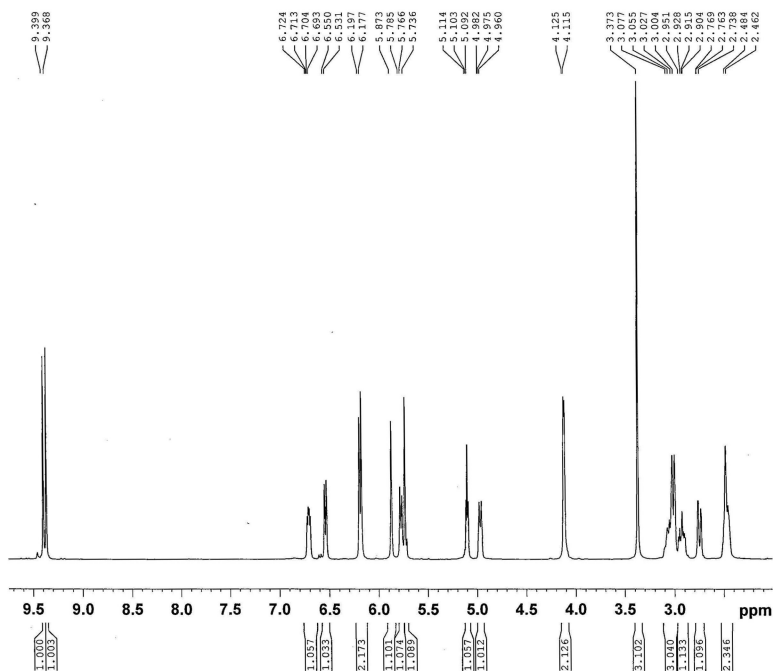


rt-24 1H 2019 05 17



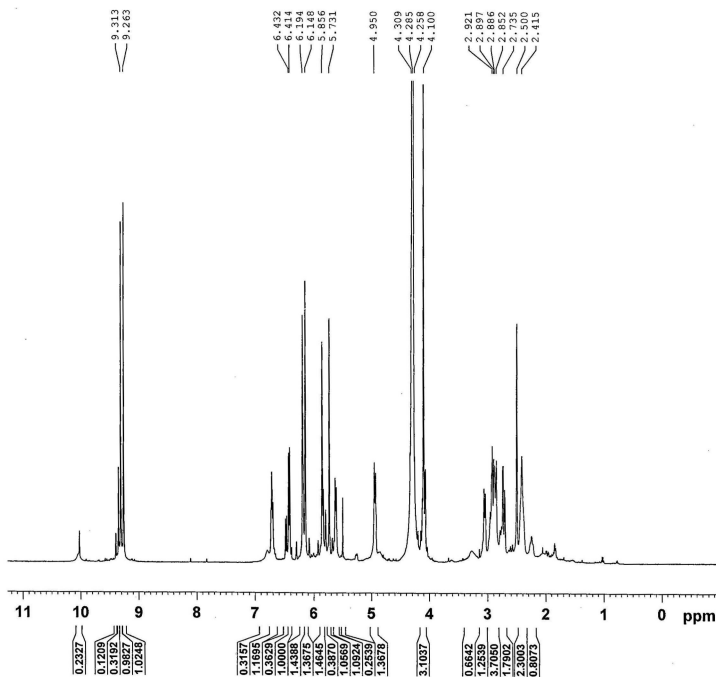
Current Data Parameters  
 NAME yrt-24  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20190517  
 Time 21.57  
 INSTRUM av500  
 PROBHD 5 mm FAPBO BB-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 4  
 DS 1  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 1.638500 sec  
 RG 45.2  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0335010 MHz

F2 - Processing parameters  
 SI 16384  
 SF 500.0300082 MHz  
 WM 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 FC 2.00

YRT-24+D2O 1H 1D 2019 11 30



Current Data Parameters  
 NAME YRT-24  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20191201  
 Time 12.19  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB-  
 PULPROG zg30  
 TD 16384  
 SOLVENT DMSO  
 NS 8  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.819300 sec  
 RG 114  
 DW 50.000 usec  
 DE 8.00 usec  
 TE 292.5 K  
 D1 1.00000000 sec  
 TDO 1

