Supporting Information

Guidongnins I-J, two new 6,7-*seco*-7,20-olide-*ent*-kaurene diterpenes with unusual structures from *Isodon rubescens*

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[†]Juan Zou and Jiang-Hai Ye contributed equally to this work.

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General Experimental Procedures

An XRC-1 micro melting point apparatus (Sichuan Weitai, Chengdu, China) was used for the measurement of compounds' melting points. Optical rotations were determined on a Jasco P-1010 polarimeter (Perkin-Elmer, Waltham, United States). The IR spectra was recorded on a VECTOR22 infrared spectrometer (Bruker, Karlsruhe, Germany) using KBr pellets method. A Bruker Avance spectrometer (600 MHz, Bruker, Karlsruhe, Germany) was used for recording the NMR spectra. The HR-ESI-MS data was obtained on a Bruker Q-TOF mass spectrometer (Bruker, Karlsruhe, Germany). X-ray data were collected on a Bruker APEX-II CCD instrument equipped with Cu Kα radiation for 1 (Bruker, Rheinstetten, Germany) and Bruker APEX-II instrument equipped with Mo Kα radiation for 2 (Bruker, Rheinstetten, Germany). Silica gel (200-300 mesh; Qingdao Haiyang Chemical, Qingdao, China) was used for column chromatography, while silica gel GF254 (0.2 mm, Qingdao Haiyang Chemical Inc., Qingdao, China) was used for analytical TLC. Prior to use, all solvents were distilled.
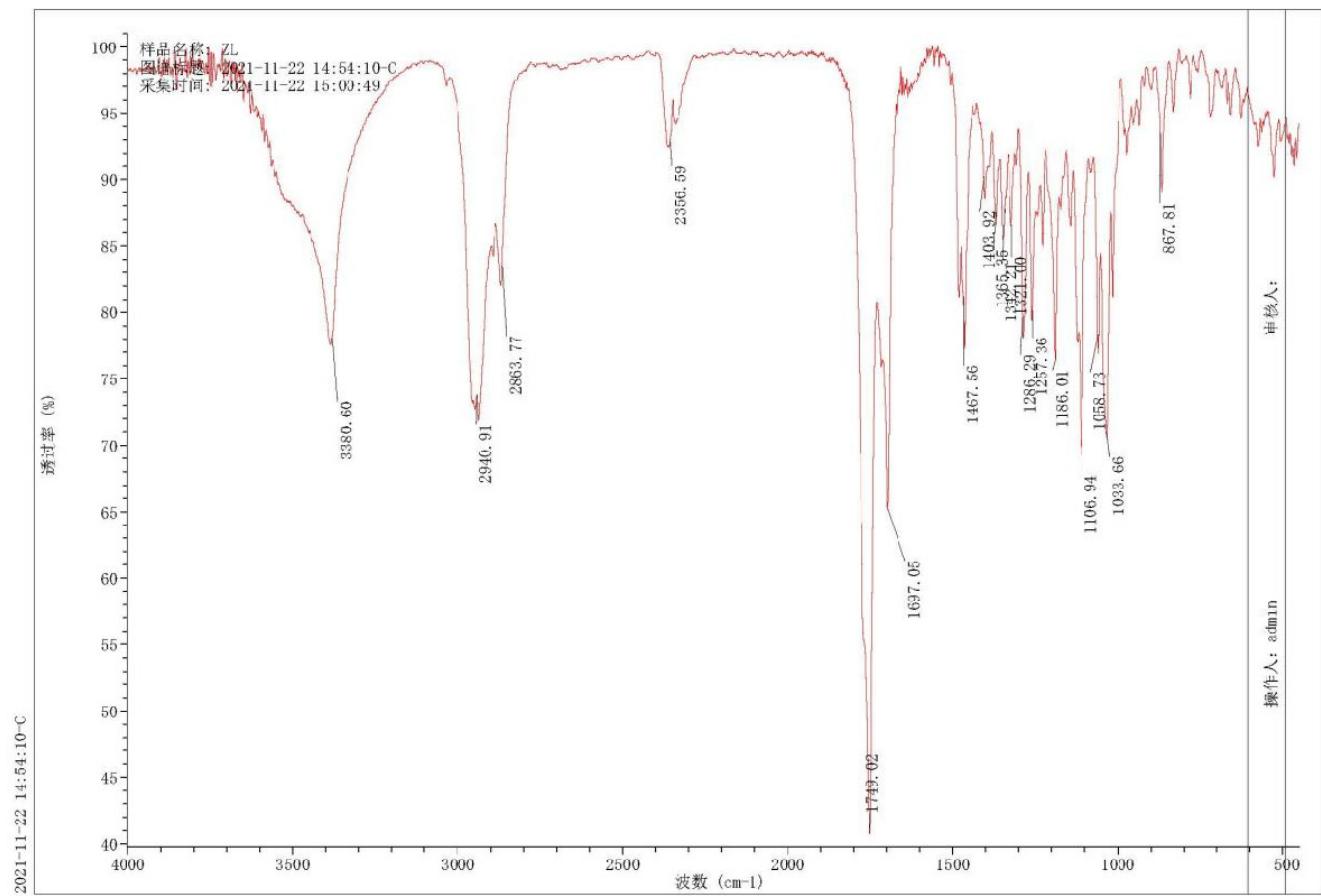
Figure S1. The IR (KBr disc) spectrum of **1.**
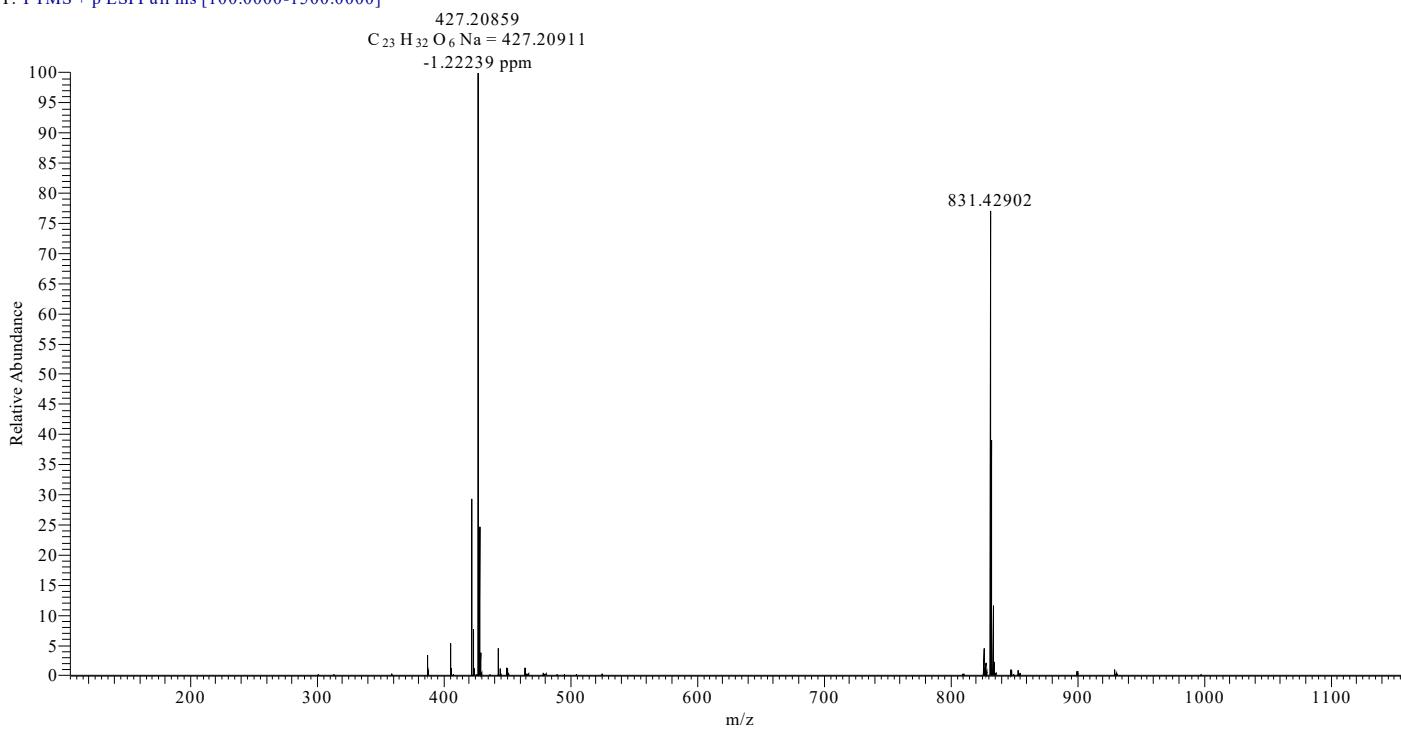
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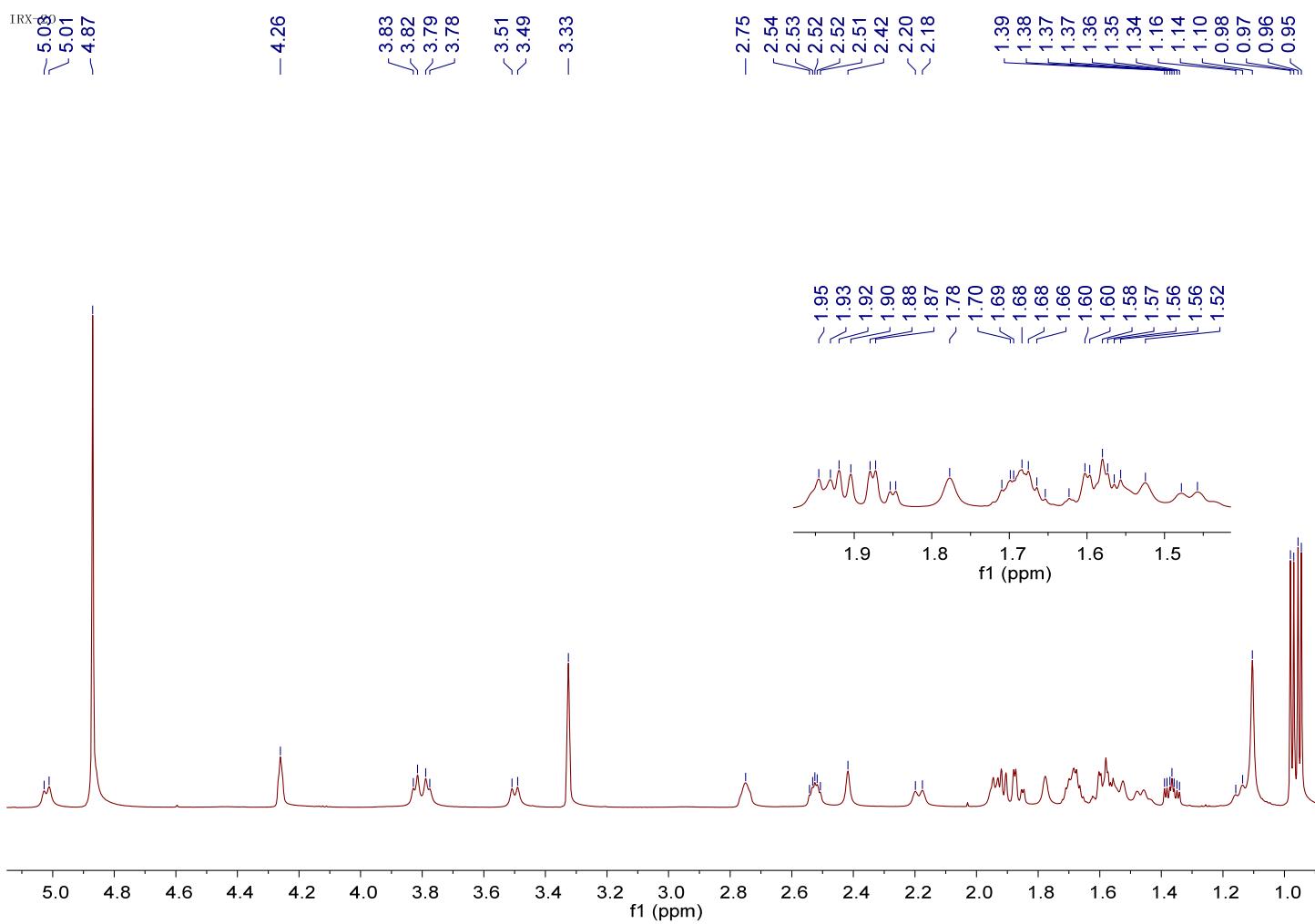
Figure S3. ^{1}H NMR spectrum of **1** in CD$_3$OD (600 MHz).
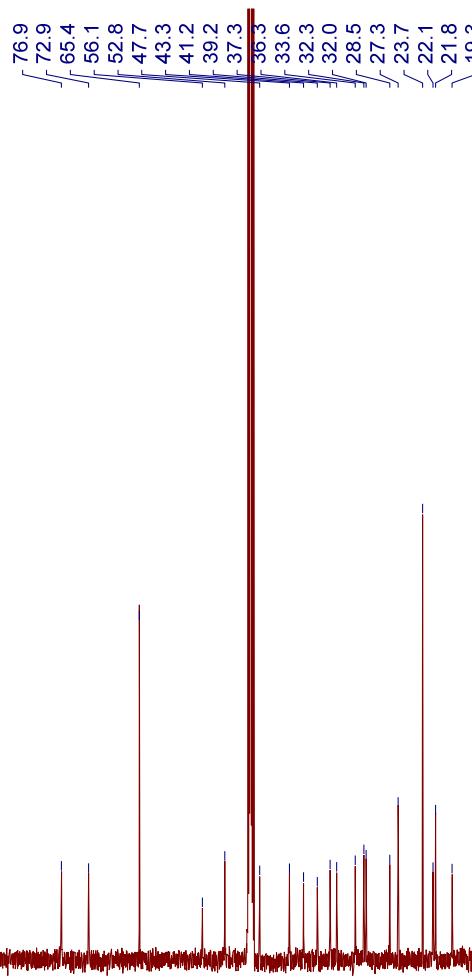
Figure S4. ^{13}C NMR spectrum of **1** in CD$_3$OD (150 MHz).
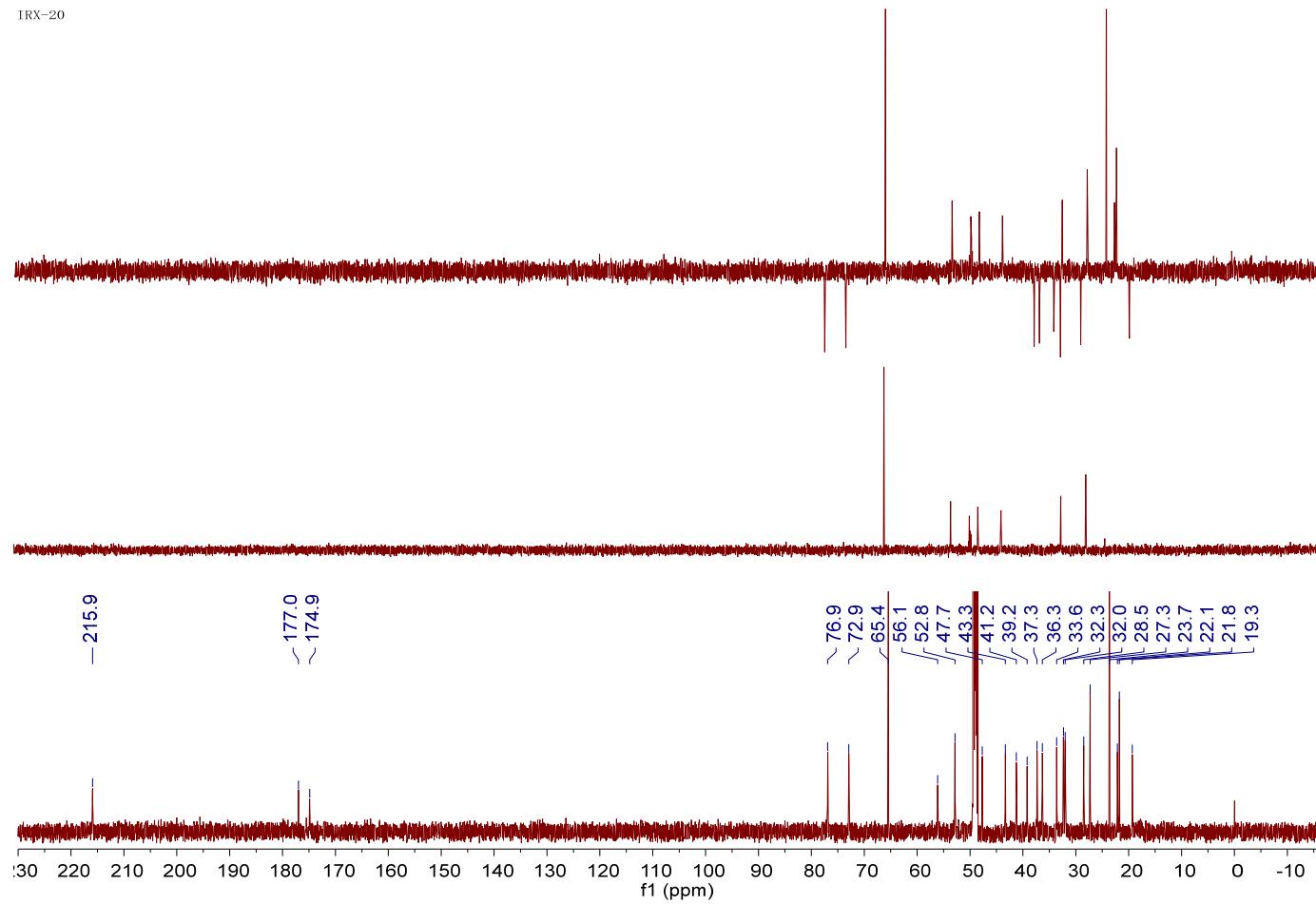
Figure S5. DEPT spectrum of **1** in CD₃OD.
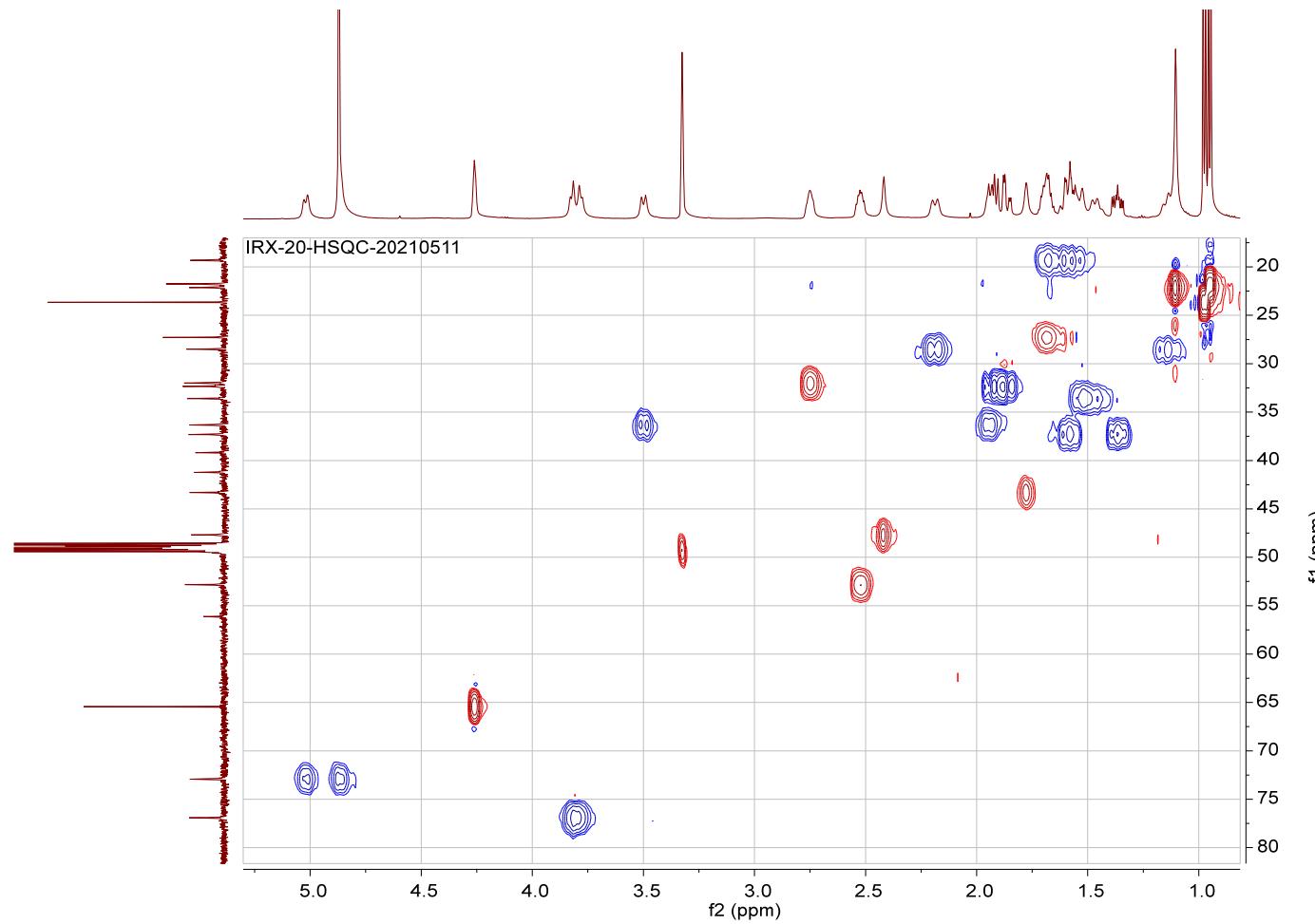
Figure S6. HSQC spectrum of **1** in CD₃OD.
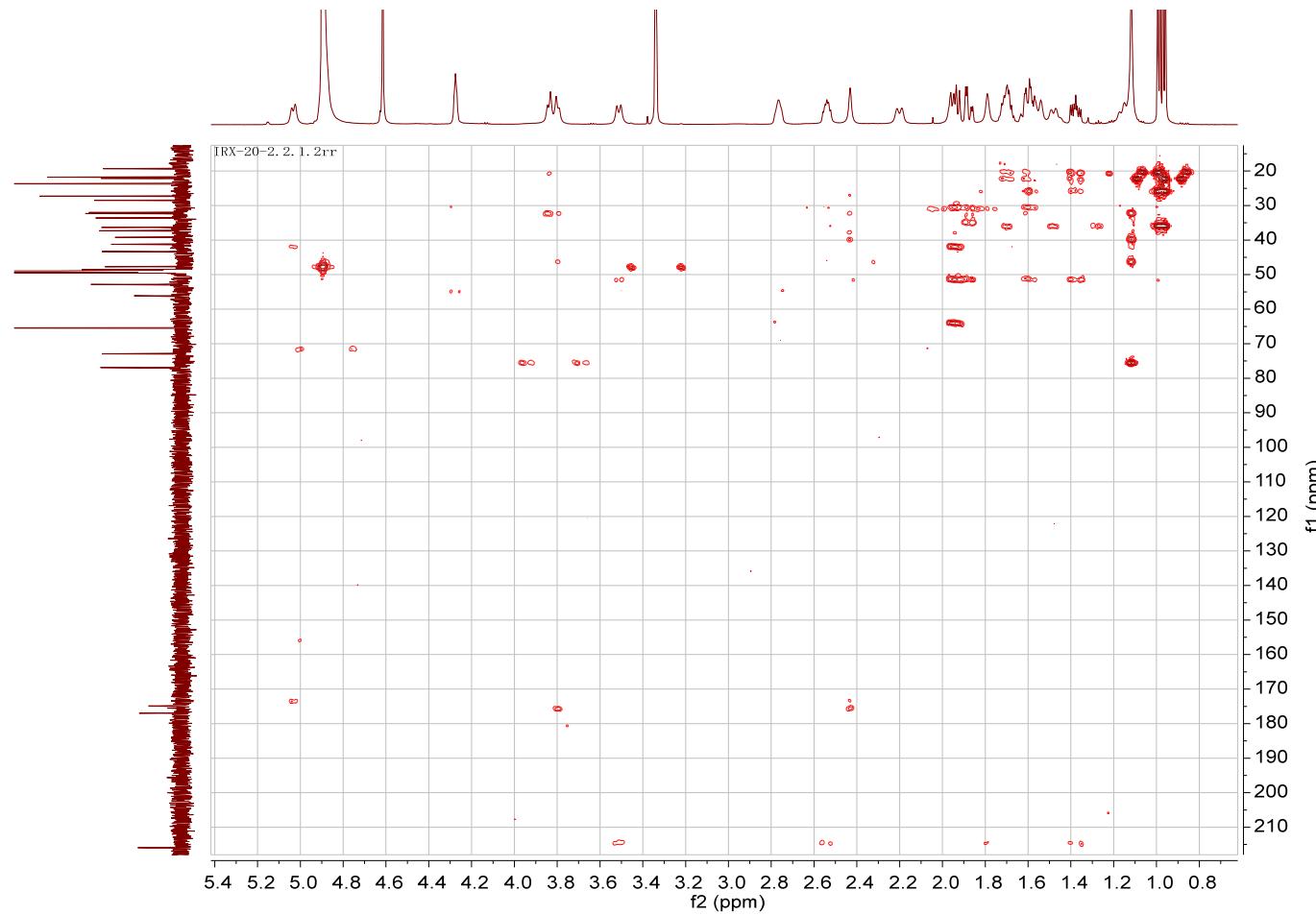
Figure S7. HMBC spectrum of **1** in CD₃OD.

