Supplementary material for publication on line

New application of 1,2,4-triazole derivatives as antitubercular agents. Structure, in vitro screening and docking studies.

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X-ray structure determination

CIF for C1

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_shelx_space_group_comment
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The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
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CrysAlisPro, Agilent Technologies,
Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb 9 2015,16:26:32)
Empirical absorption correction using spherical harmonics,
implemented in SCALE3 ABSPACK scaling algorithm.
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systematic absences.

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Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
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C45 C44 H44 119.6 . . ?
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UNIT 26 18 8 2 2
MERG 2
FMAP 2
PLAN -2
ACTA
BOND $H
CONF
L.S. 40
WGHT 0.069800 0.199700
FVAR 3.49246
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N4    3    0.706198    0.103198    0.796261   11.00000    0.04626    0.04200 =
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C3    1    0.578480    0.211067    0.847799   11.00000    0.04933    0.04307 =
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C5    1    0.839460    0.045242    0.861251   11.00000    0.04872    0.04419 =
      0.03475   -0.01199   -0.01596    0.00125
C41   1    0.698826    0.038488    0.701409   11.00000    0.04342    0.04316 =
      0.03708   -0.01593   -0.01783    0.00519
C42   1    0.784935    0.137151    0.586726   11.00000    0.04326    0.04699 =
      0.04447   -0.01733   -0.01788    0.00195
C43   1    0.786498    0.076002    0.494457   11.00000    0.05178    0.07646 =
      0.04378   -0.02492   -0.01922    0.00999
AFIX  43
H43   2    0.843831    0.146004    0.417109   11.00000   -1.50000
AFIX   0
C44   1    0.701230   -0.091247    0.519222   11.00000    0.06868    0.07558 =
      0.06622   -0.04337   -0.03725    0.01883
AFIX  43
H44   2    0.700961   -0.135316    0.457875   11.00000   -1.50000
AFIX   0
C45   1    0.616026   -0.194675    0.633824   11.00000    0.08043    0.05177 =
      0.08609   -0.03173   -0.04134    0.00176
AFIX  43
H45   2    0.559036   -0.307825    0.649135   11.00000   -1.50000
AFIX   0
C46   1    0.614630   -0.131044    0.726837   11.00000    0.06452    0.04868 =
      0.05867   -0.01688   -0.02509   -0.00209
AFIX  43
H46   2    0.558361   -0.200904    0.804367   11.00000   -1.50000
AFIX   0
C61   1    0.415255    0.305046    0.806229   11.00000    0.04988    0.03930 =
      0.04744   -0.01497   -0.01579    0.00522
C63   1    0.267226    0.408015    0.658871   11.00000    0.07601    0.05880 =
      0.07765   -0.03196   -0.04471    0.02090
AFIX  43
H63   2    0.265733    0.423433    0.581719   11.00000   -1.50000
AFIX   0
C64   1    0.116059    0.473342    0.727318   11.00000    0.05924    0.04958 =
      0.08681   -0.01773   -0.03308    0.01410
AFIX  43
H64   2    0.013450    0.527918    0.698085   11.00000   -1.50000
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AFIX   0
C65   1    0.119857    0.456291    0.839576    11.00000    0.05961    0.05882 =
      0.07603   -0.01839   -0.00901    0.01785
AFIX  43
H65   2    0.021400    0.502327    0.887567    11.00000   -1.50000
AFIX   0
C66   1    0.272095    0.369626    0.881030    11.00000    0.06530    0.06014 =
      0.05142   -0.01555   -0.01259    0.01669
AFIX  43
H66   2    0.277633    0.355350    0.957347    11.00000   -1.50000
AFIX   0
HKLF    4

REM  t1 in P-1
REM R1 =  0.0559 for    2092 Fo > 4sig(Fo)  and  0.0802 for all    2845 data
REM    175 parameters refined using      0 restraints

END

WGHT      0.0651      0.2555

REM Highest difference peak  0.697,  deepest hole -0.255,  1-sigma level  0.055
Q1    1   0.3191  0.3773  0.9534  11.00000  0.05    0.20
Q2    1   0.4976  0.2649  0.8239  11.00000  0.05    0.19
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CIF for C12

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_shelx_space_group_comment
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The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
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'-x, -y, -z'
'x, -y-1/2, z-1/2'

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CrysAlisPro, Agilent Technologies,
Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb  9 2015,16:26:32)
Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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_reflns_special_details
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 Reflections were merged by SHELXL according to the crystal
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class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of unique
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Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
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SHELXL-2014/7 (Sheldrick, 2014) and WINGX (Farrugia, 2012)
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O47 O -0.0266(2) 0.99272(19) -0.14262(14) 0.0608(5) Uani 1 1 d . . . . .
N1 N 0.3579(2) 0.37414(18) 0.05440(12) 0.0333(4) Uani 1 1 d . . . . .
H1 H 0.369(3) 0.310(3) 0.0997(17) 0.050 Uiso 1 1 d . U . . .
N2 N 0.3863(2) 0.34250(17) -0.03527(12) 0.0339(4) Uani 1 1 d . . . . .
N4 N 0.27969(18) 0.54222(16) -0.02347(11) 0.0281(4) Uani 1 1 d . . . . .
N63 N 0.3873(2) 0.34019(18) -0.32216(12) 0.0375(4) Uani 1 1 d . . . . .
C3 C 0.3377(2) 0.44692(19) -0.08155(13) 0.0280(4) Uani 1 1 d . . . . .
C5 C 0.2930(2) 0.4941(2) 0.06514(14) 0.0293(4) Uani 1 1 d . . . . .
C41 C 0.2016(2) 0.6621(2) -0.05053(13) 0.0291(4) Uani 1 1 d . . . . .
C42 C 0.2628(2) 0.7883(2) -0.04163(14) 0.0345(5) Uani 1 1 d . . . . .
H42 H 0.3530 0.7971 -0.0153 0.052 Uiso 1 1 calc R U . . .
C43 C 0.1897(3) 0.9026(2) -0.07196(16) 0.0405(5) Uani 1 1 d . . . . .
H43 H 0.2306 0.9881 -0.0660 0.061 Uiso 1 1 calc R U . . .
C44 C 0.0556(3) 0.8883(2) -0.11120(16) 0.0408(6) Uani 1 1 d . . . . .
C45 C -0.0042(3) 0.7602(3) -0.11995(17) 0.0459(6) Uani 1 1 d . . . . .
H45 H -0.0940 0.7507 -0.1466 0.069 Uiso 1 1 calc R U . . .
C46 C 0.0678(2) 0.6474(2) -0.08960(16) 0.0397(5) Uani 1 1 d . . . . .
H46 H 0.0269 0.5618 -0.0953 0.060 Uiso 1 1 calc R U . . .
C48 C 0.0307(3) 1.1257(3) -0.1398(2) 0.0671(9) Uani 1 1 d . . . . .
H481 H 0.1109 1.1311 -0.1799 0.101 Uiso 1 1 calc R U . . .
H482 H 0.0607 1.1466 -0.0783 0.101 Uiso 1 1 calc R U . . .
H483 H -0.0408 1.1894 -0.1592 0.101 Uiso 1 1 calc R U . . .
C61 C 0.3524(2) 0.45924(19) -0.18097(13) 0.0280(4) Uani 1 1 d . . . . .
C62 C 0.3647(2) 0.3412(2) -0.23250(14) 0.0338(5) Uani 1 1 d . . . . .
H62 H 0.3565 0.2584 -0.2025 0.051 Uiso 1 1 calc R U . . .
C64 C 0.3957(3) 0.4603(2) -0.36444(15) 0.0404(6) Uani 1 1 d . . . . .
H64 H 0.4110 0.4612 -0.4273 0.061 Uiso 1 1 calc R U . . .
C65 C 0.3828(3) 0.5820(2) -0.32007(15) 0.0415(6) Uani 1 1 d . . . . .

H65 H 0.3886 0.6632 -0.3523 0.062 Uiso 1 1 calc R U . . .
C66 C 0.3611(3) 0.5820(2) -0.22687(15) 0.0361(5) Uani 1 1 d . . . . .
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N2 0.0459(11) 0.0290(9) 0.0269(9) 0.0028(7) 0.0043(8) 0.0035(8)
N4 0.0357(9) 0.0265(9) 0.0221(8) 0.0001(7) 0.0016(7) 0.0021(7)
N63 0.0511(12) 0.0339(10) 0.0276(9) -0.0050(8) 0.0004(8) 0.0008(9)
C3 0.0341(11) 0.0251(10) 0.0248(10) -0.0010(8) 0.0016(8) -0.0004(8)
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C41 0.0356(11) 0.0287(10) 0.0230(9) 0.0000(8) 0.0027(8) 0.0034(9)
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C45 0.0349(12) 0.0517(15) 0.0509(15) 0.0034(12) -0.0058(11) 0.0044(11)
C46 0.0358(12) 0.0388(12) 0.0445(13) -0.0012(10) -0.0012(10) -0.0034(10)
C48 0.086(2) 0.0478(17) 0.068(2) 0.0187(14) 0.0159(16) 0.0275(16)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
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 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C48 H482 0.9600 . ?
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C65 H65 0.9300 . ?
C66 H66 0.9300 . ?