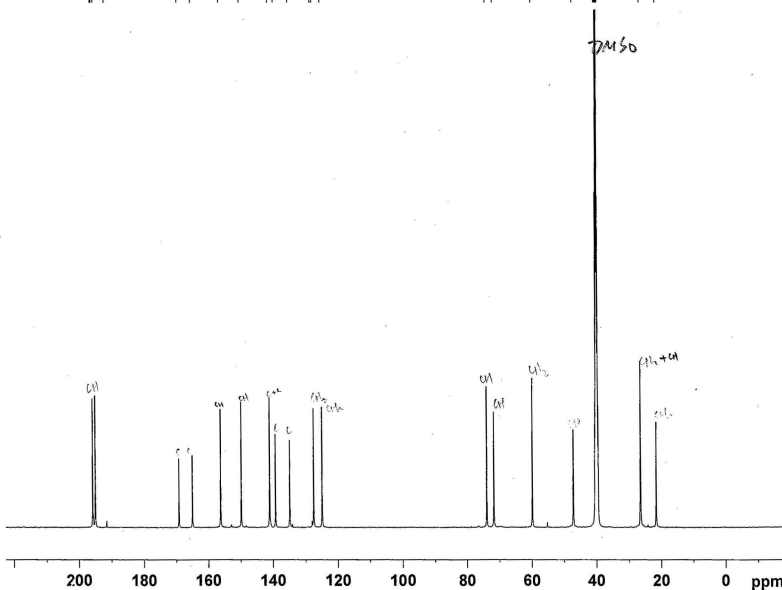
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.00 usec  
 PL1 2.00 dB  
 SFO1 500.0338500 MHz

F2 - Processing parameters  
 SI 16384  
 SF 500.0299975 MHz  
 WM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 FC 2.00

yrt-24 13C 1D 2019 05 17

195.26  
195.55  
194.95  
194.45  
169.13  
164.95  
156.24  
149.84  
141.05  
139.26  
134.88  
133.59  
124.98

73.96  
71.77  
59.94  
47.21  
40.51  
40.35  
40.01  
39.85  
39.82  
26.50  
21.63



NAME yrt-24  
EXPNO 2  
PROCNO 1  
Date 20190518  
Time 7.34  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 11271  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 5790  
DW 15.300 usec  
DE 6.00 usec  
TE 298.5 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TDO 1

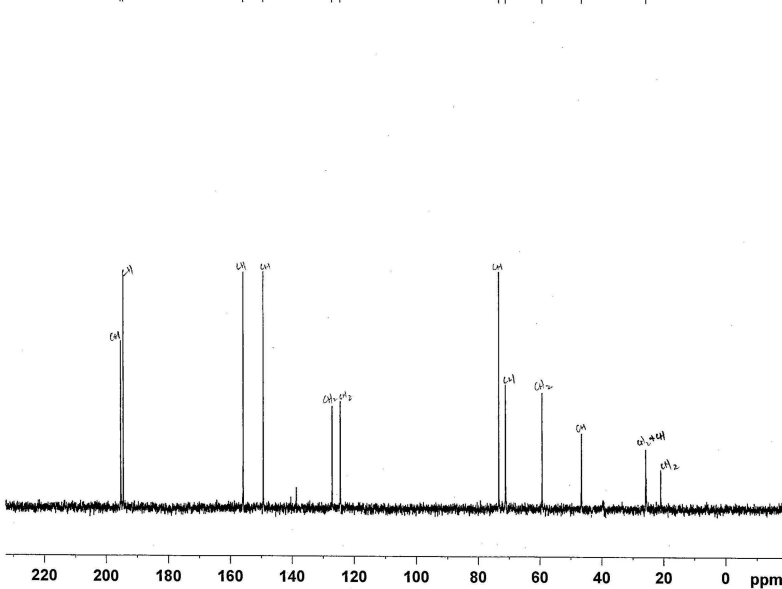
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
PL1 2.00 dB  
SF01 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 17.66 dB  
PL13 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7326421 MHz  
WDW EM  
SSB 0  
LB 8.00 Hz  
GB 0  
PC 1.00

