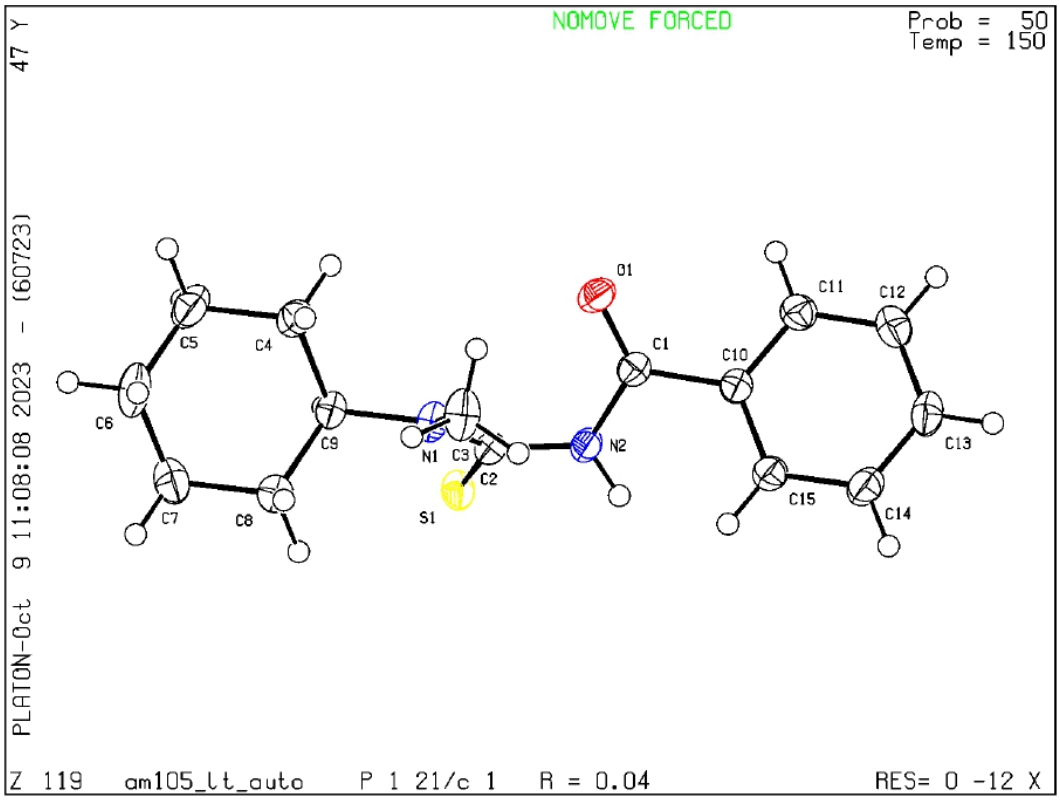

N-(cyclohexyl(methyl)carbomothioyl)-2-methylbenzamide (**TU2**)

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Datablock: shelx

```
Bond precision:   C-C = 0.0019 A           Wavelength=0.71073

Cell:             a=7.9426(3)     b=23.3394(5)          c=8.9398(3)
                  alpha=90        beta=112.789(4)       gamma=90
Temperature:      150 K

                 Calculated                Reported
Volume           1527.85(10)               1527.85(9)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C16 H22 N2 O S            C16 H22 N2 O S
Sum formula      C16 H22 N2 O S            C16 H22 N2 O S
Mr               290.42                    290.42
Dx,g cm-3        1.263                     1.262
Z                4                         4
Mu (mm-1)        0.210                     0.210
F000             624.0                     624.0
F000'            624.70
h,k,lmax         11,33,12                  10,33,12
Nref             4768                      4025
Tmin,Tmax        0.933,0.959               0.460,1.000
Tmin'            0.922

Correction method= # Reported T Limits: Tmin=0.460 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.844           Theta(max)= 30.752

R(reflections)= 0.0351( 3518)                    wR2(reflections)=
                                                 0.0909( 4025)
S = 1.054                 Npar= 183
```