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N1 N2 C3 N4 -0.1(2) . . . . ?
N1 N2 C3 C61 176.84(18) . . . . ?
C5 N4 C3 N2 0.0(2) . . . . ?
C41 N4 C3 N2 -172.29(18) . . . . ?
C5 N4 C3 C61 -176.85(19) . . . . ?
C41 N4 C3 C61 10.9(3) . . . . ?
N2 N1 C5 N4 -0.3(2) . . . . ?
N2 N1 C5 S5 179.40(16) . . . . ?
C3 N4 C5 N1 0.2(2) . . . . ?
C41 N4 C5 N1 172.53(18) . . . . ?
C3 N4 C5 S5 -179.49(16) . . . . ?
C41 N4 C5 S5 -7.1(3) . . . . ?
C3 N4 C41 C42 -107.4(2) . . . . ?
C5 N4 C41 C42 81.6(3) . . . . ?
C3 N4 C41 C46 69.4(3) . . . . ?
C5 N4 C41 C46 -101.6(2) . . . . ?
C46 C41 C42 C43 0.1(3) . . . . ?
N4 C41 C42 C43 176.85(19) . . . . ?
C41 C42 C43 C44 -0.1(3) . . . . ?
C48 O47 C44 C43 3.4(4) . . . . ?
C48 O47 C44 C45 -177.0(2) . . . . ?
C42 C43 C44 O47 179.4(2) . . . . ?
C42 C43 C44 C45 -0.1(4) . . . . ?
O47 C44 C45 C46 -179.2(2) . . . . ?
C43 C44 C45 C46 0.4(4) . . . . ?
C44 C45 C46 C41 -0.4(4) . . . . ?
C42 C41 C46 C45 0.2(3) . . . . ?
N4 C41 C46 C45 -176.6(2) . . . . ?
N2 C3 C61 C66 -151.1(2) . . . . ?
N4 C3 C61 C66 25.4(3) . . . . ?
N2 C3 C61 C62 26.0(3) . . . . ?
N4 C3 C61 C62 -157.5(2) . . . . ?
C64 N63 C62 C61 -1.4(3) . . . . ?
C66 C61 C62 N63 1.6(3) . . . . ?
C3 C61 C62 N63 -175.7(2) . . . . ?
C62 N63 C64 C65 0.3(4) . . . . ?
N63 C64 C65 C66 0.5(4) . . . . ?
C64 C65 C66 C61 -0.2(4) . . . . ?
C62 C61 C66 C65 -0.8(3) . . . . ?
C3 C61 C66 C65 176.4(2) . . . . ?

_refine_diff_density_max    0.206
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_refine_diff_density_rms    0.055
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_shelx_res_file
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    shelx.res created by SHELXL-2014/7

TITL T15 in P2(1)/c
CELL  0.71073   9.3878   9.8576  14.6003   90.000   90.586   90.000
ZERR     4.00   0.0019   0.0020   0.0029    0.000    0.030    0.000
LATT   1
SYMM  - X, 1/2 + Y, 1/2 - Z
SFAC  C    H    N    O    S
UNIT  56 48 16 4 4
MERG   2
FMAP   2
PLAN   -2
ACTA
BOND   $H
CONF
L.S.  40
WGHT    0.047900    0.439900
FVAR       1.59215
MOLE    1
S5    5    0.241152    0.564845    0.162700    11.00000    0.05339    0.04096 =
      0.02604   -0.00377    0.00773   -0.00204
O47   4   -0.026586    0.992715   -0.142623    11.00000    0.05889    0.05028 =
      0.07318    0.01492   -0.00225    0.02259
N1    3    0.357904    0.374142    0.054397    11.00000    0.04710    0.02993 =
      0.02291    0.00527    0.00323    0.00204
H1    2    0.369350    0.309782    0.099680    11.00000   -1.50000
N2    3    0.386303    0.342496   -0.035267    11.00000    0.04595    0.02904 =
      0.02690    0.00284    0.00432    0.00353
N4    3    0.279690    0.542218   -0.023475    11.00000    0.03566    0.02649 =
      0.02208    0.00014    0.00163    0.00210
N63   3    0.387341    0.340187   -0.322163    11.00000    0.05106    0.03387 =
      0.02761   -0.00500    0.00038    0.00076
C3    1    0.337663    0.446921   -0.081553    11.00000    0.03413    0.02508 =
      0.02476   -0.00100    0.00160   -0.00037
C5    1    0.292966    0.494086    0.065143    11.00000    0.03331    0.02804 =
      0.02653    0.00218    0.00134   -0.00394
C41   1    0.201632    0.662100   -0.050534    11.00000    0.03558    0.02868 =
      0.02301    0.00005    0.00271    0.00335
C42   1    0.262786    0.788329   -0.041629    11.00000    0.03895    0.03207 =
      0.03247   -0.00233   -0.00359    0.00007
AFIX  43
H42   2    0.352954    0.797135   -0.015326    11.00000   -1.50000
AFIX   0
C43   1    0.189724    0.902553   -0.071958    11.00000    0.05058    0.03017 =
      0.04085   -0.00051    0.00005    0.00319
AFIX  43
H43   2    0.230592    0.988077   -0.065969    11.00000   -1.50000
AFIX   0
```

```
C44   1    0.055558    0.888310   -0.111198    11.00000    0.04418    0.04186 =
      0.03640    0.00489    0.00432    0.01531
C45   1   -0.004195    0.760236   -0.119947    11.00000    0.03493    0.05173 =
      0.05091    0.00339   -0.00576    0.00438
AFIX  43
H45   2   -0.094001    0.750701   -0.146650    11.00000   -1.50000
AFIX   0
C46   1    0.067824    0.647373   -0.089604    11.00000    0.03575    0.03879 =
      0.04446   -0.00124   -0.00119   -0.00336
AFIX  43
H46   2    0.026942    0.561813   -0.095292    11.00000   -1.50000
AFIX   0
C48   1    0.030683    1.125674   -0.139791    11.00000    0.08629    0.04775 =
      0.06765    0.01866    0.01585    0.02747
AFIX 133
H481  2    0.110898    1.131086   -0.179885    11.00000   -1.50000
H482  2    0.060705    1.146565   -0.078342    11.00000   -1.50000
H483  2   -0.040756    1.189446   -0.159228    11.00000   -1.50000
AFIX   0
C61   1    0.352409    0.459245   -0.180969    11.00000    0.03346    0.02739 =
      0.02313   -0.00070    0.00062   -0.00035
C62   1    0.364652    0.341192   -0.232504    11.00000    0.04409    0.02796 =
      0.02932    0.00007    0.00141   -0.00009
AFIX  43
H62   2    0.356498    0.258362   -0.202517    11.00000   -1.50000
AFIX   0
C64   1    0.395672    0.460308   -0.364436    11.00000    0.05551    0.04241 =
      0.02329   -0.00254    0.00229    0.00200
AFIX  43
H64   2    0.411014    0.461188   -0.427261    11.00000   -1.50000
AFIX   0
C65   1    0.382798    0.582040   -0.320073    11.00000    0.06324    0.03215 =
      0.02927    0.00372    0.00358    0.00126
AFIX  43
H65   2    0.388619    0.663233   -0.352256    11.00000   -1.50000
AFIX   0
C66   1    0.361063    0.582008   -0.226874    11.00000    0.05436    0.02684 =
      0.02725   -0.00178    0.00210    0.00077
AFIX  43
H66   2    0.352308    0.663354   -0.195163    11.00000   -1.50000
AFIX   0
HKLF    4

REM  T15 in P2(1)/c
REM R1 =  0.0423 for    2286 Fo > 4sig(Fo)  and  0.0661 for all    3073 data
REM    184 parameters refined using      0 restraints