YRT-24 dept90 13C 1D 2019 11 01

195.34  
194.49  
155.88  
149.40  
127.13  
124.51

73.41  
71.24  
59.36  
46.61  
25.97



NAME YRT-24  
EXPNO 4  
PROCNO 1  
Date 20191101  
Time 20.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG dept90  
TD 65536  
SOLVENT DMSO  
NS 34  
DS 2  
SWH 32679.738 Hz  
FIDRES 0.498653 Hz  
AQ 1.0027661 sec  
RG 13000  
DW 15.300 usec  
DE 6.00 usec  
TE 296.6 K  
CNST2 145.0000000  
D1 4.0000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001222 sec  
TDO 1

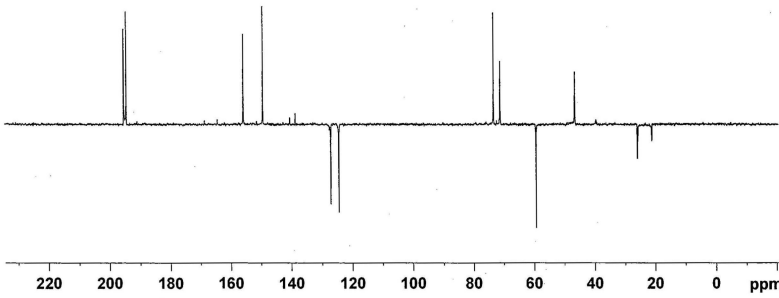
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.60 usec  
p2 19.20 usec  
PL1 2.00 dB  
SF01 125.7464750 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P3 13.50 usec  
p4 27.00 usec  
PCPD2 80.00 usec  
PL2 2.60 dB  
PL12 17.66 dB  
SFO2 500.0355000 MHz  
SI 32768  
SF 125.7327003 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 5.00

YRT-24 dept135 13C 1D 2019 11 01

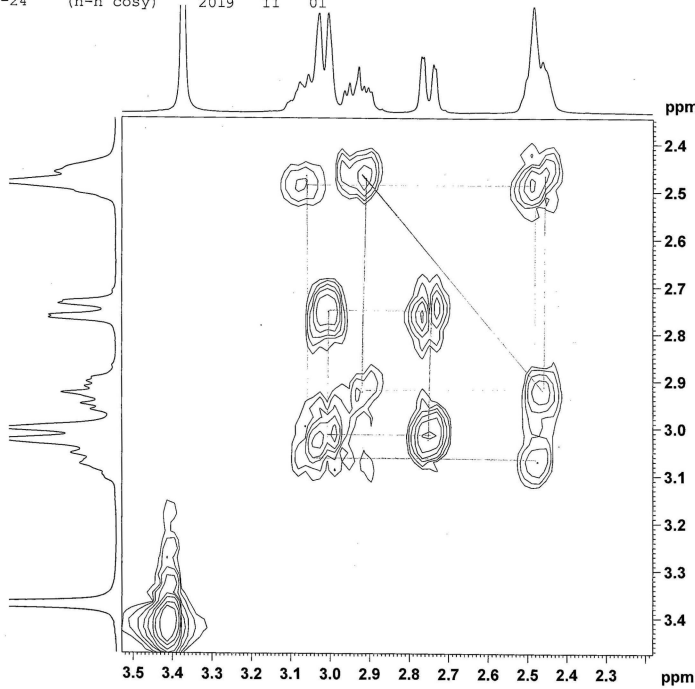


NAME YRT-24  
 EXNO 3  
 PROCNO 1  
 Date 20191101  
 Time 20.49  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG dept135  
 TD 65536  
 SOLVENT DMSO  
 NS 178  
 DS 2  
 SWH 32679.736 Hz  
 FIDRES 0.498653 Hz  
 AQ 1.0027661 sec  
 RG 13000  
 DW 15.300 usec  
 DE 6.00 usec  
 TE 296.5 K  
 CNST2 145.000000  
 D1 4.0000000 sec  
 d2 0.0034828 sec  
 d12 0.0002000 sec  
 DELTA 0.0001553 sec  
 TD 1