IRX-20-COSY-20210511
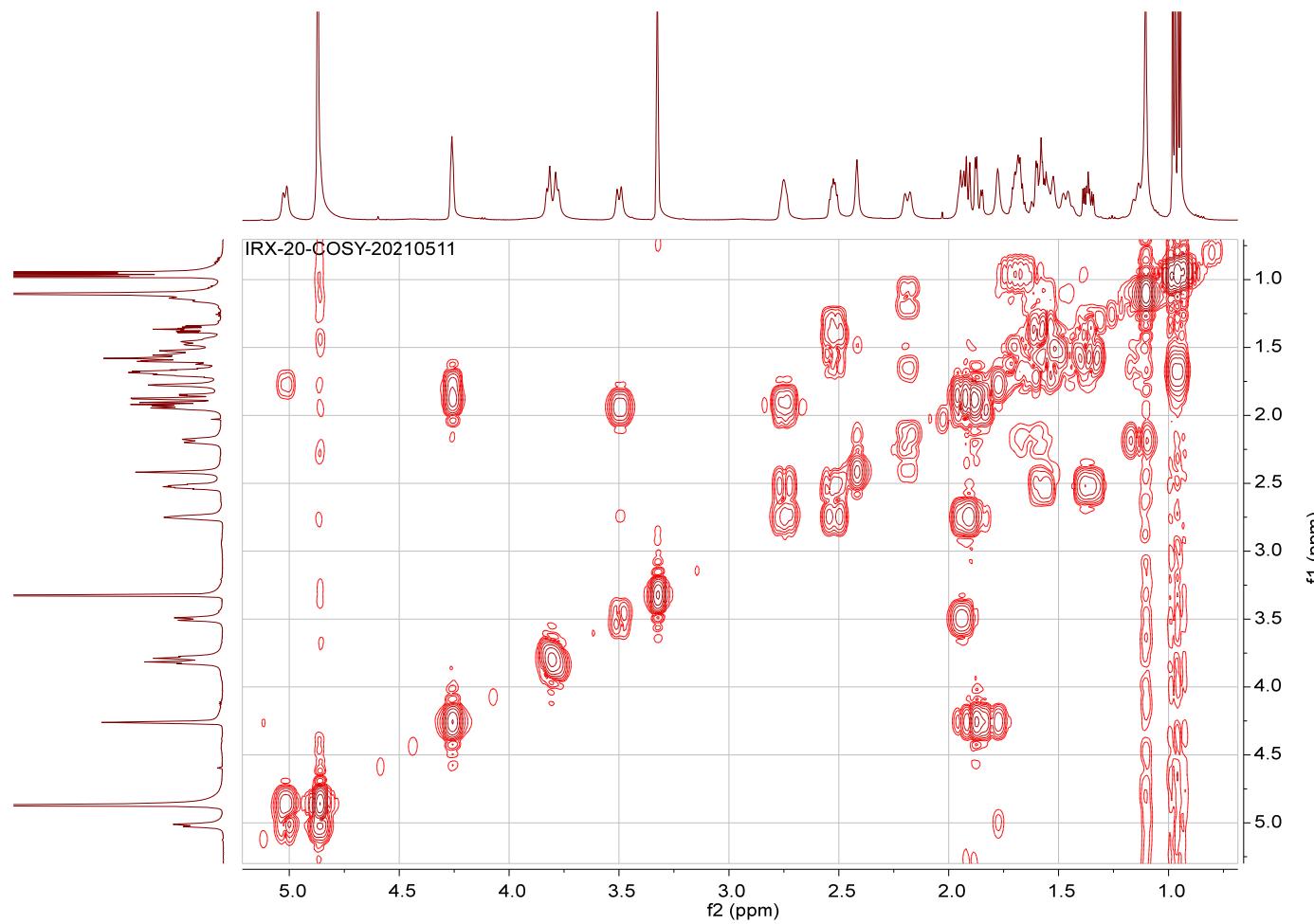
Figure S8. ^1H-^1H COSY spectrum of **1** in CD$_3$OD.