END

WGHT      0.0547      0.2965
```

REM Highest difference peak 0.206, deepest hole -0.252, 1-sigma level 0.055
Q1   1   0.0116 0.8229 -0.0904 11.00000 0.05   0.21
Q2   1   0.1945 0.9996 -0.0164 11.00000 0.05   0.19
;

CIF for C13

data_shelx

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_shelx_SHELXL_version_number   '2014/7'
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4-(2,4-dichlorophenyl)-3-(4-pyridylmethyl)-1H-1,2,4-triazole-5-thione
;
_chemical_name_common   ?
_chemical_melting_point   ?
_chemical_formula_moiety   'C14 H10 Cl2 N4 S'
_chemical_formula_sum   'C14 H10 Cl2 N4 S'
_chemical_formula_weight   337.22

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 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C' 'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H' 'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N' 'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'S' 'S'   0.1246   0.1234
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl' 'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_space_group_IT_number   2
_space_group_name_H-M_alt   'P -1'
_space_group_name_Hall   '-P 1'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
;

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 _space_group_symop_operation_xyz
 'x, y, z'
 '-x, -y, -z'

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_cell_length_b                 8.8584(9)
_cell_length_c                 11.251(2)
_cell_angle_alpha               81.356(13)
_cell_angle_beta                83.534(12)
_cell_angle_gamma               66.032(11)
_cell_volume                   757.21(19)
_cell_formula_units_Z          2
_cell_measurement_temperature  296(2)
_cell_measurement_reflns_used  1947
_cell_measurement_theta_min    1.8070
_cell_measurement_theta_max    26.5620

_exptl_crystal_description     block
_exptl_crystal_colour          colourles
_exptl_crystal_density_meas    ?
_exptl_crystal_density_method  ?
_exptl_crystal_density_diffrn  1.479
_exptl_crystal_F_000           344
_exptl_transmission_factor_min  ?
_exptl_transmission_factor_max  ?
_exptl_crystal_size_max        0.40
_exptl_crystal_size_mid        0.40
_exptl_crystal_size_min        0.10
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_shelx_estimated_absorpt_T_max  ?
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_exptl_absorpt_correction_type  'multi-scan'
_exptl_absorpt_process_details
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CrysAlisPro, Agilent Technologies,
Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb  9 2015,16:26:32)
Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
;
_exptl_absorpt_special_details  ?
_diffrn_ambient_temperature    296(2)
_diffrn_radiation_wavelength   0.71073
_diffrn_radiation_type         MoK\a
_diffrn_source                 ?
_diffrn_measurement_device_type  'KM4 CCD four-circle diffractometer'
_diffrn_measurement_method     '\w scans'
_diffrn_detector_area_resol_mean  ?
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_diffrn_reflns_number            4996
_diffrn_reflns_av_unetI/netI     0.0628
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_diffrn_reflns_limit_h_min       -11
_diffrn_reflns_limit_h_max       11
_diffrn_reflns_limit_k_min       -11
_diffrn_reflns_limit_k_max       11
_diffrn_reflns_limit_l_min       -14
_diffrn_reflns_limit_l_max       14