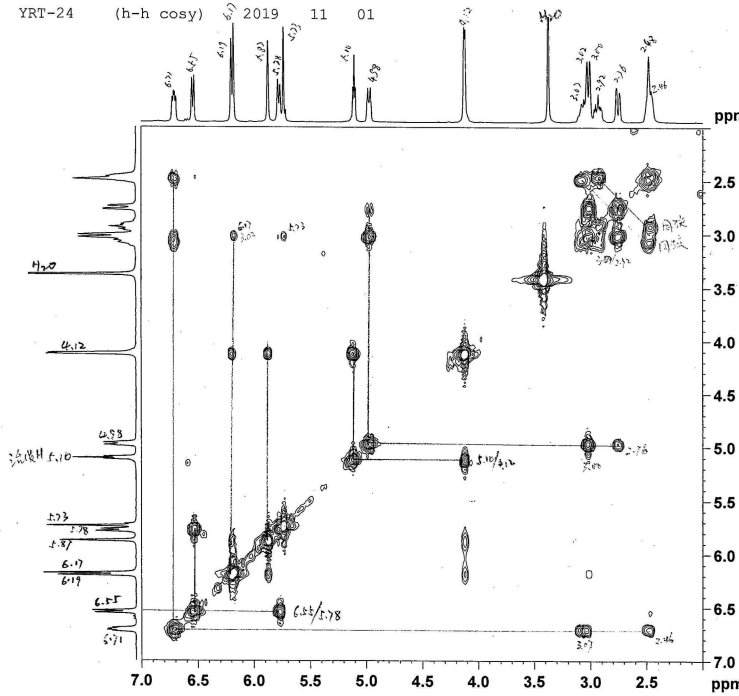
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.20 usec  
 P2 24.40 usec  
 PL1 3.00 dB  
 SFO1 125.7464750 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P3 13.00 usec  
 P4 26.00 usec  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 17.70 dB  
 SFO2 500.0355000 MHz  
 SI 32768  
 SF 125.7327092 MHz  
 WDW EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 5.00

YRT-24 (h-h cosy) 2019 11 01



Current Data Parameters  
 NSMG YRT-24  
 EXFNO 6  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20191101  
 Time 21.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosyypg  
 TD 2048  
 SOLVENT DMSO  
 NS 8  
 DS 8  
 SWH 9469.697 Hz  
 FIDRES 4.623876 Hz  
 AQ 0.1082372 sec  
 RG 80.6  
 DW 52.800 usec  
 DE 6.00 usec  
 TE 296.4 K  
 d0 0.0000300 sec  
 D1 1.48689198 sec  
 d13 0.0000000 sec  
 D16 0.0002000 sec  
 INO 0.00010525 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 P2 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0350060 MHz  
 ===== GRADIENT CHANNEL =====  
 GRFM1 SINE.100  
 SFL1 10.00 A  
 P16 1000.00 usec  
 F1 - Acquisition parameters  
 NDO 256  
 TD 256  
 SFO1 500.035 MHz  
 FIDRES 37.114014 Hz  
 SW 19.001 ppm  
 FMODE QF  
 F2 - Processing parameters  
 SI 1024  
 SF 500.0300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 F1 - Processing parameters  
 SI 1024  
 MC2 OF  
 SF 500.0300000 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