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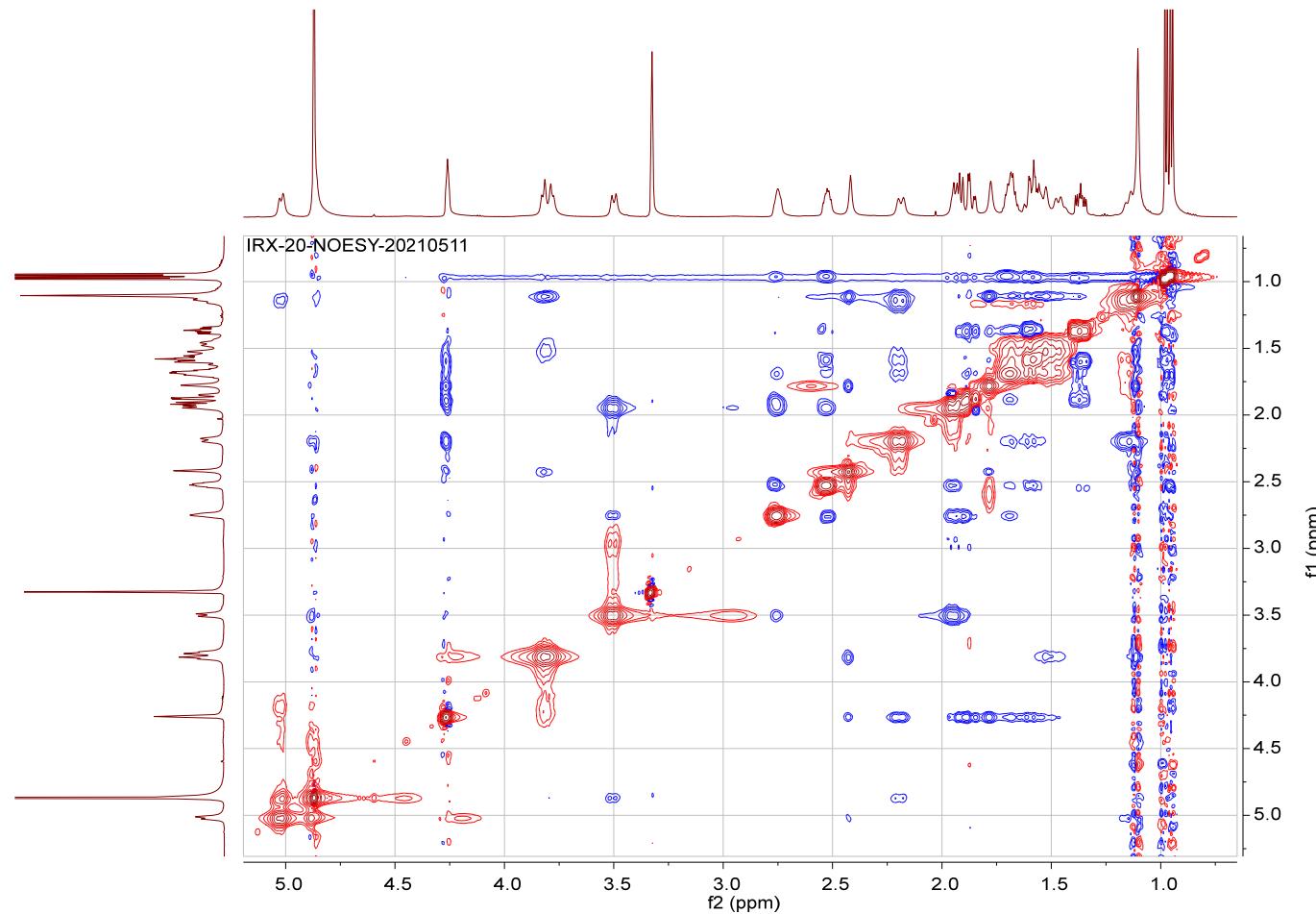
Figure S9. NOESY spectrum of **1** in CD₃OD.
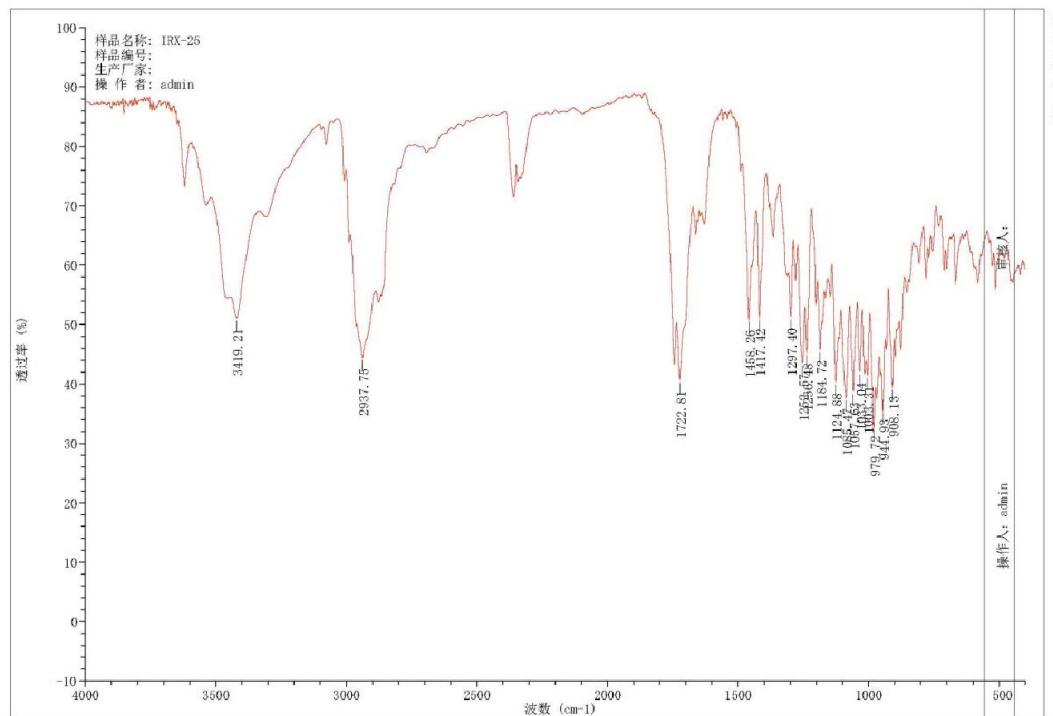
Figure S10. The IR (KBr disc) spectrum of **2.**
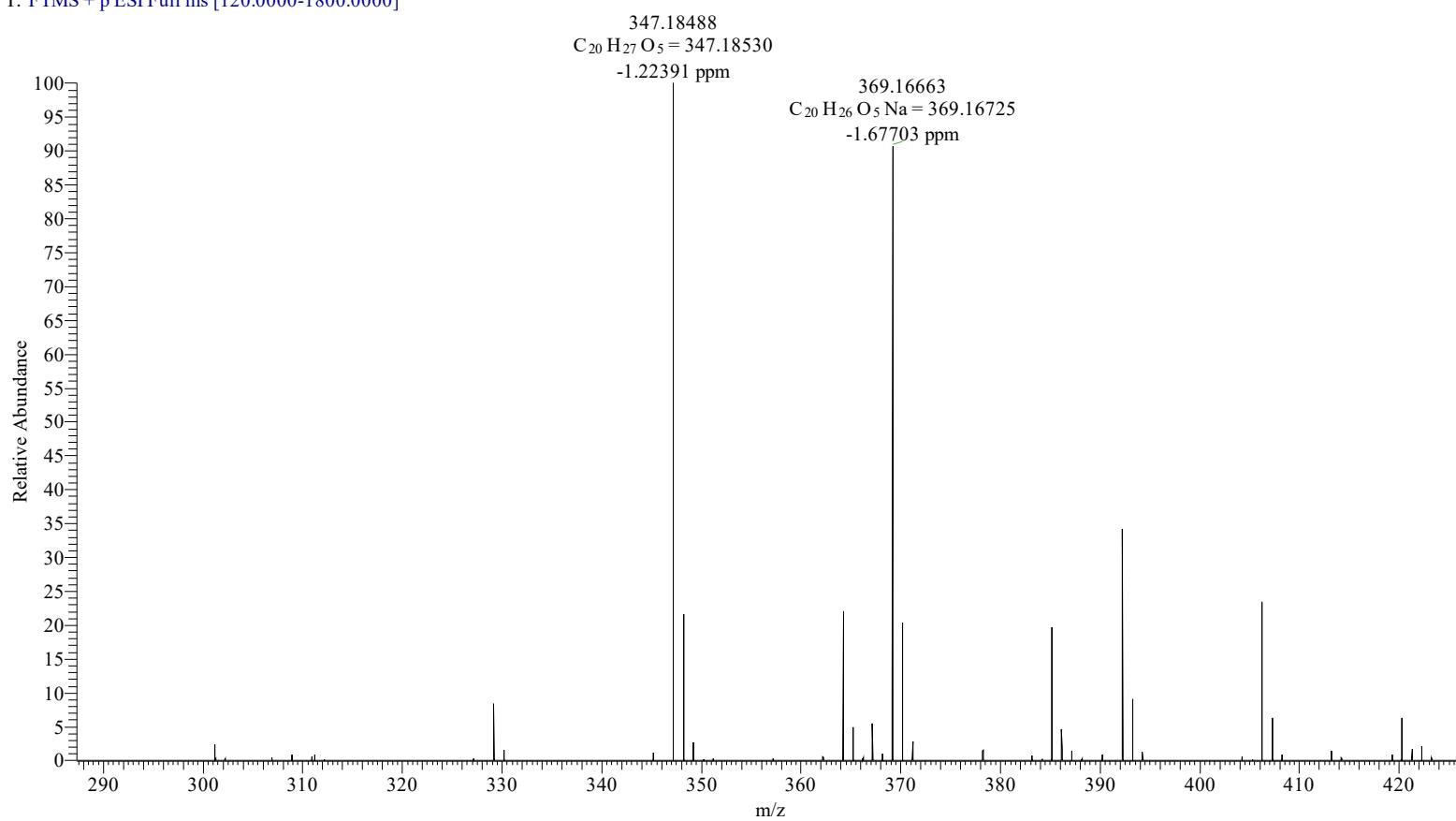
Figure S11. The HR-ESI-MS spectrum of **2**.
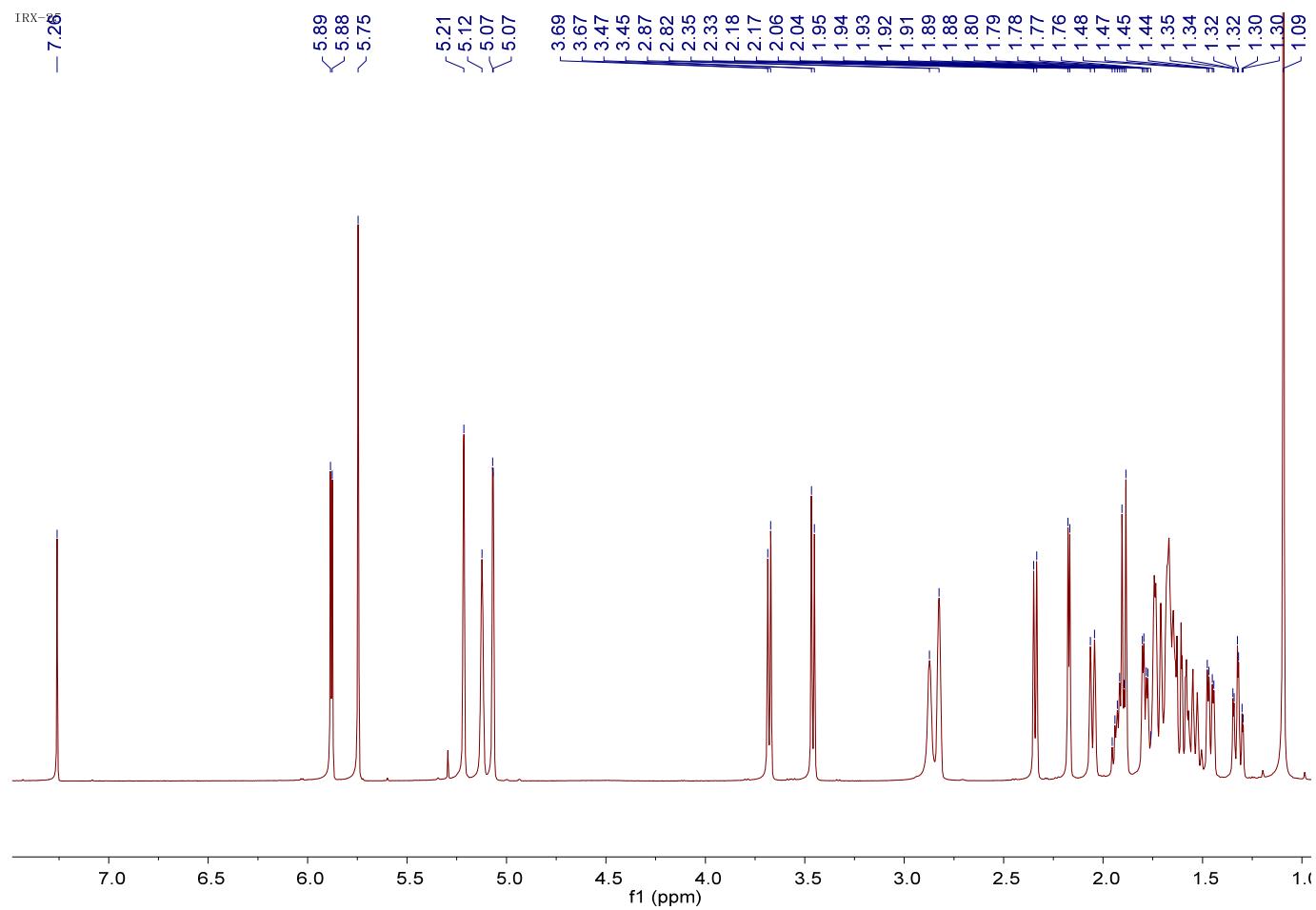
Figure S12. ^{1}H NMR spectrum of **2** in CDCl$_3$ (600 MHz)**.**
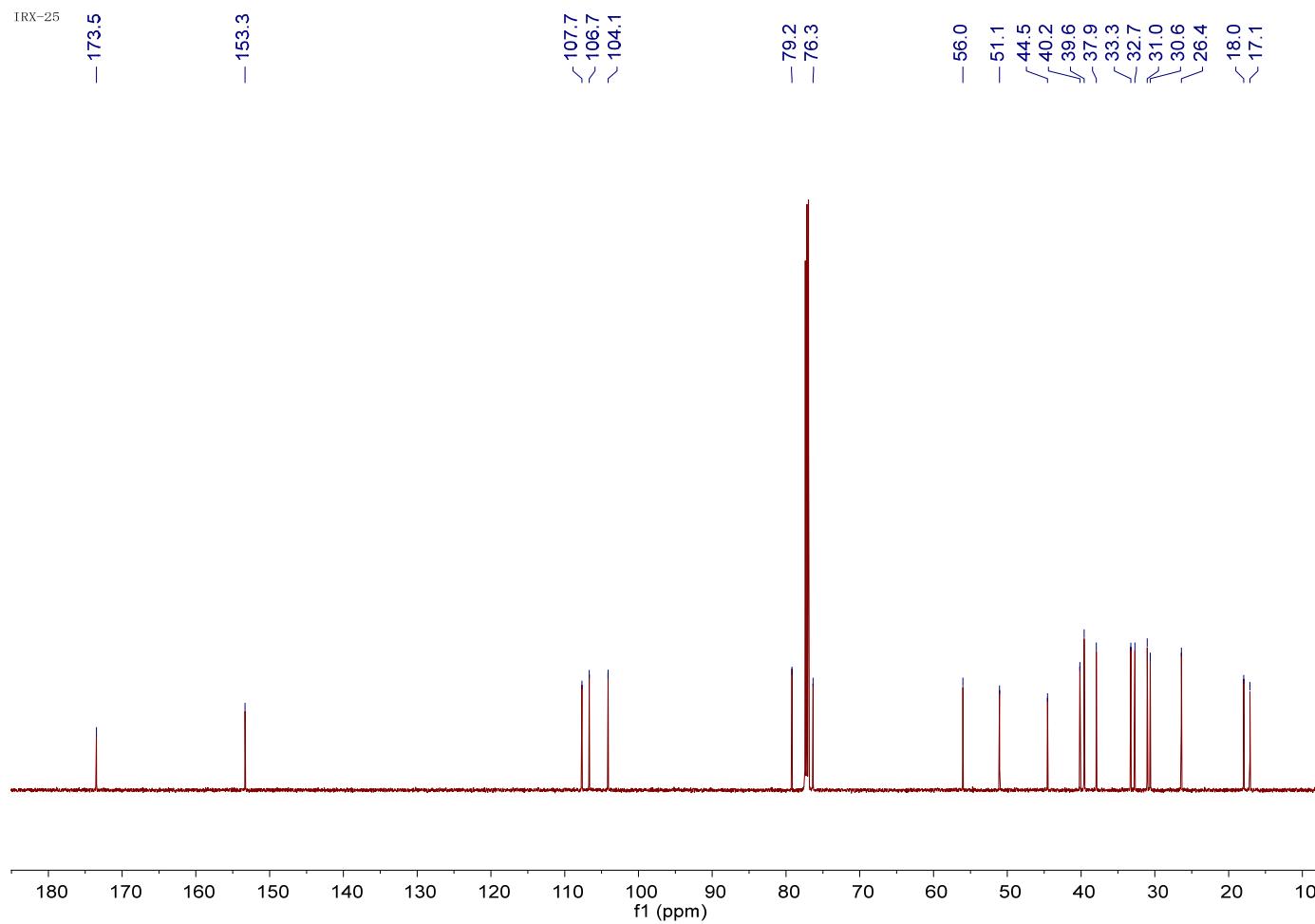
Figure S13. ^{13}C NMR spectrum of **2** in CDCl$_3$ (150 MHz).