_diffrn_reflns_theta_min         1.834
_diffrn_reflns_theta_max         28.932
_diffrn_reflns_theta_full        25.242
_diffrn_measured_fraction_theta_max   0.871
_diffrn_measured_fraction_theta_full  1.000
_diffrn_reflns_Laue_measured_fraction_max    0.871
_diffrn_reflns_Laue_measured_fraction_full   1.000
_diffrn_reflns_point_group_measured_fraction_max   0.871
_diffrn_reflns_point_group_measured_fraction_full  1.000
_reflns_number_total             4996
_reflns_number_gt                3212
_reflns_threshold_expression     'I > 2\s(I)'
_reflns_Friedel_coverage         0.000
_reflns_Friedel_fraction_max     .
_reflns_Friedel_fraction_full    .

_reflns_special_details
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 _reflns_Friedel_fraction is defined as the number of unique
 Friedel pairs measured divided by the number that would be
 possible theoretically, ignoring centric projections and
 systematic absences.
;

_computing_data_collection
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CrysAlisPro, Agilent Technologies,
Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb  9 2015,16:26:32)
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_computing_cell_refinement
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Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb  9 2015,16:26:32)
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_computing_data_reduction
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CrysAlisPro, Agilent Technologies,
Version 1.171.37.35h (release 09-02-2015 CrysAlis171 .NET)
(compiled Feb  9 2015,16:26:32)
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_computing_structure_solution     'SHELXS-2013/1 (Sheldrick, 2013)'
_computing_structure_refinement   'SHELXL-2014/7 (Sheldrick, 2014)'
_computing_molecular_graphics     'ORTEP3 for Windows (Farrugia, 2012)'
_computing_publication_material
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SHELXL-2014/7 (Sheldrick, 2014) and WINGX (Farrugia, 2012)
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 Refined as a 2-component twin.
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_refine_ls_structure_factor_coef  Fsqd
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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0582P)^2^] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    ?
_atom_sites_solution_hydrogens    mixed
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      'SHELXL-2014/7 (Sheldrick 2014'
_refine_ls_extinction_coef        0.019(4)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          4996
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_refine_ls_R_factor_all           0.0666
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_refine_ls_goodness_of_fit_ref    0.903
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 _atom_site_occupancy
 _atom_site_site_symmetry_order
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Cl42 Cl 0.00899(11) 0.27775(10) 0.11464(7) 0.0529(3) Uani 1 1 d . . . . .
Cl44 Cl 0.26017(13) -0.21174(9) 0.47456(8) 0.0683(3) Uani 1 1 d . . . . .
S5 S -0.29281(10) 0.59255(11) 0.30994(8) 0.0534(3) Uani 1 1 d . . . . .
N1 N -0.0820(3) 0.7488(3) 0.2145(2) 0.0410(6) Uani 1 1 d . . . . .
H1 H -0.177(4) 0.858(4) 0.193(3) 0.062 Uiso 1 1 d . U . . .
N2 N 0.0913(3) 0.7240(3) 0.1962(2) 0.0429(6) Uani 1 1 d . . . . .