YRT-24 (h-h cosy) 2019 11 01



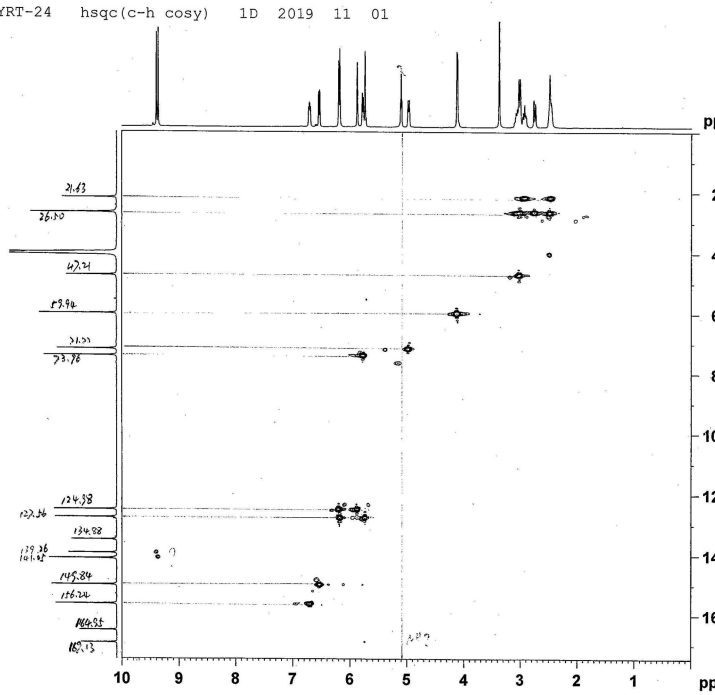
```

NAME      YRT-24
EXPNO     1
PROCNO    1
Date_     20191101
Time      21.53
INSTRUM   spect
PROBHD    5 mm FAPBO BB-
PULPROG   cosypp4f
TD         65536
SOLVENT   DMSO
NS         8
DS         8
SWH        9469.697 Hz
FIDRES     4.623876 Hz
AQ         0.1092372 sec
RG         80.6
DE         52.800 usec
TE         296.4 K
AQ         0.00000300 sec
D1         1.4868198 sec
d13        0.00000400 sec
DL6        0.00020000 sec
IN0        0.00010253 sec

===== CHANNEL f1 =====
NUC1      1H
P0         13.50 usec
P1         13.50 usec
PL1        2.20 dB
SFO1      500.0330060 MHz

===== GRADIENT CHANNEL =====
GENAM1    SINE.100
GPR1      10.00 %
P16       1000.00 usec
ND0        1
TD         256
SFO1      500.033 MHz
FIDRES     37.114014 Hz
SW         19.001 ppm
FMODE     QF
SI         1024
SF         500.0300000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         500.0300000 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

YRT-24 hsqc(c-h cosy) 1D 2019 11 01



```

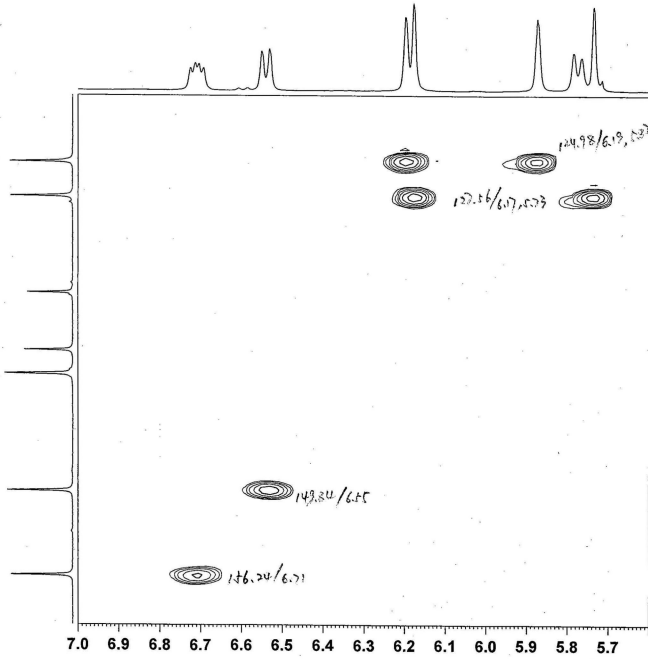
NAME      YRT-24
EXPNO     1
PROCNO    1
Date_     20191101
Time      20.59
INSTRUM   spect
PROBHD    5 mm FAPBO BB-
PULPROG   hsqc100
TD         65536
SOLVENT   DMSO
NS         8
DS         8
SWH        10000.000 Hz
FIDRES     9.765425 Hz
AQ         0.6512000 sec
RG         1400
DE         50.000 usec
TE         296.4 K
AQ         0.00000000 sec
D1         1.5000000 sec
d1         0.00172414 sec
d13        0.00000000 sec
DL1        0.00000400 sec
DL3        0.00020000 sec
DL6        0.00132200 sec
DZGTA     0.00071614 sec
IN0        0.00001990 sec
STCMT     0
EGOPTS    0