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

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    S1       --C2       .        5.2 s.u.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H2       ..H11      .       1.97 Ang.
                                                   x,y,z  =      1_555 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.96Ang From N2      .      -0.41 eA-3
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          1 Report
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        698 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         13 Info
```

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

   1 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
   1 ALERT type 3 Indicator that the structure quality may be low
   2 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

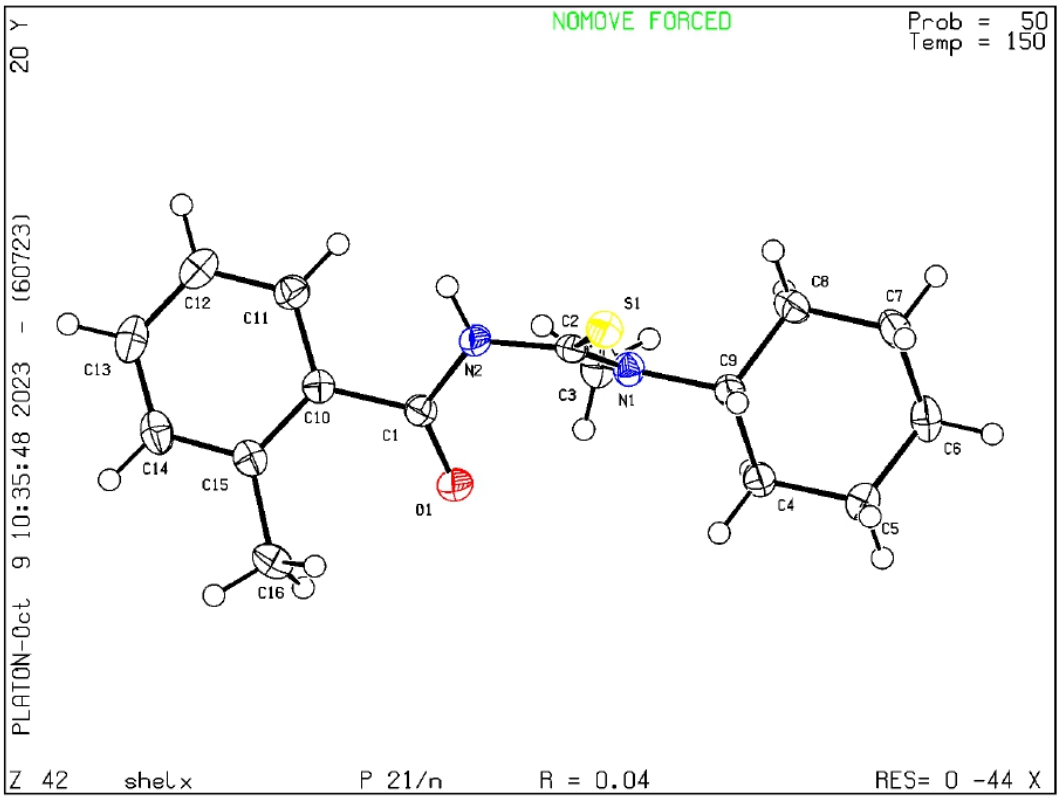
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 06/07/2023; check.def file version of 30/06/2023

Datablock shelx - ellipsoid plot



N-(diphenylcarbamothioyl)-4-nitrobenzamide (**TU6**)

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 = 0.0021 A          Wavelength=0.71073

Cell:           a=6.8186(2)       b=10.0318(2)      c=13.2816(3)
                alpha=89.529(2)   beta=78.134(2)    gamma=89.102(2)
Temperature:    150 K

                Calculated                Reported
Volume          888.97(4)                 888.96(4)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C20 H15 N3 O3 S           C20 H15 N3 O3 S
Sum formula     C20 H15 N3 O3 S           C20 H15 N3 O3 S
Mr              377.41                    377.41
Dx,g cm-3       1.410                     1.406
Z               2                         2
Mu (mm-1)       0.209                     0.209
F000            392.0                     390.0
F000'           392.41
h,k,lmax        9,14,19                   8,13,17
Nref            5649                      4318
Tmin,Tmax       0.951,0.962               0.664,1.000
Tmin'           0.951

Correction method= # Reported T Limits: Tmin=0.664 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.764          Theta(max)= 30.941

R(reflections)= 0.0389( 3503)                    wR2(reflections)=
                                                 0.1002( 4318)
S = 1.072                 Npar= 244
```

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

```
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        40 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      1037 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.5 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.         2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.         2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        11 Info
```

```
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```

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Datablock shelx - ellipsoid plot