N4 N 0.0604(3) 0.4946(2) 0.27551(19) 0.0314(6) Uani 1 1 d . . . . .
N63 N 0.6761(3) 0.0727(3) 0.1457(3) 0.0576(8) Uani 1 1 d . . . . .
C3 C 0.1758(4) 0.5688(3) 0.2346(3) 0.0349(7) Uani 1 1 d . . . . .
C5 C -0.1071(4) 0.6134(3) 0.2644(2) 0.0362(7) Uani 1 1 d . . . . .
C31 C 0.3676(4) 0.4853(3) 0.2409(3) 0.0439(8) Uani 1 1 d . . . . .
H311 H 0.3943 0.4422 0.3240 0.066 Uiso 1 1 calc R U . . .
H312 H 0.4169 0.5676 0.2165 0.066 Uiso 1 1 calc R U . . .
C41 C 0.1081(4) 0.3230(3) 0.3227(2) 0.0334(7) Uani 1 1 d . . . . .
C42 C 0.0891(4) 0.2125(3) 0.2562(3) 0.0360(7) Uani 1 1 d . . . . .
C43 C 0.1371(4) 0.0472(3) 0.3023(3) 0.0441(8) Uani 1 1 d . . . . .
H43 H 0.1234 -0.0274 0.2585 0.066 Uiso 1 1 calc R U . . .
C44 C 0.2054(4) -0.0054(3) 0.4136(3) 0.0465(8) Uani 1 1 d . . . . .
C45 C 0.2273(4) 0.1025(4) 0.4804(3) 0.0543(9) Uani 1 1 d . . . . .
H45 H 0.2750 0.0650 0.5553 0.081 Uiso 1 1 calc R U . . .
C46 C 0.1769(4) 0.2677(4) 0.4336(3) 0.0448(8) Uani 1 1 d . . . . .
H46 H 0.1897 0.3422 0.4779 0.067 Uiso 1 1 calc R U . . .
C61 C 0.4547(3) 0.3447(3) 0.1641(3) 0.0353(7) Uani 1 1 d . . . . .
C62 C 0.5869(4) 0.2000(4) 0.2084(3) 0.0486(8) Uani 1 1 d . . . . .
H62 H 0.6154 0.1911 0.2874 0.073 Uiso 1 1 calc R U . . .
C64 C 0.6335(5) 0.0882(4) 0.0334(4) 0.0595(10) Uani 1 1 d . . . . .
H64 H 0.6953 0.0008 -0.0121 0.089 Uiso 1 1 calc R U . . .
C65 C 0.5033(5) 0.2257(4) -0.0198(3) 0.0570(10) Uani 1 1 d . . . . .
H65 H 0.4767 0.2312 -0.0988 0.085 Uiso 1 1 calc R U . . .
C66 C 0.4135(4) 0.3551(4) 0.0480(3) 0.0475(8) Uani 1 1 d . . . . .
H66 H 0.3245 0.4500 0.0147 0.071 Uiso 1 1 calc R U . . .

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 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Cl42 0.0638(6) 0.0486(5) 0.0469(5) -0.0087(4) -0.0159(4) -0.0184(4)
Cl44 0.0888(8) 0.0345(5) 0.0711(6) 0.0088(4) -0.0027(5) -0.0192(5)
S5 0.0338(5) 0.0647(6) 0.0644(6) -0.0103(5) -0.0028(4) -0.0211(4)
N1 0.0307(15) 0.0252(14) 0.0610(18) -0.0079(12) -0.0058(13) -0.0029(12)
N2 0.0355(15) 0.0261(14) 0.0663(18) -0.0085(12) -0.0017(13) -0.0106(12)
N4 0.0280(13) 0.0239(12) 0.0431(14) -0.0052(10) -0.0061(11) -0.0097(11)
N63 0.0444(18) 0.0308(15) 0.083(2) -0.0055(15) -0.0057(16) -0.0003(13)
C3 0.0313(17) 0.0270(16) 0.0488(19) -0.0097(13) -0.0042(14) -0.0117(14)
C5 0.0324(17) 0.0324(16) 0.0438(18) -0.0109(13) -0.0037(14) -0.0101(14)
C31 0.0327(18) 0.0309(16) 0.070(2) -0.0099(15) -0.0072(16) -0.0119(14)
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C41 0.0351(17) 0.0288(15) 0.0390(17) -0.0057(13) -0.0021(13) -0.0147(13)
C42 0.0349(18) 0.0330(16) 0.0404(18) -0.0068(14) -0.0028(14) -0.0128(14)
C43 0.051(2) 0.0370(18) 0.049(2) -0.0127(15) 0.0029(16) -0.0219(16)
C44 0.053(2) 0.0297(16) 0.051(2) 0.0025(15) -0.0003(16) -0.0131(15)
C45 0.067(2) 0.047(2) 0.042(2) 0.0024(16) -0.0130(17) -0.0157(18)
C46 0.054(2) 0.0385(17) 0.045(2) -0.0080(15) -0.0109(16) -0.0183(16)
C61 0.0241(16) 0.0267(16) 0.053(2) -0.0001(14) -0.0023(14) -0.0098(13)
C62 0.0398(19) 0.0339(18) 0.061(2) -0.0014(16) -0.0067(16) -0.0039(15)
C64 0.061(3) 0.046(2) 0.072(3) -0.0208(19) 0.011(2) -0.0204(19)
C65 0.066(3) 0.049(2) 0.058(2) -0.0047(19) -0.002(2) -0.026(2)
C66 0.043(2) 0.0310(17) 0.064(2) 0.0071(16) -0.0125(17) -0.0121(15)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Cl44 C44 1.742(3) . ?
S5 C5 1.665(3) . ?
N1 C5 1.332(3) . ?
N1 N2 1.381(3) . ?
N1 H1 0.99(3) . ?