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f1 (ppm)
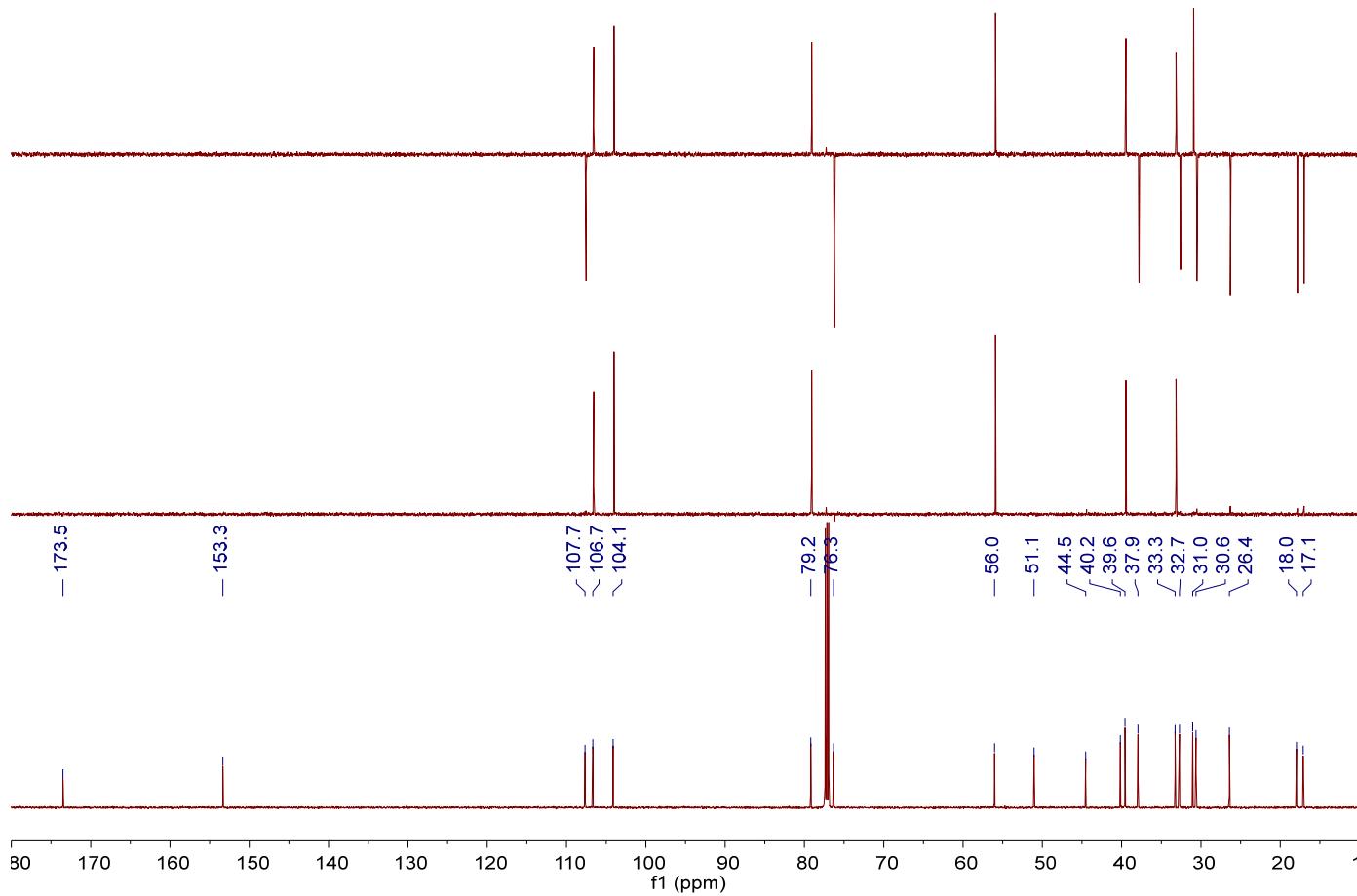
Figure S14. DEPT spectrum of **2** in CDCl₃.
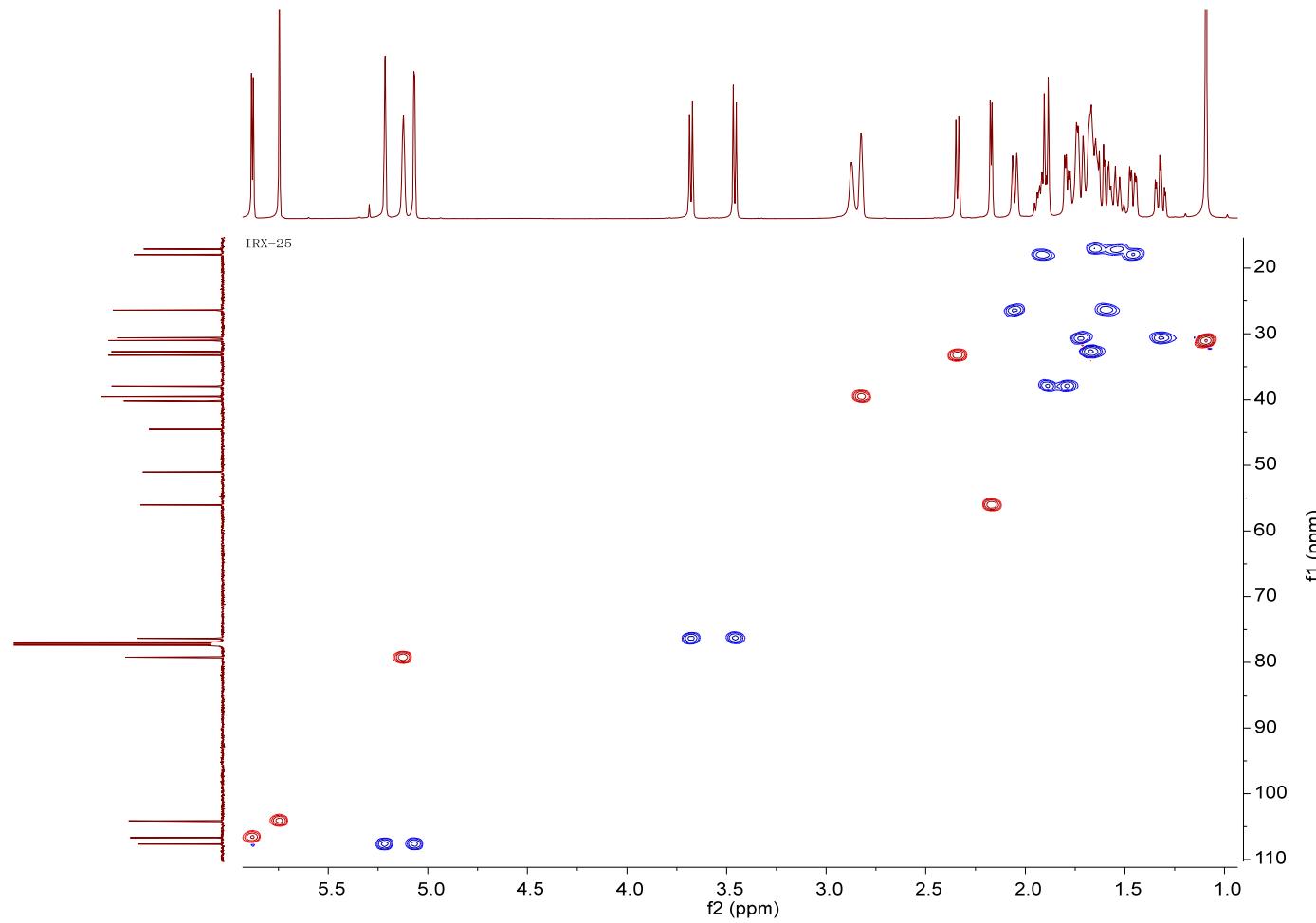
Figure S15. HSQC spectrum of **2** in CDCl₃.
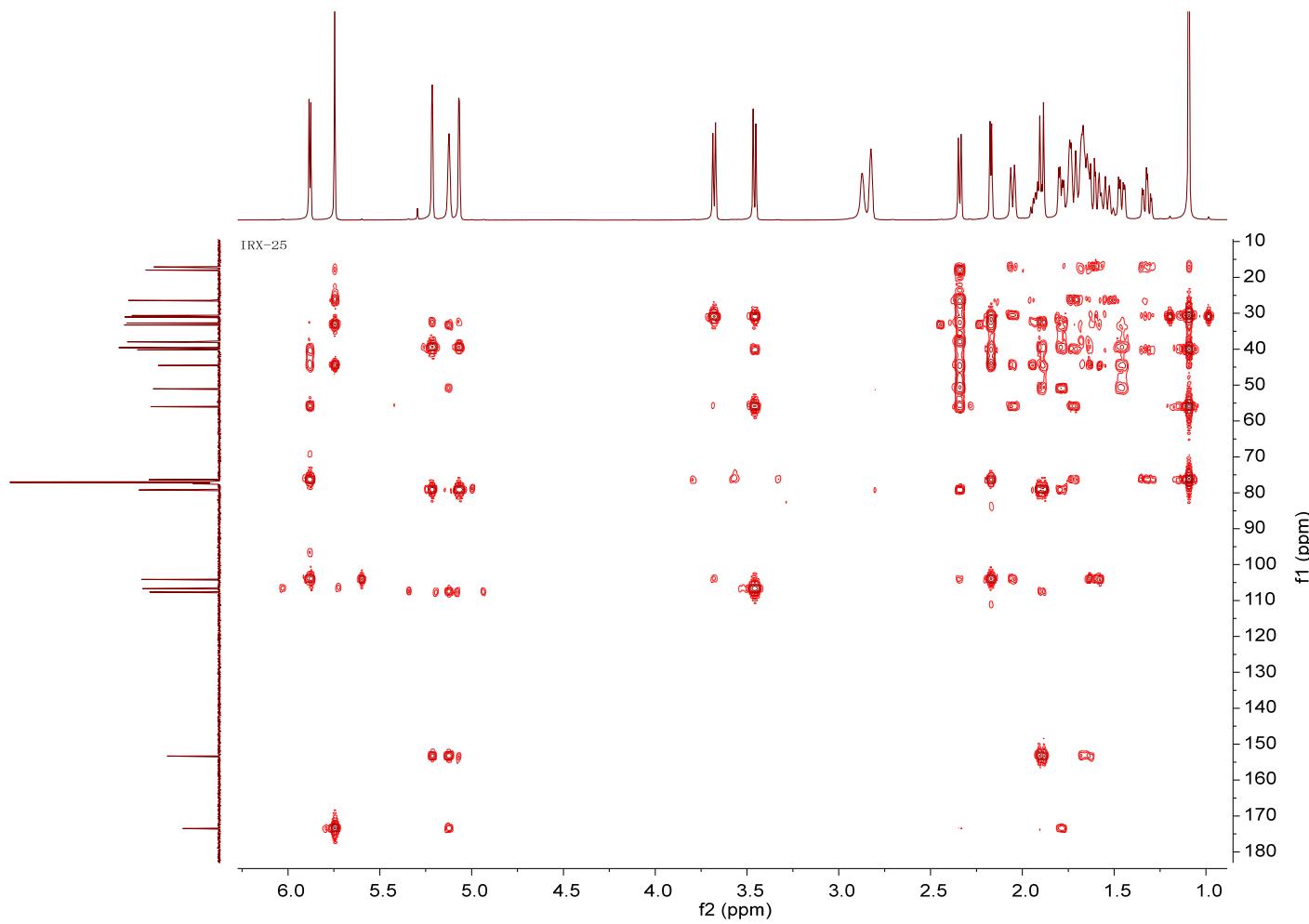
Figure S16. HMBC spectrum of **2** in CDCl3.
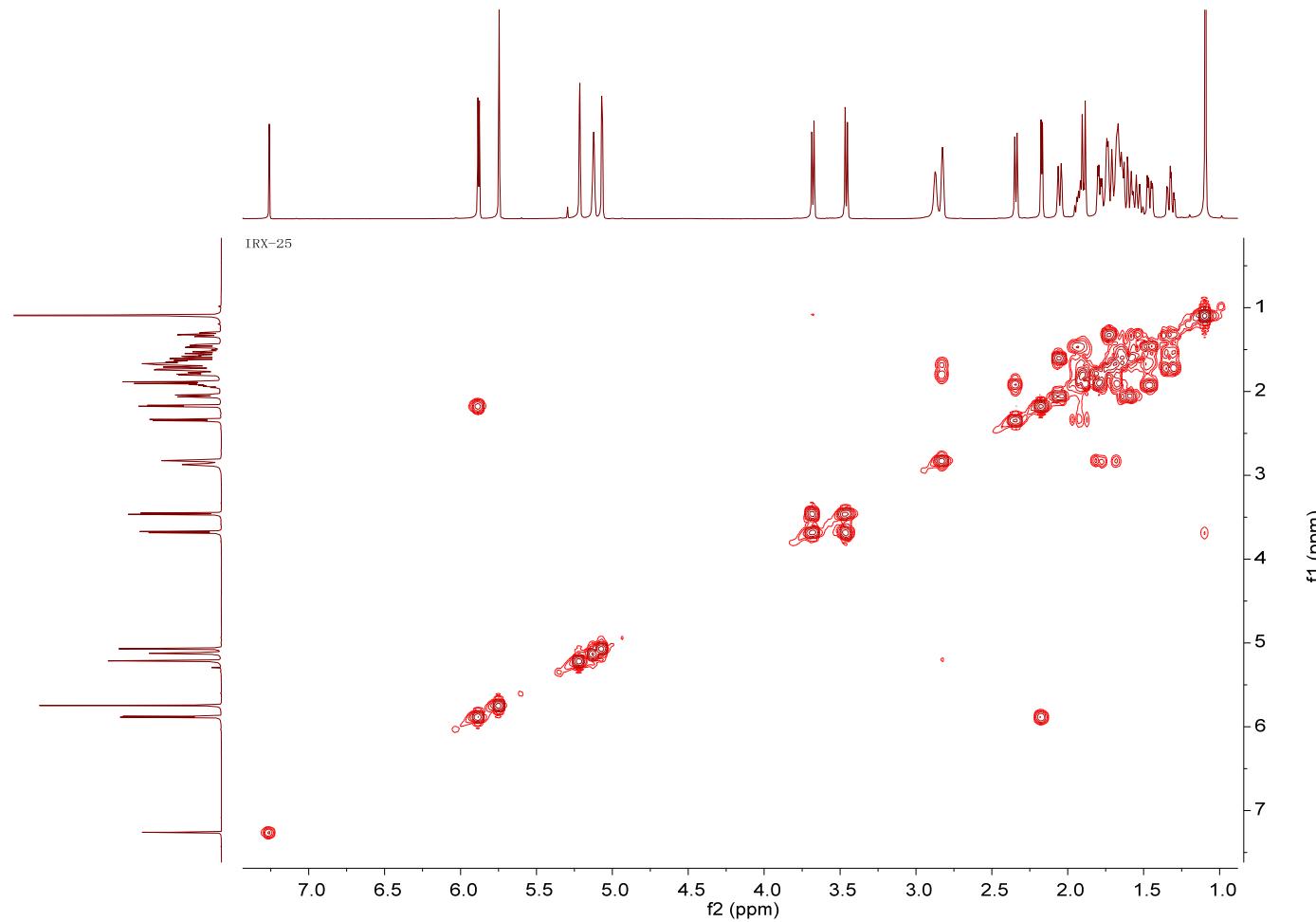
Figure S17. ^{1}H-^{1}H COSY spectrum of **2** in CDCl$_3$.
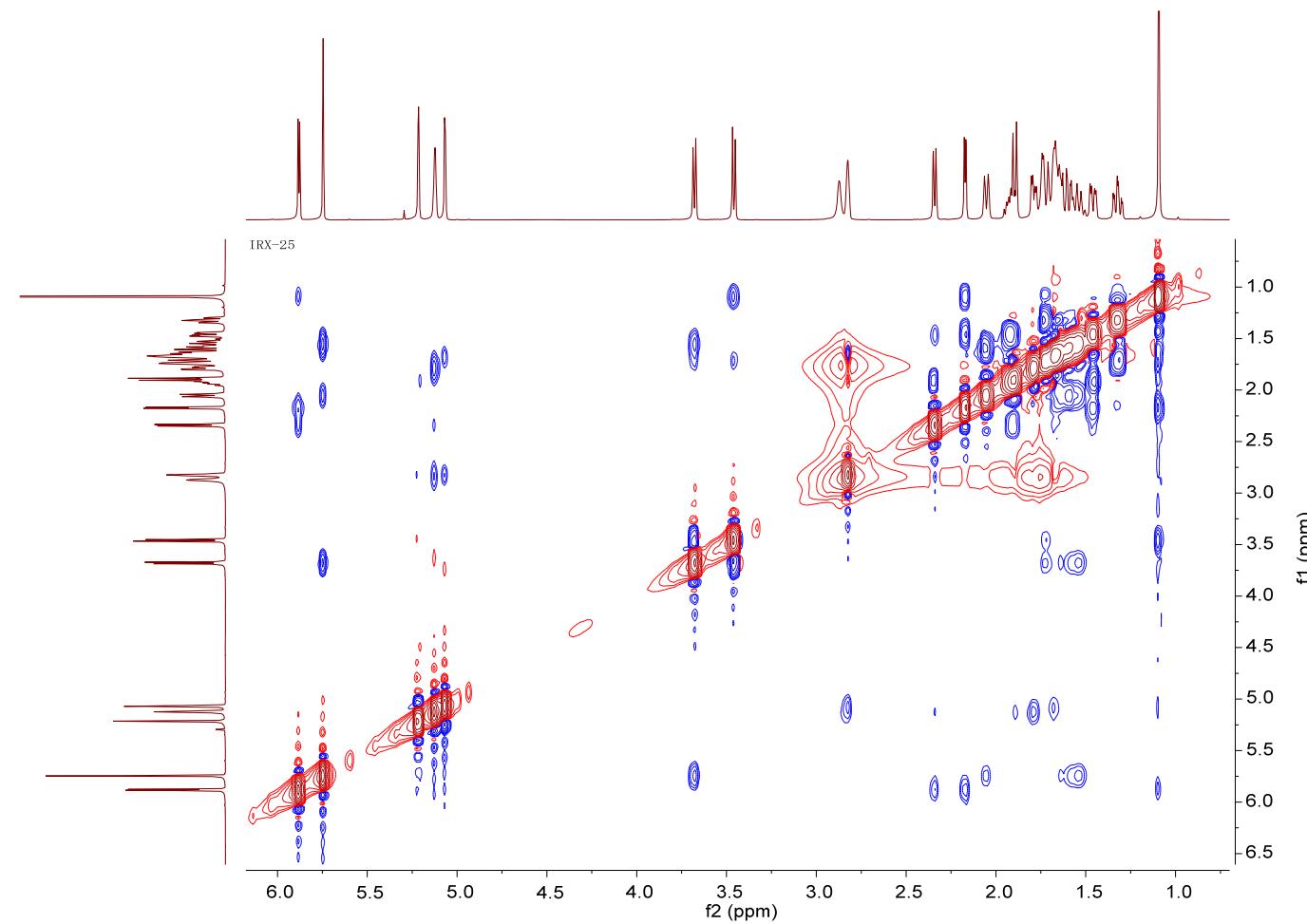
Figure S18. NOESY spectrum of **2** in CDCl₃.

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Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.
  (2009), J. Appl. Cryst. 42, 339-341.

Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.
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They are only intended as comments.
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At 1.5 times of:
All C(H,H,H) groups, All O(H) groups
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2.b Secondary CH2 refined with riding coordinates:
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C3(H3A,H3B), C2(H2A,H2B), C19(H19A,H19B)
2.c Idealised Me refined as rotating group:
C18(H18A,H18B,H18C), C23(H23A,H23B,H23C), C22(H22A,H22B,H22C)
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O1 0.0374(9) 0.0405(7) 0.0663(10) -0.0033(6) 0.0083(8) -0.0097(6)
O6 0.0469(9) 0.0519(8) 0.0458(8) 0.0088(6) -0.0030(7) -0.0132(7)
O5 0.0756(14) 0.0252(6) 0.0656(10) -0.0003(6) -0.0199(10) 0.0031(7)
O4 0.0939(18) 0.0898(13) 0.0354(8) 0.0162(9) 0.0101(10) 0.0041(13)
O2 0.0833(17) 0.0896(13) 0.0509(10) 0.0249(9) -0.0196(11) 0.0100(13)
C9 0.0337(10) 0.0223(6) 0.0282(7) 0.0001(5) -0.0012(7) -0.0011(6)
C15 0.0418(12) 0.0280(7) 0.0322(8) -0.0019(6) -0.0033(8) -0.0011(7)
C10 0.0334(10) 0.0286(7) 0.0320(8) -0.0006(6) -0.0053(7) -0.0008(7)
C16 0.0443(12) 0.0355(8) 0.0289(8) -0.0018(6) -0.0035(8) 0.0025(8)
C20 0.0378(12) 0.0349(8) 0.0496(10) -0.0004(7) -0.0128(9) 0.0034(8)
C11 0.0426(12) 0.0273(7) 0.0389(9) 0.0025(6) 0.0050(9) -0.0042(7)
C8 0.0393(11) 0.0236(6) 0.0313(8) -0.0012(6) -0.0015(8) 0.0007(7)
C14 0.0455(12) 0.0357(7) 0.0377(9) -0.0065(7) 0.0035(9) 0.0055(8)

C7 0.0479(12) 0.0244(7) 0.0423(9) -0.0010(6) -0.0050(9) 0.0060(8)
C5 0.0409(12) 0.0329(7) 0.0281(7) 0.0031(6) -0.0037(7) -0.0016(7)
C12 0.0545(14) 0.0378(8) 0.0367(9) 0.0083(7) 0.0064(10) -0.0042(9)
C1 0.0429(12) 0.0355(8) 0.0404(9) -0.0067(7) -0.0071(9) -0.0067(8)
C17 0.0477(13) 0.0471(10) 0.0353(9) 0.0048(7) -0.0028(9) 0.0097(9)
C13 0.0481(12) 0.0399(8) 0.0272(8) -0.0021(6) 0.0046(8) 0.0024(8)
C4 0.0444(12) 0.0468(10) 0.0345(9) -0.0031(7) 0.0033(9) 0.0041(9)
C21 0.0526(15) 0.0576(11) 0.0385(10) 0.0112(8) -0.0010(10) 0.0070(11)
C3 0.0622(17) 0.0455(10) 0.0473(11) -0.0140(8) 0.0014(12) 0.0095(10)
C2 0.0618(15) 0.0298(7) 0.0537(11) -0.0094(7) -0.0028(11) 0.0007(9)
C6 0.0710(18) 0.0501(10) 0.0333(10) 0.0102(8) -0.0066(11) 0.0003(12)
C18 0.0408(14) 0.0717(14) 0.0523(12) -0.0025(11) 0.0007(10) 0.0132(13)
C19 0.0663(18) 0.0762(16) 0.0478(12) 0.0040(11) 0.0188(13) 0.0002(15)
C23 0.093(3) 0.0840(19) 0.0554(15) 0.0022(13) -0.0285(17) 0.0015(19)
C22 0.112(3) 0.0673(15) 0.0616(16) 0.0209(13) -0.0081(19) 0.0332(19)

_geom_special_details
;
 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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   _geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
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O3 C20 1.457(2) . ?
O3 C7 1.328(3) . ?
O1 H1 0.8200 . ?
O1 C11 1.427(3) . ?
O6 C15 1.206(3) . ?
O5 C7 1.211(2) . ?
O4 C6 1.342(4) . ?
O4 C19 1.432(4) . ?
O2 C6 1.195(4) . ?
C9 H9 0.9800 . ?
C9 C10 1.553(2) . ?
C9 C11 1.541(2) . ?
C9 C8 1.579(2) . ?
C15 C16 1.529(2) . ?
C15 C8 1.533(3) . ?
C10 C20 1.528(3) . ?
C10 C5 1.555(3) . ?
C10 C1 1.541(2) . ?
C16 H16 0.9800 . ?
C16 C17 1.523(3) . ?
C16 C13 1.549(3) . ?
C20 H20A 0.9700 . ?
C20 H20B 0.9700 . ?
C11 H11 0.9800 . ?
C11 C12 1.536(3) . ?
C8 C14 1.551(3) . ?
C8 C7 1.509(2) . ?