===== CHANNEL f1 =====
NUC1      1H
P1         13.00 usec
P2         24.00 usec
P28        1.00 usec
PL1         2.00 dB
SFO1      500.0330060 MHz

===== CHANNEL f2 =====
CPCPRG2   gddc
NUC2       13C
P3         12.00 usec
P4         24.00 usec
PCPD2     75.00 usec
PL2        3.00 dB
PL3        18.50 dB
SFO2     125.7420210 MHz

===== GRADIENT CHANNEL =====
GPRAM2    SINE.100
GPR1      80.00 %
GPR2      20.10 %
P16       1000.00 usec
ND0        2
TD         256
SFO1     125.742 MHz
FIDRES     99.160988 Hz
SW         89.819 ppm
FMODE     Echo-AntiEcho
SI         1024
SF         500.0300000 MHz
WDW        G2SINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        Echo-AntiEcho
SF         125.7420210 MHz
WDW        G2SINE
SSB        2
LB         0.00 Hz
GB         0
  
```

YRT-24 hsqc(c-h cosy) 1E 2019 11 01



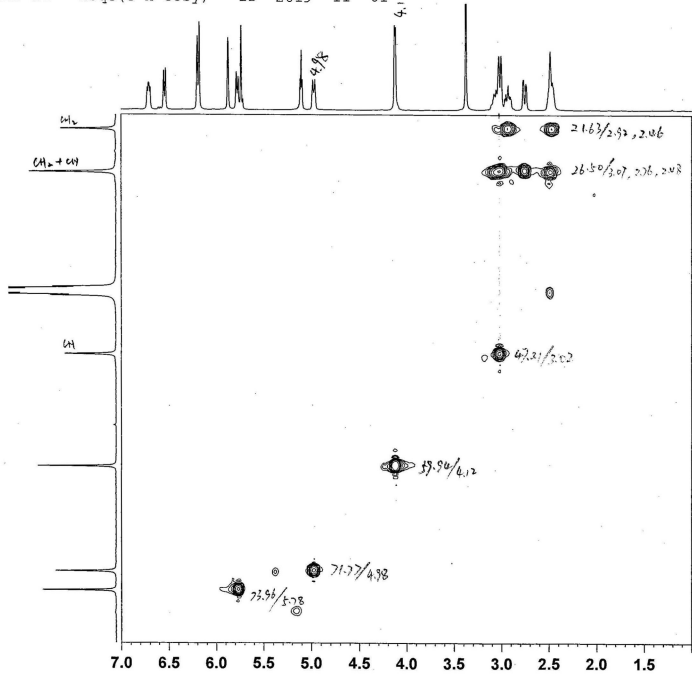
NAME YRT-24  
EXPNO 1  
PROCNO 1  
PROC 20191101  
TIME 20.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hsqc2top  
TD 1024  
SOLVENT H2O  
NS 8  
DS 8  
SWH 10000.000 Hz  
FIDRES 9.745625 Hz  
AQ 0.0513000 sec  
RG 1400  
DM 50.000 usec  
DE 4.00 usec  
TE 296.4 K  
CNS2 145.000000  
d0 0.00000000 sec  
d1 0.00000000 sec  
d4 0.00172414 sec  
d11 0.00000000 sec  
d13 0.00000400 sec  
d16 0.00000000 sec  
DELTA 0.00132000 sec  
DELTAL 0.00071614 sec  
DELTA2 0.00019900 sec  
STICNT 0  
ZGZFTR 0

----- CHANNEL f1 -----  
NUC1 1H  
P1 13.00 usec  
P2 24.00 usec  
P28 5.00 usec  
PL1 2.00 dB  
PL2 3.00 dB  
PL12 16.50 dB  
SFO1 500.0330060 MHz

----- CHANNEL f2 -----  