N2 C3 1.296(3) . ?
N4 C5 1.381(3) . ?
N4 C3 1.384(3) . ?
N4 C41 1.436(3) . ?
N63 C64 1.325(4) . ?
N63 C62 1.329(4) . ?
C3 C31 1.484(4) . ?
C31 C61 1.508(4) . ?
C31 H311 0.9700 . ?
C31 H312 0.9700 . ?
C41 C46 1.372(4) . ?
C41 C42 1.385(3) . ?
C42 C43 1.384(4) . ?
C43 C44 1.372(4) . ?
C43 H43 0.9300 . ?
C44 C45 1.380(4) . ?
C45 C46 1.383(4) . ?

C45 H45 0.9300 . ?
C46 H46 0.9300 . ?
C61 C66 1.370(4) . ?
C61 C62 1.380(4) . ?
C62 H62 0.9300 . ?
C64 C65 1.374(5) . ?
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N2 N1 H1 122.4(17) . . ?
C3 N2 N1 104.8(2) . . ?
C5 N4 C3 108.5(2) . . ?
C5 N4 C41 126.1(2) . . ?
C3 N4 C41 125.4(2) . . ?
C64 N63 C62 116.8(3) . . ?
N2 C3 N4 110.1(2) . . ?
N2 C3 C31 125.0(2) . . ?
N4 C3 C31 124.8(2) . . ?
N1 C5 N4 103.0(2) . . ?
N1 C5 S5 129.1(2) . . ?
N4 C5 S5 127.8(2) . . ?
C3 C31 C61 114.8(2) . . ?
C3 C31 H311 108.6 . . ?
C61 C31 H311 108.6 . . ?
C3 C31 H312 108.6 . . ?
C61 C31 H312 108.6 . . ?
H311 C31 H312 107.5 . . ?
C46 C41 C42 119.8(2) . . ?
C46 C41 N4 119.5(2) . . ?
C42 C41 N4 120.7(2) . . ?
C43 C42 C41 120.1(3) . . ?
C43 C42 Cl42 119.3(2) . . ?
C41 C42 Cl42 120.7(2) . . ?
C44 C43 C42 119.1(3) . . ?
C44 C43 H43 120.4 . . ?
C42 C43 H43 120.4 . . ?
C43 C44 C45 121.6(3) . . ?
C43 C44 Cl44 119.5(2) . . ?
C45 C44 Cl44 118.8(3) . . ?

C44 C45 C46 118.6(3) . . ?
C44 C45 H45 120.7 . . ?
C46 C45 H45 120.7 . . ?
C41 C46 C45 120.8(3) . . ?
C41 C46 H46 119.6 . . ?
C45 C46 H46 119.6 . . ?
C66 C61 C62 117.0(3) . . ?
C66 C61 C31 122.9(3) . . ?
C62 C61 C31 120.0(3) . . ?
N63 C62 C61 124.3(3) . . ?
N63 C62 H62 117.8 . . ?
C61 C62 H62 117.8 . . ?
N63 C64 C65 123.9(4) . . ?
N63 C64 H64 118.0 . . ?
C65 C64 H64 118.0 . . ?
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C64 C65 H65 121.2 . . ?
C66 C65 H65 121.2 . . ?
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C5 N4 C3 N2 -1.6(3) . . . . ?
C41 N4 C3 N2 179.0(2) . . . . ?
C5 N4 C3 C31 174.9(3) . . . . ?
C41 N4 C3 C31 -4.5(4) . . . . ?
N2 N1 C5 N4 -1.6(3) . . . . ?
N2 N1 C5 S5 175.3(2) . . . . ?
C3 N4 C5 N1 1.9(3) . . . . ?
C41 N4 C5 N1 -178.7(2) . . . . ?
C3 N4 C5 S5 -175.0(2) . . . . ?
C41 N4 C5 S5 4.4(4) . . . . ?
N2 C3 C31 C61 -118.1(3) . . . . ?
N4 C3 C31 C61 65.9(4) . . . . ?
C5 N4 C41 C46 -108.0(3) . . . . ?
C3 N4 C41 C46 71.3(4) . . . . ?
C5 N4 C41 C42 73.5(4) . . . . ?

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C3 N4 C41 C42 -107.2(3) . . . . ?
C46 C41 C42 C43 0.8(4) . . . . ?
N4 C41 C42 C43 179.4(2) . . . . ?
C46 C41 C42 Cl42 -178.1(2) . . . . ?
N4 C41 C42 Cl42 0.5(4) . . . . ?
C41 C42 C43 C44 -0.7(4) . . . . ?
Cl42 C42 C43 C44 178.2(2) . . . . ?
C42 C43 C44 C45 -0.1(5) . . . . ?
C42 C43 C44 Cl44 178.0(2) . . . . ?
C43 C44 C45 C46 0.8(5) . . . . ?
Cl44 C44 C45 C46 -177.4(2) . . . . ?
C42 C41 C46 C45 -0.1(5) . . . . ?
N4 C41 C46 C45 -178.7(3) . . . . ?
C44 C45 C46 C41 -0.7(5) . . . . ?
C3 C31 C61 C66 44.0(4) . . . . ?
C3 C31 C61 C62 -138.6(3) . . . . ?
C64 N63 C62 C61 0.1(5) . . . . ?
C66 C61 C62 N63 0.5(5) . . . . ?
C31 C61 C62 N63 -177.0(3) . . . . ?
C62 N63 C64 C65 -0.7(5) . . . . ?
N63 C64 C65 C66 0.6(6) . . . . ?
C62 C61 C66 C65 -0.6(4) . . . . ?
C31 C61 C66 C65 176.8(3) . . . . ?
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TITL T17 in P-1
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ZERR     2.00   0.0010   0.0009   0.0020    0.013    0.012    0.011
LATT   1
SFAC  C    H    N    S    CL