C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?
C14 C13 1.529(3) . ?
C5 H5 0.9800 . ?
C5 C4 1.548(3) . ?
C5 C6 1.535(3) . ?
C12 H12A 0.9700 . ?
C12 H12B 0.9700 . ?
C12 C13 1.545(3) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C1 C2 1.525(3) . ?
C17 H17A 0.9700 . ?
C17 H17B 0.9700 . ?
C17 C21 1.538(3) . ?
C13 H13 0.9800 . ?
C4 C3 1.543(3) . ?
C4 C18 1.529(4) . ?
C4 C19 1.530(3) . ?
C21 H21 0.9800 . ?
C21 C23 1.523(5) . ?
C21 C22 1.518(4) . ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?
C3 C2 1.514(4) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?

C18 H18C 0.9600 . ?
C19 H19A 0.9700 . ?
C19 H19B 0.9700 . ?
C23 H23A 0.9600 . ?
C23 H23B 0.9600 . ?
C23 H23C 0.9600 . ?
C22 H22A 0.9600 . ?
C22 H22B 0.9600 . ?
C22 H22C 0.9600 . ?

loop_
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  _geom_angle_site_symmetry_3
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C7 O3 C20 118.67(15) . . ?
C11 O1 H1 109.5 . . ?
C6 O4 C19 109.33(19) . . ?
C10 C9 H9 105.8 . . ?
C10 C9 C8 111.07(12) . . ?
C11 C9 H9 105.8 . . ?
C11 C9 C10 116.81(15) . . ?
C11 C9 C8 110.59(14) . . ?
C8 C9 H9 105.8 . . ?
O6 C15 C16 126.5(2) . . ?
O6 C15 C8 126.26(18) . . ?

C16 C15 C8 107.26(17) . . ?
C9 C10 C5 108.79(15) . . ?
C20 C10 C9 106.64(14) . . ?
C20 C10 C5 111.93(15) . . ?
C20 C10 C1 108.11(16) . . ?
C1 C10 C9 113.07(14) . . ?
C1 C10 C5 108.37(15) . . ?
C15 C16 H16 106.6 . . ?
C15 C16 C13 104.12(17) . . ?
C17 C16 C15 112.93(16) . . ?
C17 C16 H16 106.6 . . ?
C17 C16 C13 119.18(17) . . ?
C13 C16 H16 106.6 . . ?
O3 C20 C10 111.47(18) . . ?
O3 C20 H20A 109.3 . . ?
O3 C20 H20B 109.3 . . ?
C10 C20 H20A 109.3 . . ?
C10 C20 H20B 109.3 . . ?
H20A C20 H20B 108.0 . . ?
O1 C11 C9 109.95(15) . . ?
O1 C11 H11 108.7 . . ?
O1 C11 C12 111.09(18) . . ?
C9 C11 H11 108.7 . . ?
C12 C11 C9 109.76(16) . . ?
C12 C11 H11 108.7 . . ?
C15 C8 C9 104.39(14) . . ?
C15 C8 C14 99.73(15) . . ?
C14 C8 C9 112.52(14) . . ?
C7 C8 C9 117.51(14) . . ?

C7 C8 C15 112.25(16) . . ?
C7 C8 C14 108.96(15) . . ?
C8 C14 H14A 111.7 . . ?
C8 C14 H14B 111.7 . . ?
H14A C14 H14B 109.5 . . ?
C13 C14 C8 100.19(15) . . ?
C13 C14 H14A 111.7 . . ?
C13 C14 H14B 111.7 . . ?
O3 C7 C8 120.37(16) . . ?
O5 C7 O3 118.72(18) . . ?
O5 C7 C8 120.78(19) . . ?
C10 C5 H5 107.5 . . ?
C4 C5 C10 117.79(14) . . ?
C4 C5 H5 107.5 . . ?
C6 C5 C10 115.60(19) . . ?
C6 C5 H5 107.5 . . ?
C6 C5 C4 100.23(16) . . ?
C11 C12 H12A 108.8 . . ?
C11 C12 H12B 108.8 . . ?
C11 C12 C13 113.66(15) . . ?
H12A C12 H12B 107.7 . . ?
C13 C12 H12A 108.8 . . ?
C13 C12 H12B 108.8 . . ?
C10 C1 H1A 109.0 . . ?
C10 C1 H1B 109.0 . . ?
H1A C1 H1B 107.8 . . ?
C2 C1 C10 112.78(18) . . ?
C2 C1 H1A 109.0 . . ?
C2 C1 H1B 109.0 . . ?

C16 C17 H17A 109.0 . . ?
C16 C17 H17B 109.0 . . ?
C16 C17 C21 113.11(18) . . ?
H17A C17 H17B 107.8 . . ?
C21 C17 H17A 109.0 . . ?
C21 C17 H17B 109.0 . . ?
C16 C13 H13 110.0 . . ?
C14 C13 C16 101.84(15) . . ?
C14 C13 C12 108.59(18) . . ?
C14 C13 H13 110.0 . . ?
C12 C13 C16 115.93(17) . . ?
C12 C13 H13 110.0 . . ?
C3 C4 C5 109.2(2) . . ?
C18 C4 C5 118.19(17) . . ?
C18 C4 C3 111.2(2) . . ?
C18 C4 C19 109.0(2) . . ?
C19 C4 C5 98.64(18) . . ?
C19 C4 C3 109.8(2) . . ?
C17 C21 H21 107.9 . . ?
C23 C21 C17 111.2(2) . . ?
C23 C21 H21 107.9 . . ?
C22 C21 C17 110.8(2) . . ?
C22 C21 H21 107.9 . . ?
C22 C21 C23 110.9(3) . . ?
C4 C3 H3A 109.1 . . ?
C4 C3 H3B 109.1 . . ?
H3A C3 H3B 107.8 . . ?
C2 C3 C4 112.51(18) . . ?
C2 C3 H3A 109.1 . . ?

C2 C3 H3B 109.1 . . ?
C1 C2 H2A 109.3 . . ?
C1 C2 H2B 109.3 . . ?
C3 C2 C1 111.50(18) . . ?
C3 C2 H2A 109.3 . . ?
C3 C2 H2B 109.3 . . ?
H2A C2 H2B 108.0 . . ?
O4 C6 C5 109.6(2) . . ?
O2 C6 O4 120.4(2) . . ?
O2 C6 C5 130.1(2) . . ?
C4 C18 H18A 109.5 . . ?
C4 C18 H18B 109.5 . . ?
C4 C18 H18C 109.5 . . ?
H18A C18 H18B 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
O4 C19 C4 106.2(3) . . ?
O4 C19 H19A 110.5 . . ?
O4 C19 H19B 110.5 . . ?
C4 C19 H19A 110.5 . . ?
C4 C19 H19B 110.5 . . ?
H19A C19 H19B 108.7 . . ?
C21 C23 H23A 109.5 . . ?
C21 C23 H23B 109.5 . . ?
C21 C23 H23C 109.5 . . ?
H23A C23 H23B 109.5 . . ?
H23A C23 H23C 109.5 . . ?
H23B C23 H23C 109.5 . . ?
C21 C22 H22A 109.5 . . ?

C21 C22 H22B 109.5 . . ?
C21 C22 H22C 109.5 . . ?
H22A C22 H22B 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?

_shelx_res_file
;
     a.res created by SHELXL-2014/7

TITL a_a.res in P2(1)2(1)2(1)
REM Old TITL a in P222 #16
REM SHELXT solution in P2(1)2(1)2(1)
REM R1 0.143, Rweak 0.039, Alpha 0.006, Orientation as input
REM Flack x = 0.081 (0.065) from Parsons' quotients
REM Formula found by SHELXT: C23 N O5
CELL 1.54178 8.016 13.0903 19.9957 90 90 90
ZERR 4 0.0004 0.0006 0.0009 0 0 0
LATT -1
SYMM 0.5-X,-Y,0.5+Z
SYMM -X,0.5+Y,0.5-Z
SYMM 0.5+X,0.5-Y,-Z
SFAC C H O
UNIT 92 128 24

L.S. 4
PLAN   20
SIZE 0.17 0.15 0.18
TEMP 0

BOND $H
list 4
fmap 2
ACTA
REM <olex2.extras>
REM <HklSrc "%.\\a.hkl">
REM </olex2.extras>

WGHT   0.100000
FVAR   0.70957
O3   3   0.075257   0.548722   0.676801   11.00000   0.04973   0.02945 =
             0.05393   0.00156   -0.01424   0.00973
O1   3   -0.041258   0.320335   0.787708   11.00000   0.03737   0.04054 =
             0.06633   -0.00328   0.00831   -0.00965
AFIX 147
H1   2   -0.099206   0.268902   0.784820   11.00000   -1.50000
AFIX   0
O6   3   0.534090   0.520102   0.755513   11.00000   0.04694   0.05187 =
             0.04581   0.00879   -0.00302   -0.01316
O5   3   0.224180   0.649988   0.739878   11.00000   0.07555   0.02524 =
             0.06561   -0.00029   -0.01994   0.00313
O4   3   0.394663   0.424473   0.506859   11.00000   0.09393   0.08982 =
             0.03541   0.01623   0.01013   0.00412
O2   3   0.133108   0.466946   0.525927   11.00000   0.08328   0.08958 =
             0.05093   0.02493   -0.01962   0.01004
C9   1   0.225684   0.364347   0.737692   11.00000   0.03374   0.02227 =
             0.02819   0.00013   -0.00123   -0.00109
AFIX   13
H9   2   0.339988   0.337983   0.735597   11.00000   -1.20000

```
AFIX    0
C15   1     0.423477      0.484497      0.789136      11.00000      0.04179     0.02796 =
            0.03216    -0.00187    -0.00329    -0.00105
C10   1     0.163697      0.369205      0.664156      11.00000      0.03344     0.02858 =
            0.03198    -0.00056    -0.00529    -0.00075
C16   1     0.441352      0.437424      0.858778      11.00000      0.04434     0.03550 =
            0.02894    -0.00178    -0.00347     0.00250
AFIX   13
H16   2     0.471148      0.493297      0.889132      11.00000     -1.20000
AFIX    0
C20   1     0.018850      0.445061      0.662815      11.00000      0.03783     0.03490 =
            0.04958    -0.00040    -0.01283     0.00337
AFIX   23
H20A  2    -0.033927      0.443220      0.619178      11.00000     -1.20000
H20B  2    -0.063595      0.425139      0.695842      11.00000     -1.20000
AFIX    0
C11   1     0.130647      0.292284      0.785240      11.00000      0.04264     0.02732 =
            0.03887     0.00249     0.00500    -0.00424
AFIX   13
H11   2     0.139199      0.222397      0.768005      11.00000     -1.20000
AFIX    0
C8    1     0.239660      0.474776      0.768912      11.00000      0.03928     0.02358 =
            0.03135    -0.00124    -0.00155     0.00066
C14   1     0.156712      0.482146      0.838841      11.00000      0.04554     0.03569 =
            0.03769    -0.00652     0.00348     0.00554
AFIX   23
H14A  2     0.166773      0.550194      0.857614      11.00000     -1.20000
H14B  2     0.040036      0.462619      0.837410      11.00000     -1.20000
AFIX    0
```

```
C7    1    0.181868    0.563522    0.726680    11.00000    0.04793    0.02444 =
           0.04228    -0.00098    -0.00499    0.00600
C5    1    0.310508    0.404202    0.618807    11.00000    0.04092    0.03288 =
           0.02811    0.00306    -0.00368    -0.00164
AFIX   13
H5    2    0.362679    0.463455    0.640253    11.00000    -1.20000
AFIX   0
C12   1    0.209885    0.295911    0.855151    11.00000    0.05454    0.03777 =
           0.03674    0.00830    0.00639    -0.00420
AFIX   23
H12A  2    0.307605    0.252210    0.855530    11.00000    -1.20000
H12B  2    0.131039    0.268633    0.887327    11.00000    -1.20000
AFIX   0
C1    1    0.099267    0.265675    0.638037    11.00000    0.04292    0.03548 =
           0.04043    -0.00673    -0.00712    -0.00668
AFIX   23
H1A   2    0.016961    0.239131    0.669063    11.00000    -1.20000
H1B   2    0.044502    0.276111    0.595322    11.00000    -1.20000
AFIX   0
C17   1    0.581871    0.359430    0.862971    11.00000    0.04773    0.04707 =
           0.03530    0.00481    -0.00280    0.00965
AFIX   23
H17A  2    0.683346    0.389915    0.845646    11.00000    -1.20000
H17B  2    0.554414    0.301451    0.834839    11.00000    -1.20000
AFIX   0
C13   1    0.261708    0.404422    0.877380    11.00000    0.04807    0.03994 =
           0.02723    -0.00210    0.00462    0.00243
AFIX   13
H13   2    0.243732    0.412517    0.925567    11.00000    -1.20000
```

```
AFIX    0
C4    1    0.450198    0.325868    0.603687    11.00000    0.04438    0.04678 =
          0.03452    -0.00306    0.00328    0.00406
C21   1    0.614096    0.321400    0.934603    11.00000    0.05261    0.05759 =
          0.03848    0.01119    -0.00097    0.00704
AFIX   13
H21   2    0.506038    0.314758    0.957110    11.00000    -1.20000
AFIX    0
C3    1    0.370575    0.224160    0.581303    11.00000    0.06215    0.04548 =
          0.04729    -0.01401    0.00138    0.00946
AFIX   23
H3A   2    0.321084    0.233129    0.537427    11.00000    -1.20000
H3B   2    0.457012    0.172621    0.577551    11.00000    -1.20000
AFIX    0
C2    1    0.238036    0.187028    0.629463    11.00000    0.06182    0.02983 =
          0.05373    -0.00941    -0.00278    0.00069
AFIX   23
H2A   2    0.288735    0.173275    0.672581    11.00000    -1.20000
H2B   2    0.190822    0.123674    0.612886    11.00000    -1.20000
AFIX    0
C6    1    0.262560    0.435728    0.547411    11.00000    0.07099    0.05012 =
          0.03333    0.01019    -0.00662    0.00028
C18   1    0.584131    0.308147    0.656909    11.00000    0.04075    0.07170 =
          0.05226    -0.00252    0.00074    0.01324
AFIX 137
H18A  2    0.615289    0.372346    0.676468    11.00000    -1.50000
H18B  2    0.680174    0.277150    0.636642    11.00000    -1.50000
H18C  2    0.540999    0.263820    0.691026    11.00000    -1.50000
AFIX    0
```

```
C19    1    0.529340    0.379396    0.543497    11.00000    0.06631    0.07622 =
            0.04783    0.00403    0.01879    0.00018
AFIX   23
H19A   2    0.607161    0.431505    0.558203    11.00000    -1.20000
H19B   2    0.588770    0.330579    0.515850    11.00000    -1.20000
AFIX    0
C23    1    0.718842    0.397645    0.973977    11.00000    0.09327    0.08402 =
            0.05538    0.00224    -0.02847    0.00153
AFIX 137
H23A   2    0.828296    0.401820    0.954685    11.00000    -1.50000
H23B   2    0.727472    0.375517    1.019619    11.00000    -1.50000
H23C   2    0.666762    0.463643    0.972439    11.00000    -1.50000
AFIX    0
C22    1    0.696200    0.216914    0.933838    11.00000    0.11204    0.06732 =
            0.06159    0.02092    -0.00811    0.03322
AFIX 137
H22A   2    0.624394    0.169004    0.911643    11.00000    -1.50000
H22B   2    0.715545    0.194714    0.978934    11.00000    -1.50000
H22C   2    0.800588    0.220943    0.910454    11.00000    -1.50000
AFIX    0
HKLF 4

REM    a_a.res in P2(1)2(1)2(1)
REM R1 =   0.0451 for      4267 Fo > 4sig(Fo)   and   0.0479 for all      4524 data
REM      266 parameters refined using         0 restraints

END

WGHT       0.0864       0.1146
```