CFPRG2 gcp  
MPC1 13C  
P3 12.00 usec  
P4 24.00 usec  
P28 5.00 usec  
PL1 2.00 dB  
PL2 3.00 dB  
PL12 16.50 dB  
SFO2 125.7420210 MHz

----- GRADIENT CHANNEL -----  
GPMAX1 SINE.100  
GPMAX2 SINE.100  
GPE1 80.00 %  
GPE2 20.10 %  
P14 1000.00 usec  
MDO 2  
TD 256  
SFO1 125.742 MHz  
FIDRES 98.146988 Hz  
SW 199.819 ppm  
FAMODE Echo-Antiecho  
SF 500.0300000 MHz  
NS 8  
DS 2  
SSB 0 Hz  
LA 0  
GB 0  
PC 1.40  
SI 1024  
MPC2 echo-antiecho  
SF 125.7324440 MHz  
NS 8  
DS 2  
SSB 0 Hz  
LA 0  
GB 0

YRT-24 hsqc(c-h cosy) 1D 2019 11 01



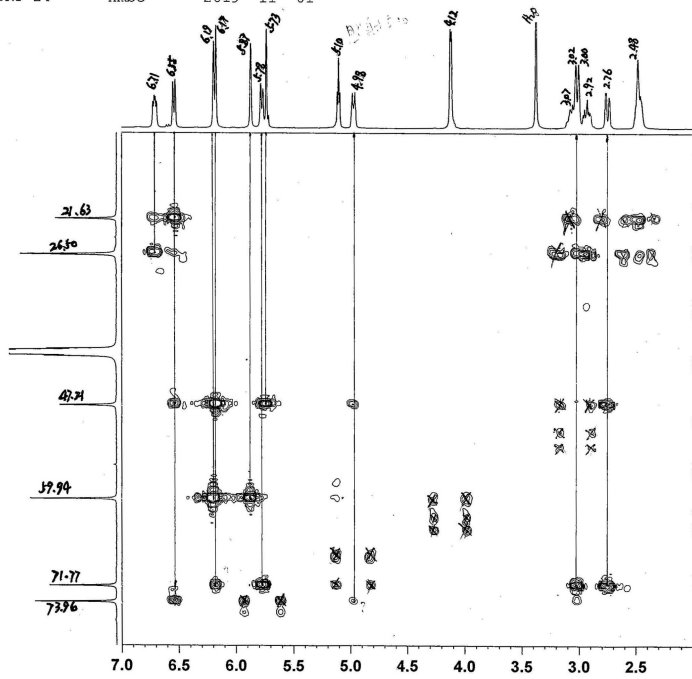
NAME YRT-24  
EXPNO 1  
PROCNO 1  
PROC 20191101  
TIME 20.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hsqc2top  
TD 1024  
SOLVENT H2O  
NS 8  
DS 8  
SWH 10000.000 Hz  
FIDRES 9.745625 Hz  
AQ 0.0513000 sec  
RG 1400  
DM 50.000 usec  
DE 4.00 usec  
TE 296.4 K  
CNS2 145.000000  
d0 0.00000000 sec  
d1 0.00000000 sec  
d4 0.00172414 sec  
d11 0.00000000 sec  
d13 0.00000400 sec  
d16 0.00000000 sec  
DELTA 0.00132000 sec  
DELTAL 0.00071614 sec  
DELTA2 0.00019900 sec  
STICNT 0  
ZGZFTR 0

----- CHANNEL f1 -----  
NUC1 1H  
P1 13.00 usec  
P2 24.00 usec  
P28 5.00 usec  
PL1 2.00 dB  
PL2 3.00 dB  
PL12 16.50 dB  
SFO1 500.0330060 MHz

----- CHANNEL f2 -----  
CFPRG2 gcp  
MPC2 13C  
P3 12.00 usec  
P4 24.00 usec  
P28 5.00 usec  
PL1 2.00 dB  
PL2 3.00 dB  
PL12 16.50 dB  
SFO2 125.7420210 MHz

----- GRADIENT CHANNEL -----  
GPMAX1 SINE.100  
GPMAX2 SINE.100  
GPE1 80.00 %  
GPE2 20.10 %  
P14 1000.00 usec  