UNIT  28 20 8 2 4
MERG   0
FMAP   2
ACTA
BOND   $H
CONF
L.S.  40
PLAN  -2
WGHT    0.058200
EXTI    0.018621
BASF   0.43793
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CL44  5    0.260172   -0.211735    0.474562    11.00000    0.08883    0.03452 =
      0.07105    0.00877   -0.00268   -0.01920
S5    4   -0.292806    0.592551    0.309938    11.00000    0.03376    0.06467 =
      0.06436   -0.01031   -0.00279   -0.02114
N1    3   -0.081959    0.748820    0.214471    11.00000    0.03070    0.02521 =
      0.06097   -0.00794   -0.00583   -0.00290
H1    2   -0.177457    0.858046    0.192663    11.00000   -1.50000
N2    3    0.091303    0.724038    0.196216    11.00000    0.03547    0.02612 =
      0.06631   -0.00853   -0.00173   -0.01063
N4    3    0.060391    0.494564    0.275511    11.00000    0.02801    0.02387 =
      0.04315   -0.00519   -0.00611   -0.00974
N63   3    0.676106    0.072723    0.145731    11.00000    0.04444    0.03081 =
      0.08333   -0.00553   -0.00574   -0.00034

C3    1    0.175794    0.568754    0.234591    11.00000    0.03129    0.02702 =
      0.04883   -0.00972   -0.00419   -0.01168
C5    1   -0.107077    0.613449    0.264356    11.00000    0.03242    0.03237 =
      0.04381   -0.01091   -0.00373   -0.01014
C31   1    0.367567    0.485272    0.240914    11.00000    0.03272    0.03089 =
      0.06995   -0.00993   -0.00717   -0.01192
AFIX  23
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H312  2    0.416930    0.567624    0.216549    11.00000   -1.50000
AFIX   0
C41   1    0.108110    0.322973    0.322657    11.00000    0.03510    0.02879 =
      0.03901   -0.00571   -0.00211   -0.01468
C42   1    0.089052    0.212459    0.256222    11.00000    0.03493    0.03303 =
      0.04039   -0.00680   -0.00280   -0.01281
C43   1    0.137148    0.047155    0.302315    11.00000    0.05148    0.03697 =
      0.04935   -0.01269    0.00288   -0.02187
AFIX  43
H43   2    0.123435   -0.027359    0.258482    11.00000   -1.50000
AFIX   0
C44   1    0.205359   -0.005386    0.413579    11.00000    0.05303    0.02966 =
      0.05064    0.00252   -0.00028   -0.01312
C45   1    0.227310    0.102517    0.480386    11.00000    0.06702    0.04690 =
      0.04213    0.00245   -0.01296   -0.01573
AFIX  43
H45   2    0.274991    0.064972    0.555250    11.00000   -1.50000
AFIX   0
C46   1    0.176887    0.267666    0.433626    11.00000    0.05409    0.03855 =
      0.04473   -0.00801   -0.01087   -0.01826
AFIX  43
H46   2    0.189740    0.342179    0.477922    11.00000   -1.50000
AFIX   0
C61   1    0.454652    0.344724    0.164084    11.00000    0.02405    0.02670 =
      0.05332   -0.00005   -0.00230   -0.00980
C62   1    0.586891    0.200032    0.208447    11.00000    0.03981    0.03386 =
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      0.06124   -0.00142   -0.00672   -0.00387
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AFIX   0
C64   1    0.633451    0.088206    0.033415    11.00000    0.06068    0.04568 =
      0.07234   -0.02078    0.01103   -0.02037
AFIX  43
H64   2    0.695308    0.000801   -0.012128    11.00000   -1.50000
AFIX   0
C65   1    0.503254    0.225714   -0.019816    11.00000    0.06577    0.04936 =
      0.05778   -0.00474   -0.00235   -0.02559
AFIX  43
H65   2    0.476729    0.231186   -0.098796    11.00000   -1.50000
AFIX   0