REM Highest difference peak   0.336,   deepest hole -0.262,   1-sigma level   0.053

Q1	1	0.1932	0.3599	0.7016	11.00000	0.05	0.34
Q2	1	0.4296	0.4532	0.8231	11.00000	0.05	0.25
Q3	1	0.2055	0.4800	0.8022	11.00000	0.05	0.24
Q4	1	0.2189	0.4107	0.7490	11.00000	0.05	0.23
Q5	1	0.2795	0.4184	0.5862	11.00000	0.05	0.20
Q6	1	0.6017	0.3369	0.8984	11.00000	0.05	0.16
Q7	1	0.4867	0.4205	0.7148	11.00000	0.05	0.16
Q8	1	0.1684	0.5031	0.4757	11.00000	0.05	0.16
Q9	1	0.0864	0.2976	0.5846	11.00000	0.05	0.15
Q10	1	0.4156	0.4591	0.6939	11.00000	0.05	0.15
Q11	1	0.5640	0.2546	0.7516	11.00000	0.05	0.15
Q12	1	0.4336	0.2521	0.7740	11.00000	0.05	0.15
Q13	1	0.5744	0.3549	0.6915	11.00000	0.05	0.15
Q14	1	-0.0159	0.4835	0.6074	11.00000	0.05	0.15
Q15	1	0.0101	0.4632	0.6076	11.00000	0.05	0.14
Q16	1	0.0456	0.2961	0.9025	11.00000	0.05	0.14
Q17	1	0.2039	0.5134	0.7510	11.00000	0.05	0.14
Q18	1	0.1756	0.3354	0.7613	11.00000	0.05	0.14
Q19	1	0.6155	0.4196	0.7004	11.00000	0.05	0.14
Q20	1	0.4727	0.3860	0.7720	11.00000	0.05	0.14

Crystal Structure Report for Compound **2**

data_20190801WYXIRX25_0m_a

_audit_creation_method   'SHELXL-2018/3'
_shelx_SHELXL_version_number   '2018/3'
_chemical_name_systematic   ?
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 'C20 H26 O5'
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 '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'

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'O'   'O'     0.0106     0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'


_space_group_crystal_system          monoclinic
_space_group_IT_number                   4
_space_group_name_H-M_alt            'P 21'
_space_group_name_Hall               'P 2yb'


_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+1/2, -z'


_cell_length_a                     6.4646(2)
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_cell_length_c                     12.3769(5)
_cell_angle_alpha                  90
_cell_angle_beta                   94.1000(10)
_cell_angle_gamma                   90
_cell_volume                       1713.86(11)
_cell_formula_units_Z               4
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_exptl_crystal_colour                 ?
_exptl_crystal_density_meas           ?
_exptl_crystal_density_method         ?
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_exptl_crystal_F_000                  744
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_exptl_transmission_factor_max        ?
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_exptl_crystal_size_mid               ?
_exptl_crystal_size_min               ?
_exptl_absorpt_coefficient_mu         0.095
_shelx_estimated_absorpt_T_min        ?
_shelx_estimated_absorpt_T_max        ?
_exptl_absorpt_correction_type        multi-scan
_exptl_absorpt_correction_T_min    0.7060
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_exptl_absorpt_process_details
;
  SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D.,
  J. Appl. Cryst. 48 (2015) 3-10
;
_exptl_absorpt_special_details        ?
_diffrn_ambient_temperature           300(2)
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_diffrn_reflns_number                     57561
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_diffrn_reflns_limit_k_max               36
_diffrn_reflns_limit_l_min              -20
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_diffrn_reflns_theta_max                 37.058
_diffrn_reflns_theta_full               25.243
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_diffrn_measured_fraction_theta_full    0.993
_diffrn_reflns_Laue_measured_fraction_max       0.997
_diffrn_reflns_Laue_measured_fraction_full      0.993
_diffrn_reflns_point_group_measured_fraction_max     0.994
_diffrn_reflns_point_group_measured_fraction_full   0.993
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_reflns_threshold_expression           'I > 2\s(I)'
_reflns_Friedel_coverage                 0.954
_reflns_Friedel_fraction_max             0.991
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_reflns_Friedel_fraction_full   0.993

_reflns_special_details
;
  Reflections were merged by SHELXL according to the crystal
  class for the calculation of statistics and refinement.

  _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.
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_computing_cell_refinement   ?
_computing_data_reduction   ?
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_computing_structure_refinement 'SHELXL-2018/3 (Sheldrick, 2018)'
_computing_molecular_graphics   ?
_computing_publication_material   ?
_refine_special_details   ?
_refine_ls_structure_factor_coef   Fsqd
_refine_ls_matrix_type   full
_refine_ls_weighting_scheme   calc
_refine_ls_weighting_details
'w=1/[\s^2^(Fo^2^)+(0.0642P)^2^+0.0285P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   ?
_atom_sites_solution_hydrogens   geom

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_refine_ls_extinction_coef               .
_refine_ls_abs_structure_details
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  Flack x determined using 4495 quotients [(I+)-(I-)]/[(I+)+(I-)]
  (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
;
_refine_ls_abs_structure_Flack       -0.09(16)
_chemical_absolute_configuration    ?
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_refine_ls_number_parameters          456
_refine_ls_number_restraints           1
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_refine_ls_R_factor_gt                0.0466
_refine_ls_wR_factor_ref              0.1242
_refine_ls_wR_factor_gt               0.1086
_refine_ls_goodness_of_fit_ref       1.018
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_refine_ls_shift/su_mean              0.000

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O1 O -0.0372(2) 0.38817(6) 0.23593(9) 0.0462(3) Uani 1 1 d . . . . .
C1 C -0.1750(3) 0.39256(9) -0.05779(14) 0.0410(3) Uani 1 1 d . . . . .
H1A H -0.090981 0.386557 -0.118817 0.049 Uiso 1 1 calc R U . . .
H1AB H -0.285972 0.362070 -0.063575 0.049 Uiso 1 1 calc R U . . .
O2 O -0.2733(2) 0.31873(7) 0.16099(12) 0.0498(3) Uani 1 1 d . . . . .
C2 C -0.2691(4) 0.45773(11) -0.06413(17) 0.0557(5) Uani 1 1 d . . . . .
H2A H -0.350489 0.462602 -0.132550 0.067 Uiso 1 1 calc R U . . .
H2AB H -0.361049 0.463054 -0.006216 0.067 Uiso 1 1 calc R U . . .
O3 O -0.3011(2) 0.21873(7) 0.15082(13) 0.0516(3) Uani 1 1 d . . . . .
C3 C -0.1017(4) 0.50690(9) -0.05463(16) 0.0541(5) Uani 1 1 d . . . . .
H3A H -0.166421 0.547642 -0.059884 0.065 Uiso 1 1 calc R U . . .
H3AB H -0.015280 0.502590 -0.115097 0.065 Uiso 1 1 calc R U . . .
O4 O 0.2536(2) 0.21498(7) 0.17380(9) 0.0432(3) Uani 1 1 d . . . . .
H4 H 0.369(5) 0.2186(14) 0.1543(8) 0.065 Uiso 1 1 calc R U . . .
C4 C 0.0360(3) 0.50349(7) 0.05091(14) 0.0404(3) Uani 1 1 d . . . . .
O5 O 0.0324(3) 0.49479(7) 0.23976(11) 0.0506(3) Uani 1 1 d . . . . .
C5 C 0.1025(2) 0.43620(7) 0.08362(12) 0.0308(3) Uani 1 1 d . . . . .
H5 H 0.243347 0.428261 0.062575 0.037 Uiso 1 1 calc R U . . .
C6 C 0.1006(3) 0.43555(8) 0.20852(13) 0.0383(3) Uani 1 1 d . . . . .
H6 H 0.240154 0.427226 0.241601 0.046 Uiso 1 1 calc R U . . .

C7 C -0.2060(2) 0.26404(8) 0.12566(12) 0.0353(3) Uani 1 1 d . . . . .
C8 C -0.0306(2) 0.26095(7) 0.05123(11) 0.0286(2) Uani 1 1 d . . . . .
C9 C 0.09464(19) 0.32160(6) 0.04707(10) 0.0249(2) Uani 1 1 d . . . . .
H9 H 0.180382 0.322867 0.115607 0.030 Uiso 1 1 calc R U . . .
C10 C -0.0409(2) 0.38108(7) 0.04721(11) 0.0276(2) Uani 1 1 d . . . . .
C12 C 0.1897(3) 0.28024(8) -0.14346(13) 0.0388(3) Uani 1 1 d . . . . .
H12A H 0.097553 0.304162 -0.192905 0.047 Uiso 1 1 calc R U . . .
H12B H 0.312983 0.270231 -0.180236 0.047 Uiso 1 1 calc R U . . .
C11 C 0.2507(2) 0.31966(8) -0.04219(12) 0.0326(3) Uani 1 1 d . . . . .
H11A H 0.274063 0.362048 -0.065503 0.039 Uiso 1 1 calc R U . . .
H11B H 0.381726 0.304038 -0.009951 0.039 Uiso 1 1 calc R U . . .
C13 C 0.0818(3) 0.22008(8) -0.11324(13) 0.0380(3) Uani 1 1 d . . . . .
H13 H 0.054951 0.192676 -0.175989 0.046 Uiso 1 1 calc R U . . .
C14 C -0.1180(3) 0.23752(8) -0.06143(13) 0.0365(3) Uani 1 1 d . . . . .
H14A H -0.207779 0.201707 -0.055198 0.044 Uiso 1 1 calc R U . . .
H14B H -0.193201 0.270067 -0.101886 0.044 Uiso 1 1 calc R U . . .
C15 C 0.1138(2) 0.20458(7) 0.08336(12) 0.0335(3) Uani 1 1 d . . . . .
H15 H 0.024119 0.169921 0.101626 0.040 Uiso 1 1 calc R U . . .
C16 C 0.2072(3) 0.18767(7) -0.02171(13) 0.0353(3) Uani 1 1 d . . . . .
C17 C 0.3726(3) 0.15253(9) -0.03023(17) 0.0454(4) Uani 1 1 d . . . . .
H17A H 0.422869 0.145669 -0.097758 0.055 Uiso 1 1 calc R U . . .
H17B H 0.438881 0.134623 0.031296 0.055 Uiso 1 1 calc R U . . .
C18 C 0.2303(4) 0.54336(9) 0.0434(2) 0.0628(6) Uani 1 1 d . . . . .
H18A H 0.309812 0.527670 -0.013332 0.094 Uiso 1 1 calc R U . . .
H18B H 0.312569 0.541789 0.111033 0.094 Uiso 1 1 calc R U . . .
H18C H 0.190630 0.585658 0.027653 0.094 Uiso 1 1 calc R U . . .
C19 C -0.0761(3) 0.52468(9) 0.14936(15) 0.0461(4) Uani 1 1 d . . . . .
H19A H -0.069790 0.569606 0.157061 0.055 Uiso 1 1 calc R U . . .
H19B H -0.220381 0.511907 0.142672 0.055 Uiso 1 1 calc R U . . .

C20 C -0.1733(3) 0.37657(8) 0.14455(14) 0.0379(3) Uani 1 1 d . . . . .
H20 H -0.278376 0.409527 0.138831 0.046 Uiso 1 1 calc R U . . .
C1_1 C 0.7001(3) 0.68442(10) 0.55496(16) 0.0464(4) Uani 1 1 d . . . . .
H1A_1 H 0.668846 0.676647 0.629261 0.056 Uiso 1 1 calc R U . . .
H1AB_1 H 0.795605 0.652342 0.534666 0.056 Uiso 1 1 calc R U . . .
O1_1 O 0.3708(3) 0.69379(8) 0.30023(10) 0.0570(4) Uani 1 1 d . . . . .
C2_1 C 0.8066(3) 0.74738(13) 0.5494(2) 0.0568(5) Uani 1 1 d . . . . .
H2A_1 H 0.927276 0.748086 0.600740 0.068 Uiso 1 1 calc R U . . .
H2AB_1 H 0.853788 0.753261 0.477494 0.068 Uiso 1 1 calc R U . . .
O2_1 O 0.5851(3) 0.61058(8) 0.32462(11) 0.0557(4) Uani 1 1 d . . . . .
C3_1 C 0.6635(4) 0.80004(11) 0.57461(18) 0.0546(5) Uani 1 1 d . . . . .
H3A_1 H 0.737833 0.839080 0.570172 0.065 Uiso 1 1 calc R U . . .
H3AB_1 H 0.624623 0.795456 0.648452 0.065 Uiso 1 1 calc R U . . .
O3_1 O 0.5223(3) 0.51119(8) 0.31487(13) 0.0594(4) Uani 1 1 d . . . . .
C4_1 C 0.4666(3) 0.80312(9) 0.49886(14) 0.0435(4) Uani 1 1 d . . . . .
O4_1 O 0.0431(2) 0.53472(8) 0.45117(11) 0.0490(3) Uani 1 1 d . . . . .
H4_1 H 0.012091 0.523513 0.388769 0.074 Uiso 1 1 calc R U . . .
C5_1 C 0.3649(3) 0.73897(8) 0.47610(12) 0.0353(3) Uani 1 1 d . . . . .
H5_1 H 0.248497 0.733842 0.521912 0.042 Uiso 1 1 calc R U . . .
O5_1 O 0.3371(3) 0.80133(8) 0.31643(13) 0.0665(5) Uani 1 1 d . . . . .
C6_1 C 0.2805(3) 0.74293(10) 0.35606(15) 0.0476(4) Uani 1 1 d . . . . .
H6_1 H 0.129218 0.738681 0.350595 0.057 Uiso 1 1 calc R U . . .
C7_1 C 0.5066(3) 0.55795(9) 0.36600(14) 0.0423(4) Uani 1 1 d . . . . .
C8_1 C 0.4229(2) 0.56001(8) 0.47695(12) 0.0354(3) Uani 1 1 d . . . . .
C9_1 C 0.3526(2) 0.62514(7) 0.51032(11) 0.0323(3) Uani 1 1 d . . . . .
H9_1 H 0.223002 0.632712 0.466263 0.039 Uiso 1 1 calc R U . . .
C10_1 C 0.4985(2) 0.67894(8) 0.48164(11) 0.0339(3) Uani 1 1 d . . . . .
C11_1 C 0.2909(3) 0.62560(9) 0.62927(12) 0.0423(4) Uani 1 1 d . . . . .
H11A_1 H 0.304470 0.667851 0.656576 0.051 Uiso 1 1 calc R U . . .

H11B_1 H 0.145668 0.614233 0.629322 0.051 Uiso 1 1 calc R U . . .
C12_1 C 0.4157(4) 0.58248(10) 0.70800(14) 0.0546(5) Uani 1 1 d . . . . .
H12A_1 H 0.340347 0.576144 0.772110 0.065 Uiso 1 1 calc R U . . .
H12B_1 H 0.547357 0.601920 0.730306 0.065 Uiso 1 1 calc R U . . .
C13_1 C 0.4552(4) 0.51932(10) 0.65529(16) 0.0549(5) Uani 1 1 d . . . . .
H13_1 H 0.522711 0.490025 0.707300 0.066 Uiso 1 1 calc R U . . .
C14_1 C 0.5853(3) 0.53033(10) 0.55913(17) 0.0494(4) Uani 1 1 d . . . . .
H14A_1 H 0.638753 0.491596 0.531977 0.059 Uiso 1 1 calc R U . . .
H14B_1 H 0.699696 0.558510 0.577517 0.059 Uiso 1 1 calc R U . . .
C15_1 C 0.2421(3) 0.51231(8) 0.48458(14) 0.0406(3) Uani 1 1 d . . . . .
H15_1 H 0.271123 0.475826 0.440559 0.049 Uiso 1 1 calc R U . . .
C16_1 C 0.2574(4) 0.49306(9) 0.60296(15) 0.0492(4) Uani 1 1 d . . . . .
C17_1 C 0.1174(5) 0.45913(13) 0.6492(2) 0.0674(6) Uani 1 1 d . . . . .
H17A_1 H 0.136544 0.449129 0.722293 0.081 Uiso 1 1 calc R U . . .
H17B_1 H -0.000236 0.445289 0.608484 0.081 Uiso 1 1 calc R U . . .
C18_1 C 0.3092(4) 0.84631(10) 0.5474(2) 0.0580(5) Uani 1 1 d . . . . .
H18A_1 H 0.371423 0.886321 0.561767 0.087 Uiso 1 1 calc R U . . .
H18B_1 H 0.267351 0.828738 0.613745 0.087 Uiso 1 1 calc R U . . .
H18C_1 H 0.190073 0.850948 0.497117 0.087 Uiso 1 1 calc R U . . .
C19_1 C 0.5051(4) 0.82555(11) 0.38483(17) 0.0587(5) Uani 1 1 d . . . . .
H19A_1 H 0.506970 0.870682 0.381894 0.070 Uiso 1 1 calc R U . . .
H19B_1 H 0.636539 0.809921 0.362920 0.070 Uiso 1 1 calc R U . . .
C20_1 C 0.5459(3) 0.67154(9) 0.36283(14) 0.0445(4) Uani 1 1 d . . . . .
H20_1 H 0.664683 0.698035 0.349252 0.053 Uiso 1 1 calc R U . . .

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_atom_site_aniso_U_33
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C1 0.0442(8) 0.0452(8) 0.0320(7) 0.0002(6) -0.0084(6) 0.0072(7)
O2 0.0441(6) 0.0519(7) 0.0568(7) -0.0016(6) 0.0277(6) -0.0086(6)
C2 0.0616(12) 0.0618(12) 0.0413(9) 0.0043(8) -0.0125(8) 0.0271(10)
O3 0.0450(7) 0.0547(8) 0.0566(8) 0.0131(6) 0.0130(6) -0.0158(6)
C3 0.0854(15) 0.0413(9) 0.0360(8) 0.0085(7) 0.0068(9) 0.0219(10)
O4 0.0426(6) 0.0576(7) 0.0287(5) 0.0052(5) -0.0025(4) 0.0077(6)
C4 0.0539(9) 0.0282(7) 0.0401(8) 0.0023(6) 0.0107(7) 0.0086(6)
O5 0.0730(9) 0.0434(7) 0.0345(6) -0.0101(5) -0.0033(6) 0.0138(6)
C5 0.0344(6) 0.0269(6) 0.0314(6) 0.0001(5) 0.0043(5) 0.0017(5)
C6 0.0474(8) 0.0353(7) 0.0311(7) -0.0052(6) -0.0032(6) 0.0045(6)
C7 0.0299(6) 0.0450(8) 0.0308(6) 0.0074(6) 0.0021(5) -0.0082(6)
C8 0.0282(6) 0.0320(6) 0.0256(5) 0.0033(5) 0.0012(4) -0.0053(5)
C9 0.0248(5) 0.0282(5) 0.0217(5) 0.0020(4) 0.0021(4) -0.0025(5)
C10 0.0280(6) 0.0314(6) 0.0238(5) 0.0023(5) 0.0031(4) 0.0004(5)
C12 0.0514(9) 0.0388(8) 0.0275(6) 0.0010(6) 0.0110(6) 0.0009(7)
C11 0.0339(6) 0.0321(6) 0.0332(6) 0.0000(5) 0.0114(5) -0.0041(6)
C13 0.0506(9) 0.0353(7) 0.0276(6) -0.0049(5) -0.0009(6) -0.0031(6)
C14 0.0396(7) 0.0371(7) 0.0317(6) 0.0000(6) -0.0061(5) -0.0082(6)
C15 0.0376(7) 0.0309(6) 0.0318(6) 0.0057(5) 0.0010(5) -0.0039(5)
C16 0.0426(7) 0.0290(6) 0.0339(7) -0.0020(5) -0.0001(6) -0.0043(6)
C17 0.0499(9) 0.0395(8) 0.0467(9) -0.0067(7) 0.0022(7) 0.0019(7)
C18 0.0719(14) 0.0301(8) 0.0893(17) 0.0047(9) 0.0258(13) -0.0019(8)
C19 0.0601(10) 0.0397(8) 0.0387(8) -0.0035(7) 0.0047(7) 0.0159(8)
C20 0.0382(7) 0.0411(8) 0.0360(7) 0.0005(6) 0.0132(6) 0.0012(6)

C1_1 0.0370(7) 0.0583(10) 0.0429(9) -0.0033(8) -0.0028(7) 0.0019(8)
O1_1 0.0813(10) 0.0616(9) 0.0270(5) -0.0050(5) -0.0038(6) 0.0097(8)
C2_1 0.0396(9) 0.0700(13) 0.0600(12) -0.0074(10) -0.0017(8) -0.0118(9)
O2_1 0.0744(10) 0.0574(8) 0.0387(6) -0.0084(6) 0.0263(7) 0.0059(7)
C3_1 0.0594(11) 0.0585(11) 0.0460(10) -0.0110(9) 0.0049(9) -0.0164(9)
O3_1 0.0626(9) 0.0637(9) 0.0543(8) -0.0260(7) 0.0202(7) 0.0015(7)
C4_1 0.0544(9) 0.0429(9) 0.0345(7) -0.0023(6) 0.0117(7) -0.0063(7)
O4_1 0.0419(6) 0.0657(9) 0.0392(6) -0.0133(6) 0.0009(5) -0.0004(6)
C5_1 0.0383(7) 0.0401(7) 0.0277(6) 0.0001(6) 0.0038(5) 0.0009(6)
O5_1 0.1024(13) 0.0534(8) 0.0421(7) 0.0134(6) -0.0068(8) -0.0029(9)
C6_1 0.0580(10) 0.0494(10) 0.0344(8) 0.0041(7) -0.0050(7) 0.0030(8)
C7_1 0.0374(7) 0.0559(10) 0.0340(7) -0.0123(7) 0.0056(6) 0.0065(7)
C8_1 0.0370(7) 0.0413(8) 0.0278(6) -0.0061(6) 0.0010(5) 0.0069(6)
C9_1 0.0357(7) 0.0395(7) 0.0220(5) -0.0034(5) 0.0034(5) 0.0044(6)
C10_1 0.0353(6) 0.0438(8) 0.0229(5) -0.0035(5) 0.0040(5) 0.0023(6)
C11_1 0.0594(10) 0.0424(8) 0.0261(6) -0.0038(6) 0.0110(7) 0.0023(7)
C12_1 0.0833(14) 0.0537(11) 0.0257(7) 0.0005(7) -0.0030(8) -0.0016(10)
C13_1 0.0765(14) 0.0490(10) 0.0370(8) 0.0058(8) -0.0114(9) 0.0083(10)
C14_1 0.0511(9) 0.0478(10) 0.0475(9) -0.0025(8) -0.0091(8) 0.0145(8)
C15_1 0.0482(8) 0.0414(8) 0.0324(7) -0.0091(6) 0.0042(6) 0.0020(7)
C16_1 0.0700(12) 0.0390(8) 0.0389(8) -0.0010(7) 0.0064(8) 0.0045(8)
C17_1 0.0896(18) 0.0575(13) 0.0569(13) 0.0054(10) 0.0180(12) -0.0035(12)
C18_1 0.0784(15) 0.0396(9) 0.0582(12) -0.0044(8) 0.0203(11) 0.0031(9)
C19_1 0.0841(15) 0.0526(11) 0.0411(9) 0.0036(9) 0.0154(9) -0.0147(11)
C20_1 0.0542(9) 0.0507(10) 0.0300(7) -0.0021(7) 0.0119(7) 0.0003(8)

_geom_special_details
;
 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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O1 C20 1.405(2) . ?
O1 C6 1.410(2) . ?
C1 C2 1.526(3) . ?
C1 C10 1.530(2) . ?
C1 H1A 0.9700 . ?
C1 H1AB 0.9700 . ?
O2 C7 1.337(2) . ?
O2 C20 1.422(2) . ?
C2 C3 1.511(4) . ?
C2 H2A 0.9700 . ?
C2 H2AB 0.9700 . ?
O3 C7 1.204(2) . ?
C3 C4 1.529(3) . ?
C3 H3A 0.9700 . ?
C3 H3AB 0.9700 . ?
O4 C15 1.405(2) . ?

O4 H4 0.80(3) . ?
C4 C18 1.529(3) . ?
C4 C19 1.531(2) . ?
C4 C5 1.553(2) . ?
O5 C6 1.409(2) . ?
O5 C19 1.430(2) . ?
C5 C6 1.547(2) . ?
C5 C10 1.550(2) . ?
C5 H5 0.9800 . ?
C6 H6 0.9800 . ?
C7 C8 1.513(2) . ?
C8 C9 1.5365(19) . ?
C8 C14 1.550(2) . ?
C8 C15 1.563(2) . ?
C9 C11 1.5490(18) . ?
C9 C10 1.5490(19) . ?
C9 H9 0.9800 . ?
C10 C20 1.530(2) . ?
C12 C13 1.527(2) . ?
C12 C11 1.540(2) . ?
C12 H12A 0.9700 . ?
C12 H12B 0.9700 . ?
C11 H11A 0.9700 . ?
C11 H11B 0.9700 . ?
C13 C16 1.514(2) . ?
C13 C14 1.529(2) . ?
C13 H13 0.9800 . ?
C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?

C15 C16 1.516(2) . ?
C15 H15 0.9800 . ?
C16 C17 1.319(3) . ?
C17 H17A 0.9300 . ?
C17 H17B 0.9300 . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C19 H19A 0.9700 . ?
C19 H19B 0.9700 . ?
C20 H20 0.9800 . ?
C1_1 C2_1 1.521(3) . ?
C1_1 C10_1 1.538(2) . ?
C1_1 H1A_1 0.9700 . ?
C1_1 H1AB_1 0.9700 . ?
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O1_1 C6_1 1.410(3) . ?
C2_1 C3_1 1.508(3) . ?
C2_1 H2A_1 0.9700 . ?
C2_1 H2AB_1 0.9700 . ?
O2_1 C7_1 1.354(3) . ?
O2_1 C20_1 1.421(2) . ?
C3_1 C4_1 1.527(3) . ?
C3_1 H3A_1 0.9700 . ?
C3_1 H3AB_1 0.9700 . ?
O3_1 C7_1 1.195(2) . ?
C4_1 C19_1 1.528(3) . ?
C4_1 C18_1 1.531(3) . ?
C4_1 C5_1 1.544(2) . ?

O4_1 C15_1 1.408(2) . ?
O4_1 H4_1 0.8200 . ?
C5_1 C6_1 1.548(2) . ?
C5_1 C10_1 1.551(2) . ?
C5_1 H5_1 0.9800 . ?
O5_1 C6_1 1.405(3) . ?
O5_1 C19_1 1.427(3) . ?
C6_1 H6_1 0.9800 . ?
C7_1 C8_1 1.512(2) . ?
C8_1 C9_1 1.536(2) . ?
C8_1 C14_1 1.546(2) . ?
C8_1 C15_1 1.562(3) . ?
C9_1 C10_1 1.549(2) . ?
C9_1 C11_1 1.553(2) . ?
C9_1 H9_1 0.9800 . ?
C10_1 C20_1 1.532(2) . ?
C11_1 C12_1 1.532(3) . ?
C11_1 H11A_1 0.9700 . ?
C11_1 H11B_1 0.9700 . ?
C12_1 C13_1 1.534(3) . ?
C12_1 H12A_1 0.9700 . ?
C12_1 H12B_1 0.9700 . ?
C13_1 C16_1 1.502(3) . ?
C13_1 C14_1 1.524(3) . ?
C13_1 H13_1 0.9800 . ?
C14_1 H14A_1 0.9700 . ?
C14_1 H14B_1 0.9700 . ?
C15_1 C16_1 1.519(3) . ?
C15_1 H15_1 0.9800 . ?

C16_1 C17_1 1.323(3) . ?
C17_1 H17A_1 0.9300 . ?
C17_1 H17B_1 0.9300 . ?
C18_1 H18A_1 0.9600 . ?
C18_1 H18B_1 0.9600 . ?
C18_1 H18C_1 0.9600 . ?
C19_1 H19A_1 0.9700 . ?
C19_1 H19B_1 0.9700 . ?
C20_1 H20_1 0.9800 . ?

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C20 O1 C6 107.73(12) . . ?
C2 C1 C10 113.02(14) . . ?
C2 C1 H1A 109.0 . . ?
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C2 C1 H1AB 109.0 . . ?
C10 C1 H1AB 109.0 . . ?
H1A C1 H1AB 107.8 . . ?
C7 O2 C20 123.96(11) . . ?
C3 C2 C1 110.87(17) . . ?
C3 C2 H2A 109.5 . . ?
C1 C2 H2A 109.5 . . ?

C3 C2 H2AB 109.5 . . ?
C1 C2 H2AB 109.5 . . ?
H2A C2 H2AB 108.1 . . ?
C2 C3 C4 113.78(16) . . ?
C2 C3 H3A 108.8 . . ?
C4 C3 H3A 108.8 . . ?
C2 C3 H3AB 108.8 . . ?
C4 C3 H3AB 108.8 . . ?
H3A C3 H3AB 107.7 . . ?
C15 O4 H4 109.5 . . ?
C18 C4 C3 110.60(17) . . ?
C18 C4 C19 108.66(17) . . ?
C3 C4 C19 112.71(16) . . ?
C18 C4 C5 108.88(15) . . ?
C3 C4 C5 113.61(14) . . ?
C19 C4 C5 101.95(13) . . ?
C6 O5 C19 109.65(12) . . ?
C6 C5 C10 103.68(12) . . ?
C6 C5 C4 104.30(12) . . ?
C10 C5 C4 119.08(13) . . ?
C6 C5 H5 109.7 . . ?
C10 C5 H5 109.7 . . ?
C4 C5 H5 109.7 . . ?
O5 C6 O1 111.71(14) . . ?
O5 C6 C5 106.91(13) . . ?
O1 C6 C5 107.28(12) . . ?
O5 C6 H6 110.3 . . ?
O1 C6 H6 110.3 . . ?
C5 C6 H6 110.3 . . ?

O3 C7 O2 116.17(14) . . ?
O3 C7 C8 122.76(16) . . ?
O2 C7 C8 120.90(13) . . ?
C7 C8 C9 113.76(12) . . ?
C7 C8 C14 108.74(12) . . ?
C9 C8 C14 113.82(11) . . ?
C7 C8 C15 109.83(12) . . ?
C9 C8 C15 111.01(11) . . ?
C14 C8 C15 98.64(12) . . ?
C8 C9 C11 111.88(11) . . ?
C8 C9 C10 113.55(10) . . ?
C11 C9 C10 114.86(11) . . ?
C8 C9 H9 105.1 . . ?
C11 C9 H9 105.1 . . ?
C10 C9 H9 105.1 . . ?
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C1 C10 C9 114.71(12) . . ?
C20 C10 C9 107.28(11) . . ?
C1 C10 C5 114.50(12) . . ?
C20 C10 C5 100.13(12) . . ?
C9 C10 C5 107.66(11) . . ?
C13 C12 C11 111.13(12) . . ?
C13 C12 H12A 109.4 . . ?
C11 C12 H12A 109.4 . . ?
C13 C12 H12B 109.4 . . ?
C11 C12 H12B 109.4 . . ?
H12A C12 H12B 108.0 . . ?
C12 C11 C9 116.94(12) . . ?
C12 C11 H11A 108.1 . . ?

C9 C11 H11A 108.1 . . ?
C12 C11 H11B 108.1 . . ?
C9 C11 H11B 108.1 . . ?
H11A C11 H11B 107.3 . . ?
C16 C13 C12 110.05(14) . . ?
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C13 C14 C8 101.08(12) . . ?
C13 C14 H14A 111.6 . . ?
C8 C14 H14A 111.6 . . ?
C13 C14 H14B 111.6 . . ?
C8 C14 H14B 111.6 . . ?
H14A C14 H14B 109.4 . . ?
O4 C15 C16 116.65(13) . . ?
O4 C15 C8 114.72(13) . . ?
C16 C15 C8 103.56(12) . . ?
O4 C15 H15 107.1 . . ?
C16 C15 H15 107.1 . . ?
C8 C15 H15 107.1 . . ?
C17 C16 C13 126.63(16) . . ?
C17 C16 C15 125.46(16) . . ?
C13 C16 C15 107.88(13) . . ?
C16 C17 H17A 120.0 . . ?
C16 C17 H17B 120.0 . . ?
H17A C17 H17B 120.0 . . ?
C4 C18 H18A 109.5 . . ?

C4 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C4 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
O5 C19 C4 104.82(14) . . ?
O5 C19 H19A 110.8 . . ?
C4 C19 H19A 110.8 . . ?
O5 C19 H19B 110.8 . . ?
C4 C19 H19B 110.8 . . ?
H19A C19 H19B 108.9 . . ?
O1 C20 O2 107.75(14) . . ?
O1 C20 C10 105.63(13) . . ?
O2 C20 C10 116.98(13) . . ?
O1 C20 H20 108.7 . . ?
O2 C20 H20 108.7 . . ?
C10 C20 H20 108.7 . . ?
C2_1 C1_1 C10_1 114.11(17) . . ?
C2_1 C1_1 H1A_1 108.7 . . ?
C10_1 C1_1 H1A_1 108.7 . . ?
C2_1 C1_1 H1AB_1 108.7 . . ?
C10_1 C1_1 H1AB_1 108.7 . . ?
H1A_1 C1_1 H1AB_1 107.6 . . ?
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C3_1 C2_1 C1_1 111.77(17) . . ?
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C1_1 C2_1 H2A_1 109.3 . . ?
C3_1 C2_1 H2AB_1 109.3 . . ?
C1_1 C2_1 H2AB_1 109.3 . . ?

H2A_1 C2_1 H2AB_1 107.9 . . ?
C7_1 O2_1 C20_1 124.23(13) . . ?
C2_1 C3_1 C4_1 113.73(17) . . ?
C2_1 C3_1 H3A_1 108.8 . . ?
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H3A_1 C3_1 H3AB_1 107.7 . . ?
C3_1 C4_1 C19_1 113.39(18) . . ?
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C10_1 C5_1 H5_1 109.2 . . ?
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O1_1 C6_1 C5_1 107.43(15) . . ?
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O3_1 C7_1 O2_1 116.92(16) . . ?