C66   1    0.413493    0.355082    0.047964    11.00000    0.04295    0.03096 =
      0.06434    0.00706   -0.01250   -0.01212
AFIX  43
H66   2    0.324488    0.449954    0.014741    11.00000   -1.50000
AFIX   0
HKLF    5

REM  T17 in P-1
REM R1 =  0.0397 for    3212 Fo > 4sig(Fo)  and  0.0666 for all    4996 data
REM    195 parameters refined using      0 restraints

END

WGHT      0.0582      0.0000

REM Highest difference peak  0.263,  deepest hole -0.250,  1-sigma level  0.072
Q1    1  -0.4070  0.5775  0.2774  11.00000  0.05    0.26
Q2    1   0.5058  0.1623  0.0052  11.00000  0.05    0.23
;
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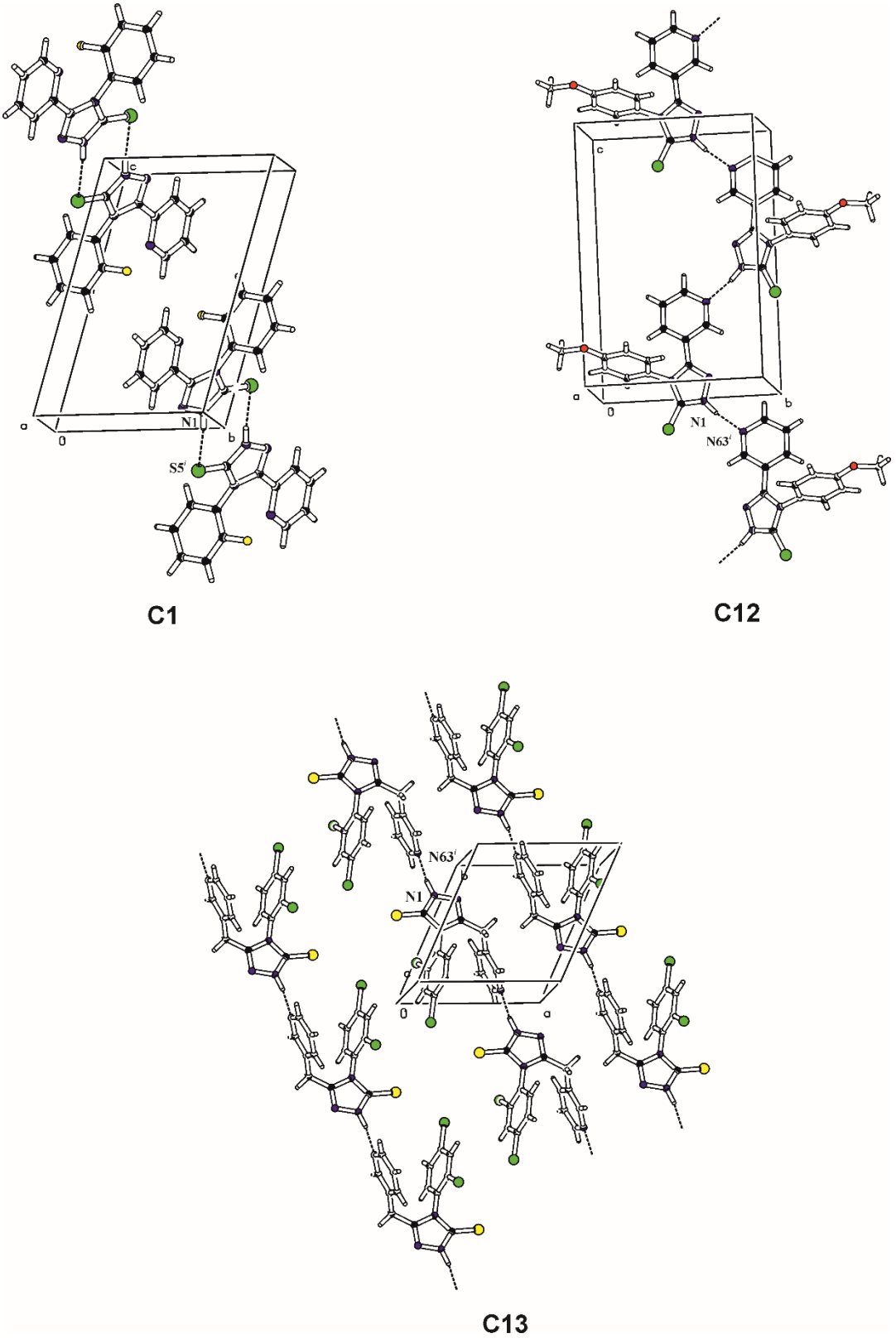
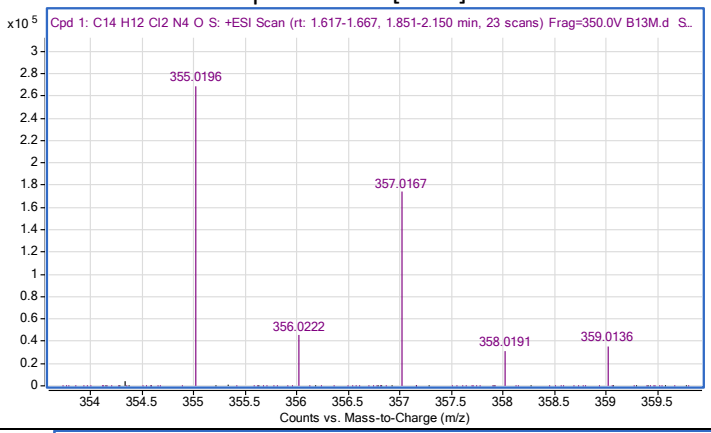
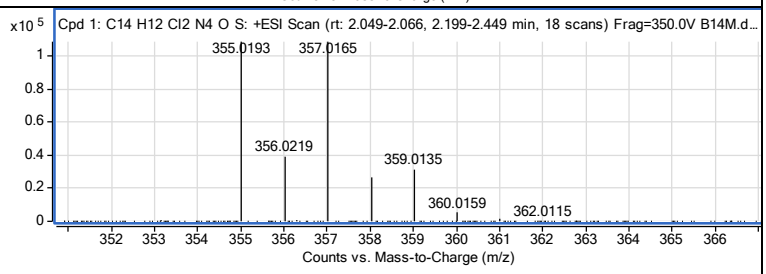
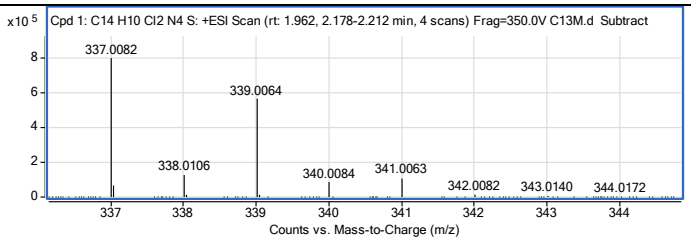
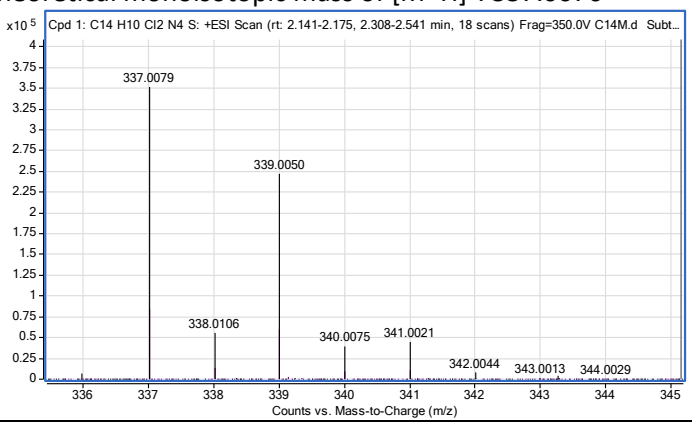


Figure 1S. The molecular packing of **C1, C12** and **C13**. Dashed lines indicate intermolecular hydrogen bonds; **C1** *i* = -*x*, 2-*y*, -*z*; **C12:** *i* = *x*, 3/2-*y*, -1/2+*z*; **C13**: *i* = -1+*x*, 1+*y*, *z*.

MS analysis for new compounds

Table 1S.

LP.	Compound formula, thoretical and measured monoisotopic mass, and mass difference in ppm	Theoretical monoisotopic mass of protonated ion and acquired LC/QTOF HRMS spectra
B13	C14H12N4OSCl2 Calculated monoisotopic mass: 354.0109 Measured monoisotopic mass: 354.0122 Mass error: 3.84 ppm	Theoretical monoisotopic mass of $[M+H]^+$: 355.0182 
B14	C14H12ON4SCl2 Calculated monoisotopic mass: 354.0109 Measured monoisotopic mass: 354.012 Mass error: 3.13 ppm	
C13	C14H10N4SCl2 Calculated monoisotopic mass: 336.0003 Measured monoisotopic mass: 336.0017 Mass error: 3.96 ppm	
C14	C14H10N4SCl2 Calculated monoisotopic mass: 336.0003 Measured monoisotopic mass: 336.0006 Mass error: 0.78 ppm	Theoretical monoisotopic mass of $[M+H]^+$: 337.0076 

Theoretical calculation

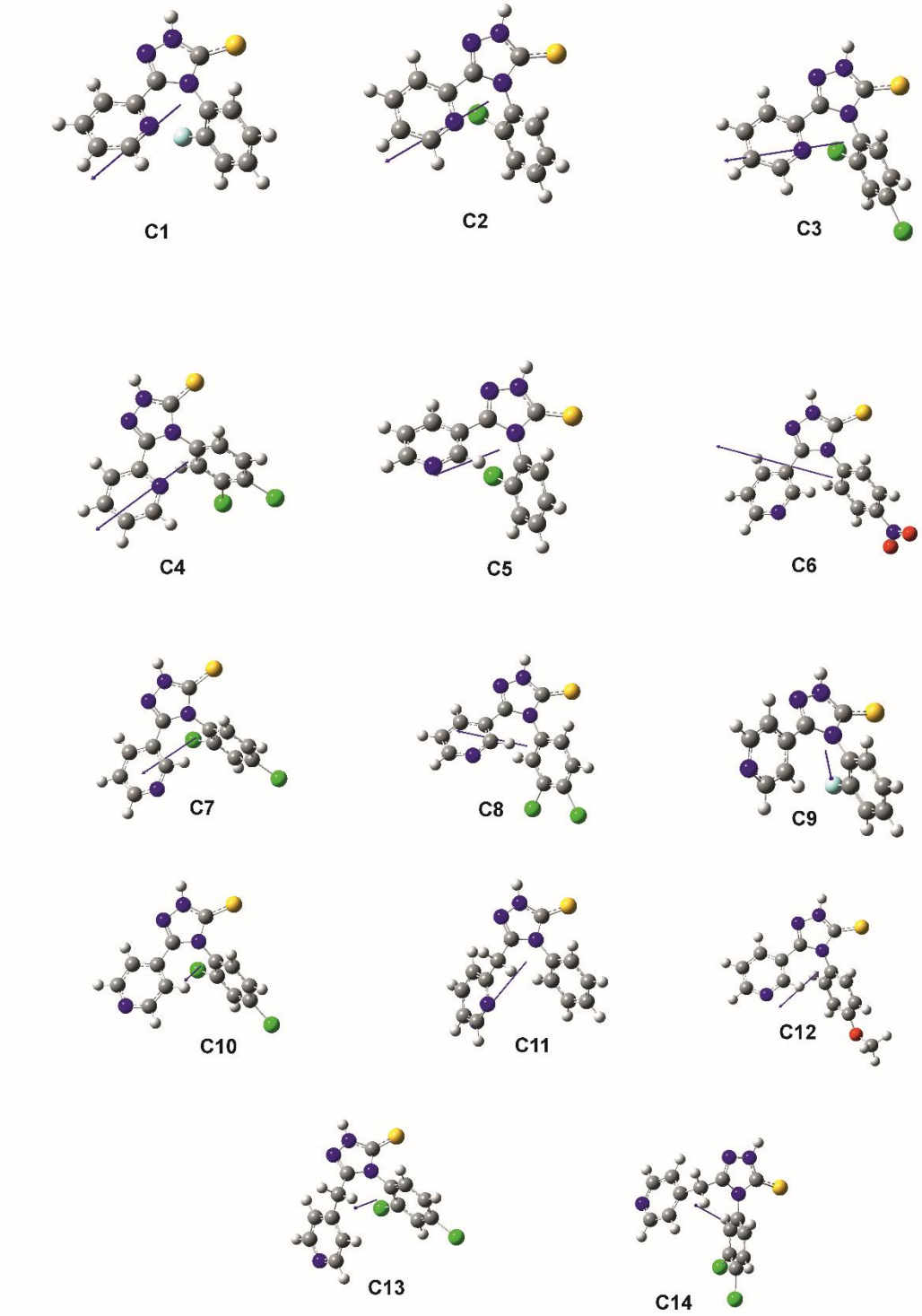


Figure 2S. A view of the molecules **C1**–**C14** with the vectors of dipole moments in the low-energy conformation calculated at the DFT/B3LYP/6-311++G(d,p) level.

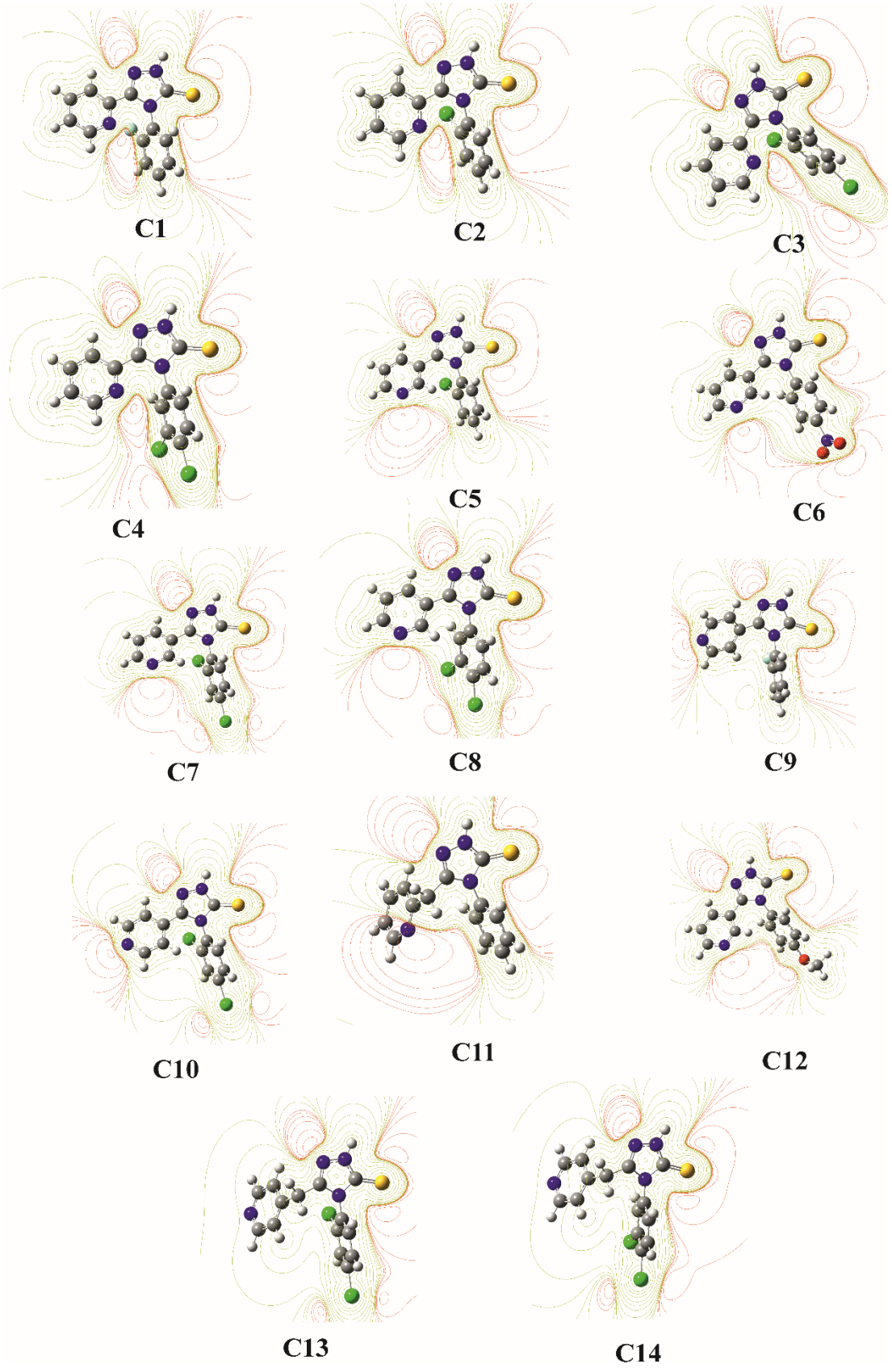

C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14

Fig. 3S. The contour maps of molecular electrostatic potential for compounds **C1**–**C14** in the plane of 1,2,4-triazole ring; the red lines represent regions with the negative electrostatic potential and yellow lines represent regions with the positive electrostatic potential.

Molecular docking

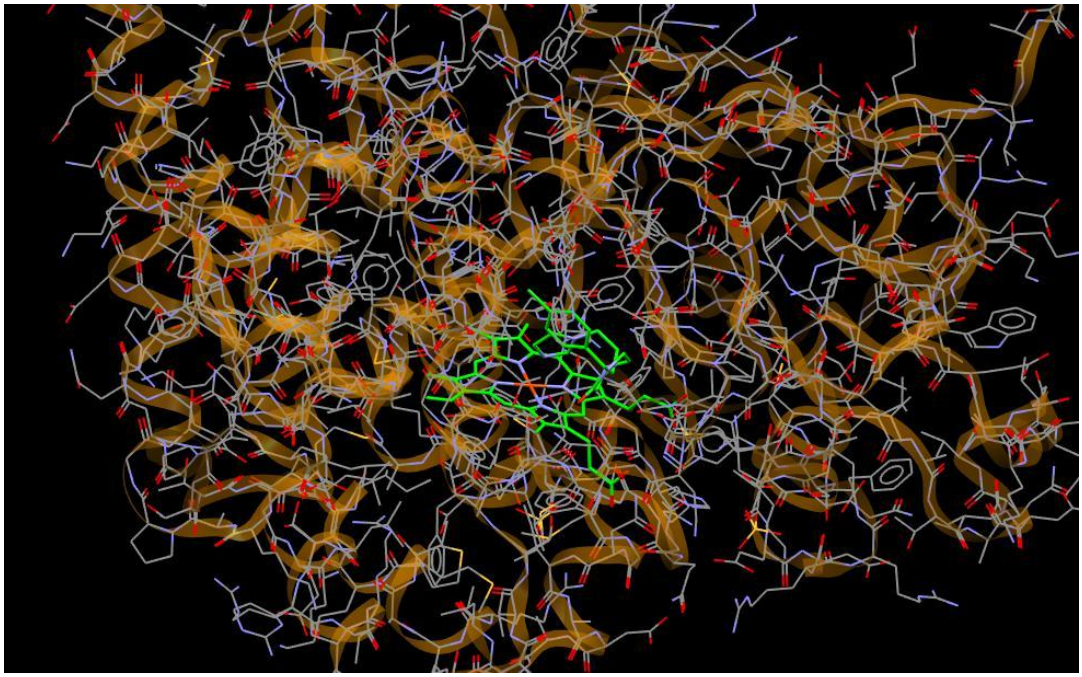


Fig. 4S. The crystal structure of the cytochrome P450 CYP121 of Mycobacterium tuberculosis obtained from expression system *Escherichia coli* in complex with 1-[(4-chlorophenyl)methyl]-4-(3-imidazol-1-ylpropyl)piperazin-2-one (9KE) and heme.

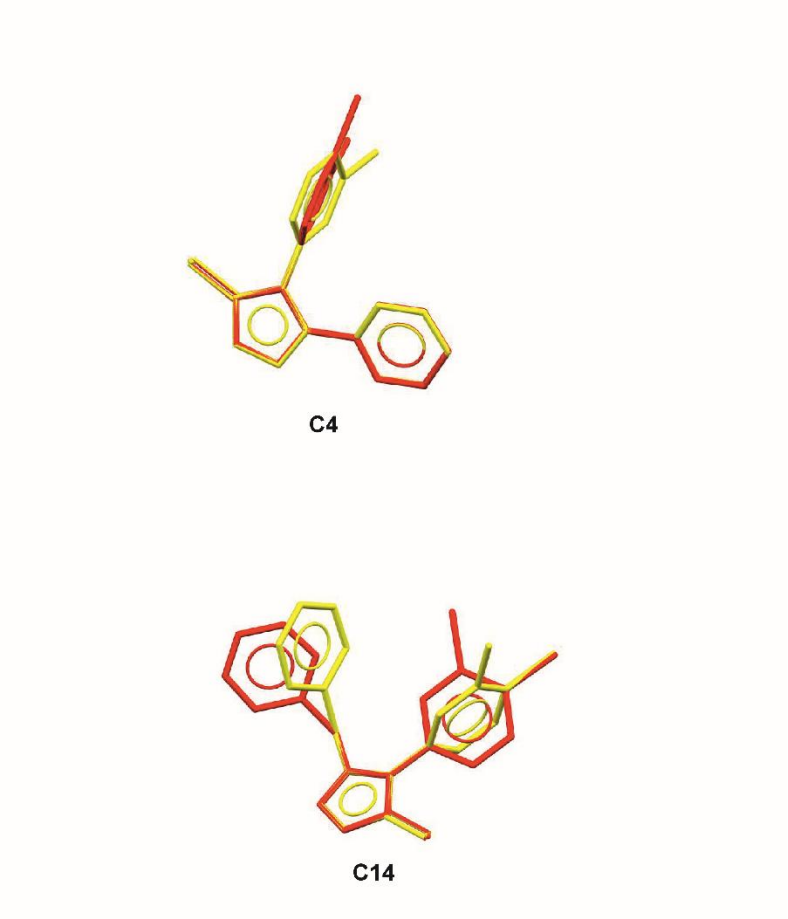
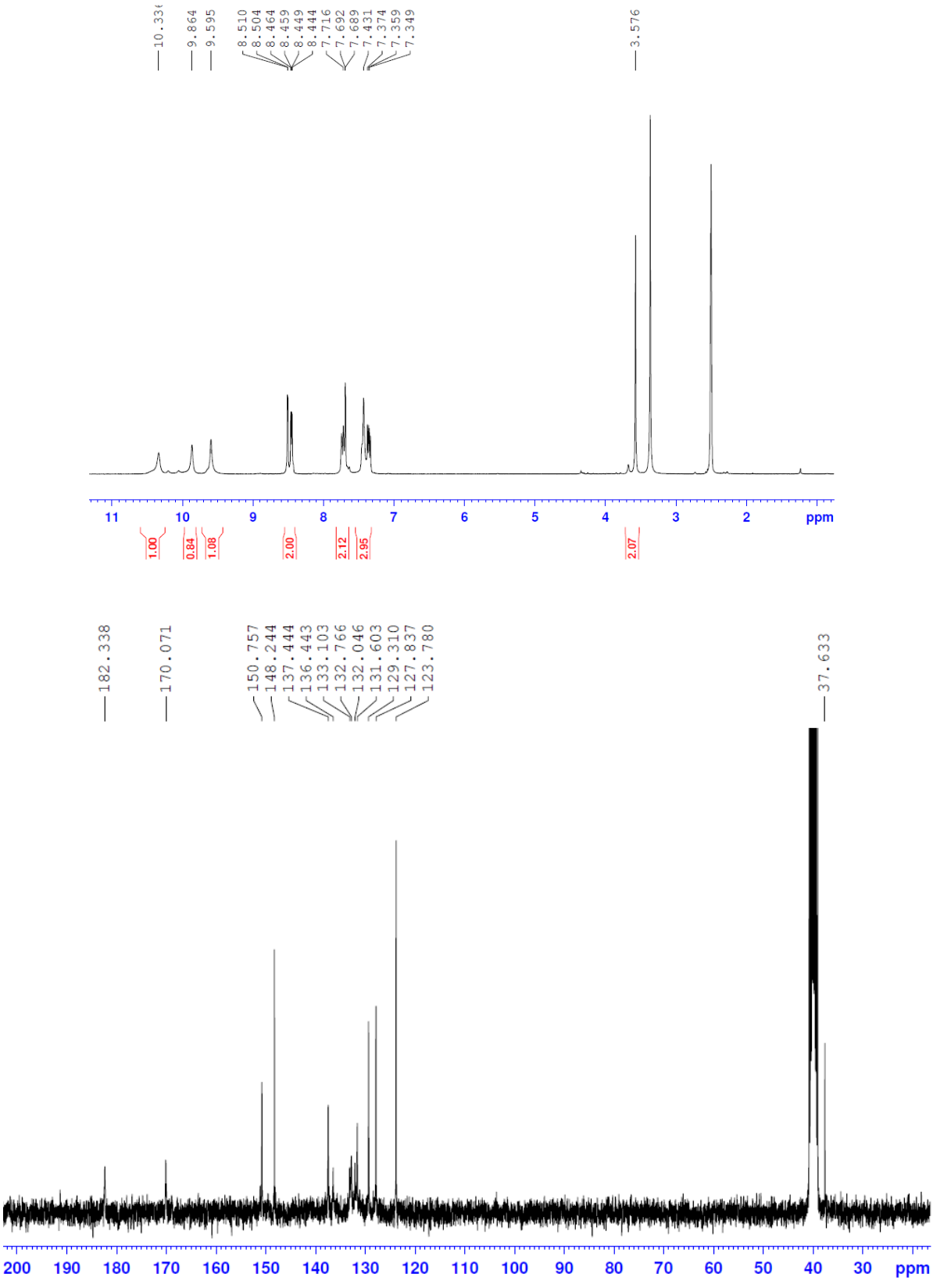


Fig. 5S. The overlay of molecules **C4** and **C14** in conformations observed in binding site of the cytochrome P450 CYP121 9red) and to their starting conformations for the docking process obtained as a result of energy minimization and energy optimization at DFT level (yellow).

Spectral data for new compounds:

Compound B13



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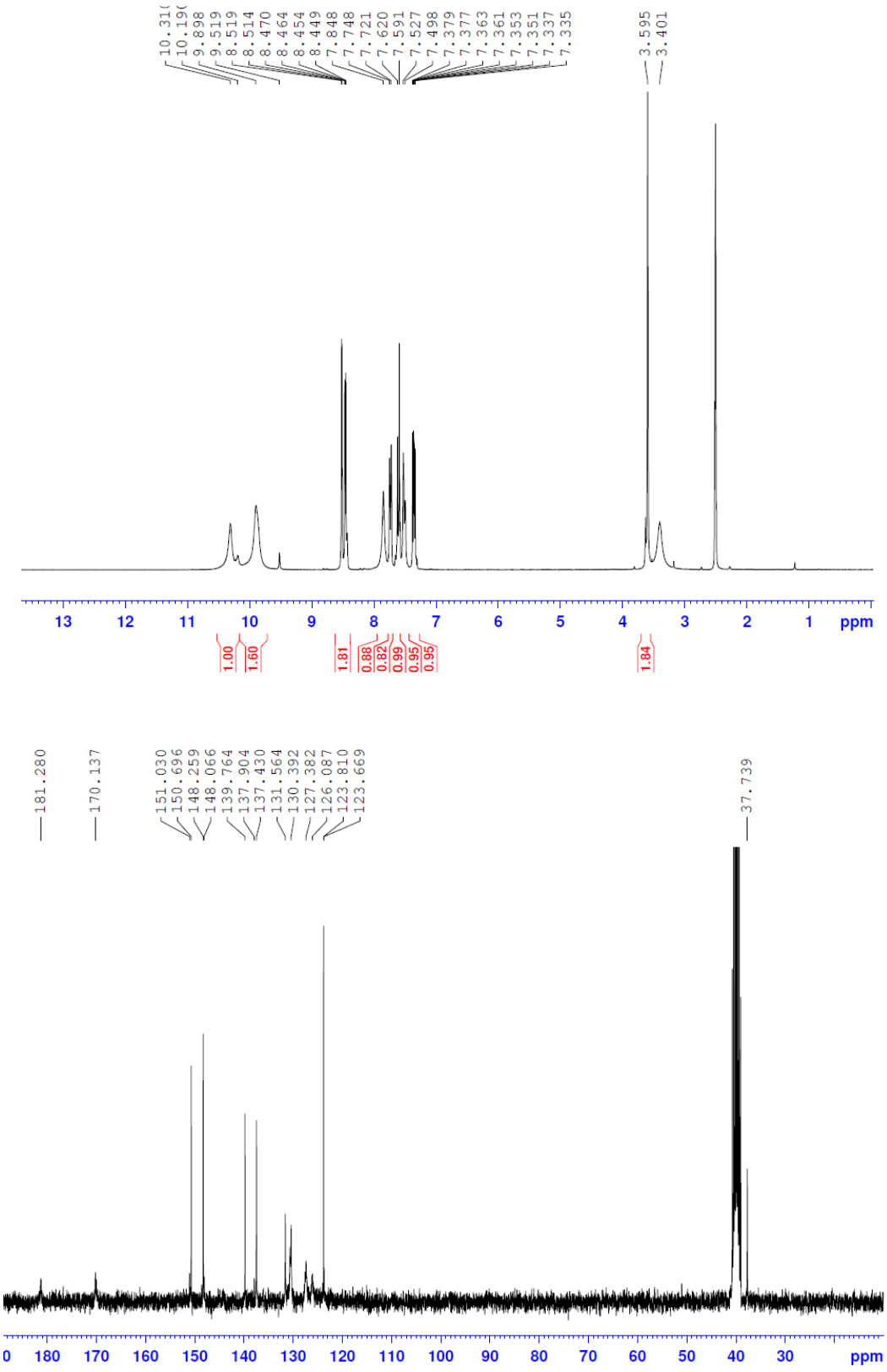
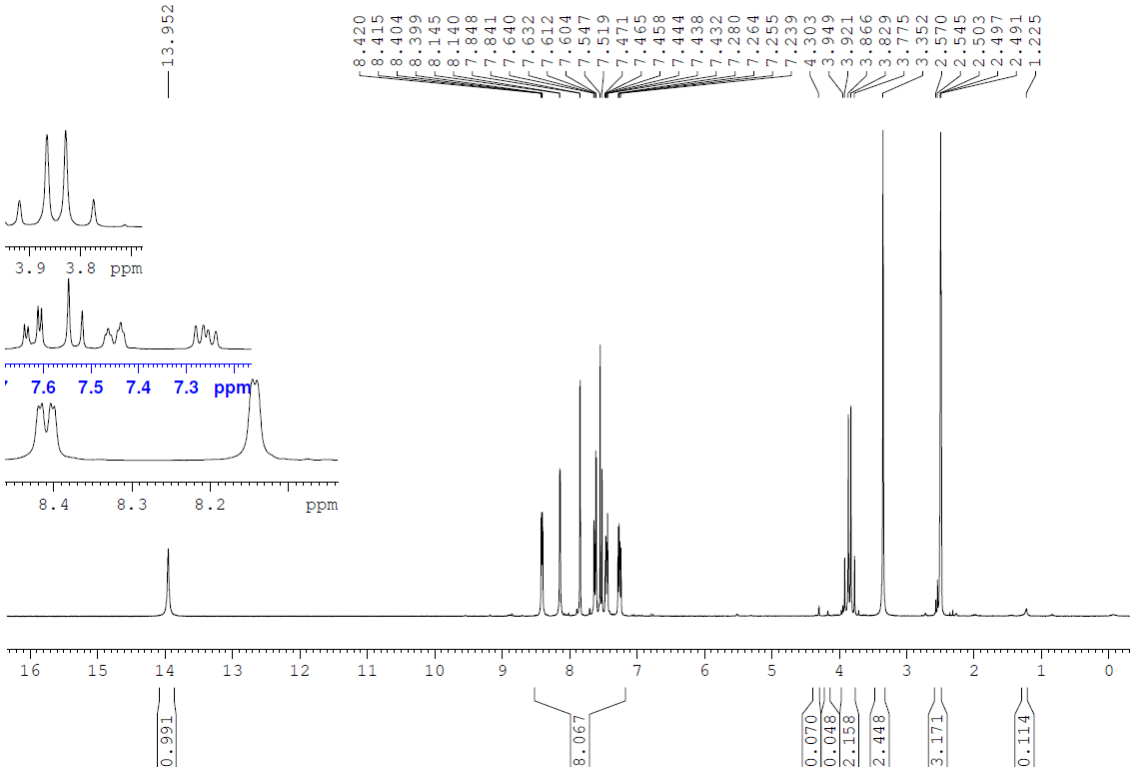


Compound C13



Compound C14