O3_1 C7_1 C8_1 123.70(19) . . ?
O2_1 C7_1 C8_1 119.14(15) . . ?
C7_1 C8_1 C9_1 113.75(14) . . ?
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C9_1 C8_1 C15_1 110.11(13) . . ?
C14_1 C8_1 C15_1 99.53(15) . . ?
C8_1 C9_1 C10_1 114.89(12) . . ?
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C10_1 C9_1 C11_1 114.49(13) . . ?
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C20_1 C10_1 C9_1 108.02(13) . . ?
C1_1 C10_1 C9_1 115.21(14) . . ?
C20_1 C10_1 C5_1 101.12(13) . . ?
C1_1 C10_1 C5_1 114.11(14) . . ?
C9_1 C10_1 C5_1 106.49(12) . . ?
C12_1 C11_1 C9_1 116.10(15) . . ?
C12_1 C11_1 H11A_1 108.3 . . ?
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C12_1 C11_1 H11B_1 108.3 . . ?
C9_1 C11_1 H11B_1 108.3 . . ?
H11A_1 C11_1 H11B_1 107.4 . . ?
C11_1 C12_1 C13_1 111.10(15) . . ?
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C13_1 C12_1 H12A_1 109.4 . . ?

C11_1 C12_1 H12B_1 109.4 . . ?
C13_1 C12_1 H12B_1 109.4 . . ?
H12A_1 C12_1 H12B_1 108.0 . . ?
C16_1 C13_1 C14_1 102.82(16) . . ?
C16_1 C13_1 C12_1 110.67(19) . . ?
C14_1 C13_1 C12_1 108.22(18) . . ?
C16_1 C13_1 H13_1 111.6 . . ?
C14_1 C13_1 H13_1 111.6 . . ?
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C13_1 C14_1 H14A_1 111.6 . . ?
C8_1 C14_1 H14A_1 111.6 . . ?
C13_1 C14_1 H14B_1 111.6 . . ?
C8_1 C14_1 H14B_1 111.6 . . ?
H14A_1 C14_1 H14B_1 109.4 . . ?
O4_1 C15_1 C16_1 111.80(15) . . ?
O4_1 C15_1 C8_1 115.47(15) . . ?
C16_1 C15_1 C8_1 103.86(15) . . ?
O4_1 C15_1 H15_1 108.5 . . ?
C16_1 C15_1 H15_1 108.5 . . ?
C8_1 C15_1 H15_1 108.5 . . ?
C17_1 C16_1 C13_1 127.5(2) . . ?
C17_1 C16_1 C15_1 124.6(2) . . ?
C13_1 C16_1 C15_1 107.97(17) . . ?
C16_1 C17_1 H17A_1 120.0 . . ?
C16_1 C17_1 H17B_1 120.0 . . ?
H17A_1 C17_1 H17B_1 120.0 . . ?
C4_1 C18_1 H18A_1 109.5 . . ?
C4_1 C18_1 H18B_1 109.5 . . ?

H18A_1 C18_1 H18B_1 109.5 . . ?
C4_1 C18_1 H18C_1 109.5 . . ?
H18A_1 C18_1 H18C_1 109.5 . . ?
H18B_1 C18_1 H18C_1 109.5 . . ?
O5_1 C19_1 C4_1 105.41(18) . . ?
O5_1 C19_1 H19A_1 110.7 . . ?
C4_1 C19_1 H19A_1 110.7 . . ?
O5_1 C19_1 H19B_1 110.7 . . ?
C4_1 C19_1 H19B_1 110.7 . . ?
H19A_1 C19_1 H19B_1 108.8 . . ?
O1_1 C20_1 O2_1 106.55(16) . . ?
O1_1 C20_1 C10_1 106.56(15) . . ?
O2_1 C20_1 C10_1 117.90(15) . . ?
O1_1 C20_1 H20_1 108.5 . . ?
O2_1 C20_1 H20_1 108.5 . . ?
C10_1 C20_1 H20_1 108.5 . . ?

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_refine_diff_density_rms   0.035

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     20190801WYXIRX25_0m_a.res
     created by SHELXL-2018/3 at 11:28:29 on 06-Feb-2022
REM Old TITL Integration of 20190801WYXIRX25
REM SHELXT solution in P2(1)
REM R1 0.133,   Rweak 0.038,   Alpha 0.007,   Orientation as input

REM Flack x =   0.022 (0.123) from Parsons' quotients

REM Formula found by SHELXT: C39 O11

CELL   0.71076   6.4646   21.4751   12.3769   90.000   94.100   90.000

ZERR   4.000   0.0002   0.0008   0.0005   0.000   0.001   0.000

LATT -1

SYMM -X, 1/2+Y, -Z

SFAC C H O

UNIT 80 104 20

TEMP 26.870

ACTA

L.S. 10

BOND $H

LIST 4

FMAP 2

PLAN 5

WGHT   0.064200   0.028500

FVAR   1.33315

O1   3   -0.037212   0.388166   0.235929   11.00000   0.06588   0.04843 =
            0.02499   0.00080   0.00819   -0.00410

C1   1   -0.175015   0.392555   -0.057790   11.00000   0.04423   0.04524 =
            0.03198   0.00020   -0.00836   0.00720

AFIX   23

H1A   2   -0.090981   0.386557   -0.118817   11.00000   -1.20000

H1AB   2   -0.285972   0.362070   -0.063575   11.00000   -1.20000

AFIX   0

O2   3   -0.273343   0.318733   0.160985   11.00000   0.04410   0.05185 =
            0.05683   -0.00159   0.02770   -0.00858

C2   1   -0.269137   0.457726   -0.064134   11.00000   0.06164   0.06179 =
            0.04129   0.00433   -0.01247   0.02708

```
AFIX    23
H2A     2    -0.350489      0.462602      -0.132550      11.00000    -1.20000
H2AB    2    -0.361049      0.463054      -0.006216      11.00000    -1.20000
AFIX    0
O3      3    -0.301143      0.218732      0.150816       11.00000     0.04497    0.05467 =
             0.05660       0.01311       0.01298       -0.01577
C3      1    -0.101731      0.506896      -0.054625      11.00000     0.08544    0.04131 =
             0.03599       0.00852       0.00681        0.02190
AFIX    23
H3A     2    -0.166421      0.547642      -0.059884      11.00000    -1.20000
H3AB    2    -0.015280      0.502590      -0.115097      11.00000    -1.20000
AFIX    0
O4      3     0.253600      0.214978      0.173796       11.00000     0.04261    0.05755 =
             0.02874       0.00524       -0.00248       0.00769
AFIX 148
H4      2     0.368507      0.218597      0.154343       11.00000    -1.50000
AFIX    0
C4      1     0.035956      0.503492      0.050915       11.00000     0.05390    0.02821 =
             0.04008       0.00232       0.01073        0.00855
O5      3     0.032427      0.494786      0.239757       11.00000     0.07295    0.04336 =
             0.03446       -0.01011      -0.00328       0.01384
C5      1     0.102452      0.436195      0.083618       11.00000     0.03444    0.02694 =
             0.03144       0.00008       0.00434        0.00175
AFIX    13
H5      2     0.243347      0.428261      0.062575       11.00000    -1.20000
AFIX    0
C6      1     0.100620      0.435546      0.208522       11.00000     0.04745    0.03534 =
             0.03110       -0.00519      -0.00324       0.00450
AFIX    13
```

```
H6      2      0.240154      0.427226      0.241601      11.00000     -1.20000
AFIX    0
C7      1     -0.205983      0.264040      0.125661      11.00000      0.02992      0.04503 =
            0.03082      0.00737      0.00214     -0.00819
C8      1     -0.030596      0.260948      0.051233      11.00000      0.02819      0.03201 =
            0.02558      0.00330      0.00116     -0.00531
C9      1      0.094637      0.321604      0.047066      11.00000      0.02475      0.02818 =
            0.02172      0.00202      0.00210     -0.00250
AFIX   13
H9      2      0.180382      0.322867      0.115607      11.00000     -1.20000
AFIX    0
C10     1     -0.040906      0.381084      0.047209      11.00000      0.02795      0.03137 =
            0.02375      0.00228      0.00305      0.00035
C12     1      0.189658      0.280239     -0.143458      11.00000      0.05137      0.03884 =
            0.02749      0.00101      0.01103      0.00085
AFIX   23
H12A    2      0.097553      0.304162     -0.192905      11.00000     -1.20000
H12B    2      0.312983      0.270231     -0.180236      11.00000     -1.20000
AFIX    0
C11     1      0.250702      0.319660     -0.042192      11.00000      0.03392      0.03207 =
            0.03317     -0.00001      0.01137     -0.00411
AFIX   23
H11A    2      0.274063      0.362048     -0.065503      11.00000     -1.20000
H11B    2      0.381726      0.304038     -0.009951      11.00000     -1.20000
AFIX    0
C13     1      0.081844      0.220077     -0.113237      11.00000      0.05058      0.03531 =
            0.02760     -0.00489     -0.00087     -0.00310
AFIX   13
H13     2      0.054951      0.192676     -0.175989      11.00000     -1.20000
```

```
AFIX     0
C14   1    -0.117977      0.237521     -0.061430      11.00000     0.03959     0.03706 =
           0.03170     -0.00003     -0.00608     -0.00818
AFIX    23
H14A  2    -0.207779      0.201707     -0.055198      11.00000     -1.20000
H14B  2    -0.193201      0.270067     -0.101886      11.00000     -1.20000
AFIX     0
C15   1     0.113840      0.204584      0.083360      11.00000     0.03765     0.03090 =
           0.03184      0.00574      0.00096     -0.00387
AFIX    13
H15   2     0.024119      0.169921      0.101626      11.00000     -1.20000
AFIX     0
C16   1     0.207195      0.187675     -0.021712      11.00000     0.04261     0.02899 =
           0.03387     -0.00204     -0.00011     -0.00430
C17   1     0.372571      0.152535     -0.030228      11.00000     0.04989     0.03952 =
           0.04672     -0.00673      0.00224      0.00190
AFIX    93
H17A  2     0.422869      0.145669     -0.097758      11.00000     -1.20000
H17B  2     0.438881      0.134623      0.031296      11.00000     -1.20000
AFIX     0
C18   1     0.230321      0.543361      0.043365      11.00000     0.07192     0.03012 =
           0.08927      0.00473      0.02578     -0.00193
AFIX 137
H18A  2     0.309812      0.527670     -0.013332      11.00000     -1.50000
H18B  2     0.312569      0.541789      0.111033      11.00000     -1.50000
H18C  2     0.190630      0.585658      0.027653      11.00000     -1.50000
AFIX     0
C19   1    -0.076113      0.524682      0.149362      11.00000     0.06006     0.03968 =
           0.03875     -0.00355      0.00473      0.01590
```

```
AFIX    23
H19A   2    -0.069790     0.569606     0.157061     11.00000    -1.20000
H19B   2    -0.220381     0.511907     0.142672     11.00000    -1.20000
AFIX    0
C20    1    -0.173300     0.376572     0.144555     11.00000     0.03818     0.04115 =
            0.03600      0.00054     0.01322      0.00116
AFIX    13
H20    2    -0.278376     0.409527     0.138831     11.00000    -1.20000
AFIX    0
RESI 1
C1     1     0.700096     0.684416     0.554960     11.00000     0.03701     0.05834 =
            0.04293     -0.00331    -0.00280      0.00195
AFIX    23
H1A    2     0.668846     0.676647     0.629261     11.00000    -1.20000
H1AB   2     0.795605     0.652342     0.534666     11.00000    -1.20000
AFIX    0
O1     3     0.370810     0.693792     0.300227     11.00000     0.08127     0.06164 =
            0.02695     -0.00501    -0.00379      0.00968
C2     1     0.806612     0.747382     0.549448     11.00000     0.03959     0.07003 =
            0.05998     -0.00738    -0.00173     -0.01176
AFIX    23
H2A    2     0.927276     0.748086     0.600740     11.00000    -1.20000
H2AB   2     0.853788     0.753261     0.477494     11.00000    -1.20000
AFIX    0
O2     3     0.585064     0.610576     0.324616     11.00000     0.07438     0.05738 =
            0.03865     -0.00837     0.02631      0.00593
C3     1     0.663453     0.800040     0.574605     11.00000     0.05936     0.05852 =
            0.04597     -0.01102     0.00494     -0.01635
AFIX    23
```

```
H3A     2      0.737833      0.839080      0.570172      11.00000     -1.20000
H3AB    2      0.624623      0.795456      0.648452      11.00000     -1.20000
AFIX    0
O3      3      0.522306      0.511195      0.314874      11.00000      0.06257      0.06372 =
               0.05434     -0.02599      0.02019      0.00154
C4      1      0.466624      0.803119      0.498855      11.00000      0.05440      0.04289 =
               0.03454     -0.00228      0.01173     -0.00625
O4      3      0.043128      0.534717      0.451166      11.00000      0.04185      0.06566 =
               0.03923     -0.01333      0.00095     -0.00036
AFIX 147
H4      2      0.012091      0.523513      0.388769      11.00000     -1.50000
AFIX    0
C5      1      0.364852      0.738968      0.476100      11.00000      0.03833      0.04008 =
               0.02771      0.00013      0.00381      0.00090
AFIX    13
H5      2      0.248497      0.733842      0.521912      11.00000     -1.20000
AFIX    0
O5      3      0.337095      0.801334      0.316435      11.00000      0.10239      0.05339 =
               0.04213      0.01337     -0.00683     -0.00294
C6      1      0.280542      0.742929      0.356064      11.00000      0.05797      0.04936 =
               0.03441      0.00409     -0.00500      0.00297
AFIX    13
H6      2      0.129218      0.738681      0.350595      11.00000     -1.20000
AFIX    0
C7      1      0.506634      0.557948      0.366002      11.00000      0.03740      0.05592 =
               0.03402     -0.01234      0.00559      0.00647
C8      1      0.422908      0.560010      0.476952      11.00000      0.03697      0.04135 =
               0.02777     -0.00614      0.00102      0.00689
C9      1      0.352602      0.625139      0.510320      11.00000      0.03565      0.03946 =
```

```
            0.02200      -0.00343      0.00340       0.00445
AFIX   13
H9     2     0.223002      0.632712      0.466263      11.00000    -1.20000
AFIX    0
C10    1     0.498508      0.678943      0.481640      11.00000     0.03532      0.04382 =
            0.02288      -0.00352      0.00404       0.00229
C11    1     0.290878      0.625602      0.629269      11.00000     0.05943      0.04241 =
            0.02612      -0.00375      0.01104       0.00225
AFIX   23
H11A   2     0.304470      0.667851      0.656576      11.00000    -1.20000
H11B   2     0.145668      0.614233      0.629322      11.00000    -1.20000
AFIX    0
C12    1     0.415740      0.582477      0.708003      11.00000     0.08334      0.05367 =
            0.02571       0.00048      -0.00300      -0.00159
AFIX   23
H12A   2     0.340347      0.576144      0.772110      11.00000    -1.20000
H12B   2     0.547357      0.601920      0.730306      11.00000    -1.20000
AFIX    0
C13    1     0.455201      0.519317      0.655289      11.00000     0.07647      0.04901 =
            0.03696       0.00577      -0.01138       0.00834
AFIX   13
H13    2     0.522711      0.490025      0.707300      11.00000    -1.20000
AFIX    0
C14    1     0.585293      0.530330      0.559128      11.00000     0.05110      0.04783 =
            0.04755      -0.00248      -0.00914       0.01446
AFIX   23
H14A   2     0.638753      0.491596      0.531977      11.00000    -1.20000
H14B   2     0.699696      0.558510      0.577517      11.00000    -1.20000
AFIX    0
```

```
C15    1     0.242132      0.512307      0.484583      11.00000     0.04823     0.04135 =
           0.03241    -0.00909      0.00424      0.00203
AFIX   13
H15    2     0.271123      0.475826      0.440559      11.00000    -1.20000
AFIX    0
C16    1     0.257372      0.493062      0.602956      11.00000     0.07001     0.03897 =
           0.03895    -0.00100      0.00645      0.00449
C17    1     0.117354      0.459132      0.649155      11.00000     0.08958     0.05754 =
           0.05689     0.00536      0.01800     -0.00348
AFIX   93
H17A   2     0.136544      0.449129      0.722293      11.00000    -1.20000
H17B   2    -0.000236      0.445289      0.608484      11.00000    -1.20000
AFIX    0
C18    1     0.309185      0.846309      0.547398      11.00000     0.07843     0.03962 =
           0.05816    -0.00437      0.02034      0.00306
AFIX 137
H18A   2     0.371423      0.886321      0.561767      11.00000    -1.50000
H18B   2     0.267351      0.828738      0.613745      11.00000    -1.50000
H18C   2     0.190073      0.850948      0.497117      11.00000    -1.50000
AFIX    0
C19    1     0.505123      0.825551      0.384834      11.00000     0.08410     0.05259 =
           0.04106     0.00357      0.01539     -0.01471
AFIX   23
H19A   2     0.506970      0.870682      0.381894      11.00000    -1.20000
H19B   2     0.636539      0.809921      0.362920      11.00000    -1.20000
AFIX    0
C20    1     0.545876      0.671537      0.362833      11.00000     0.05416     0.05071 =
           0.02995    -0.00213      0.01190      0.00028
AFIX   13
```

H20   2   0.664683   0.698035   0.349252   11.00000   -1.20000
RESI 0
AFIX   0
HKLF 4

REM   20190801WYXIRX25_0m_a.res in P2(1)
REM wR2 = 0.124171, GooF = S = 1.01847, Restrained GooF = 1.01844 for all data
REM R1 = 0.046581 for 11735 Fo > 4sig(Fo) and 0.081328 for all 17341 data
REM 456 parameters refined using 1 restraints