MDO 2  
TD 256  
SFO1 125.742 MHz  
FIDRES 98.146988 Hz  
SW 199.819 ppm  
FAMODE Echo-Antiecho  
SF 500.0300000 MHz  
NS 8  
DS 2  
SSB 0 Hz  
LA 0  
GB 0  
PC 1.40  
SI 1024  
MPC2 echo-antiecho  
SF 125.7324440 MHz  
NS 8  
DS 2  
SSB 0 Hz  
LA 0  
GB 0

YRT-24 hmbc 2019 11 01



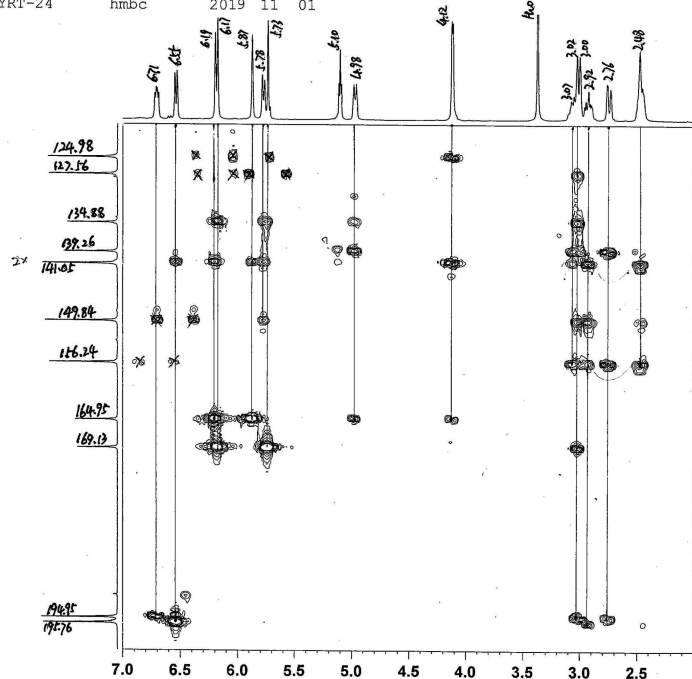
NAME YRT-24  
 EXPNO 7  
 PROCNO 1  
 Date\_ 20191101  
 Time 22.49  
 INSTRUM spect  
 F2PROG 5 mm PABBO BB-  
 PULPROG hmbcsp1pndgf  
 TD 1024  
 SOLVENT DMSO  
 NS 16  
 DS 16  
 SWH 7507.507 Hz  
 FIDRES 7.331550 Hz  
 AQ 0.0683150 sec  
 RG 23100  
 DW 66.600 usec  
 DE 6.00 usec  
 TE 296.1 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 d0 0.0000000 sec  
 d1 1.5000000 sec  
 d2 0.00344628 sec  
 d6 0.0500000 sec  
 D16 0.0002000 sec  
 INO 0.0001325 sec

----- CHANNEL F1 -----  
 NU1 1H  
 P1 13.50 usec  
 P2 27.00 usec  
 F11 2.20 GB  
 SFO1 500.0330060 MHz

----- CHANNEL F2 -----  
 NU2 13C  
 P3 10.20 usec  
 P4 2.20 GB  
 SFO2 125.7452173 MHz

----- GRADIENT CHANNEL -----  
 GRNAM1 SINE.100  
 GRNAM2 SINE.100  
 GRNAM3 SINE.100  
 GP1 50.00 %  
 GP2 30.00 %  
 GP3 40.10 %  
 P16 1000.00 usec  
 NDO 2  
 TD 512  
 SFO1 125.7452 MHz  
 FIDRES 73.702827 Hz  
 SW 300.098 ppm  
 FMODE QF  
 SF 500.0330000 MHz  
 SINE  
 L8 0.00 Hz  
 L9 0.00 Hz  
 PC 1.40  
 SI 1024  
 MC2 QF  
 SF 125.7326440 MHz  
 SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 FC 1.40  
 SI 1024  
 MC2 QF  
 SF 125.7326440 MHz  
 SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

YRT-24 hmbc 2019 11 01



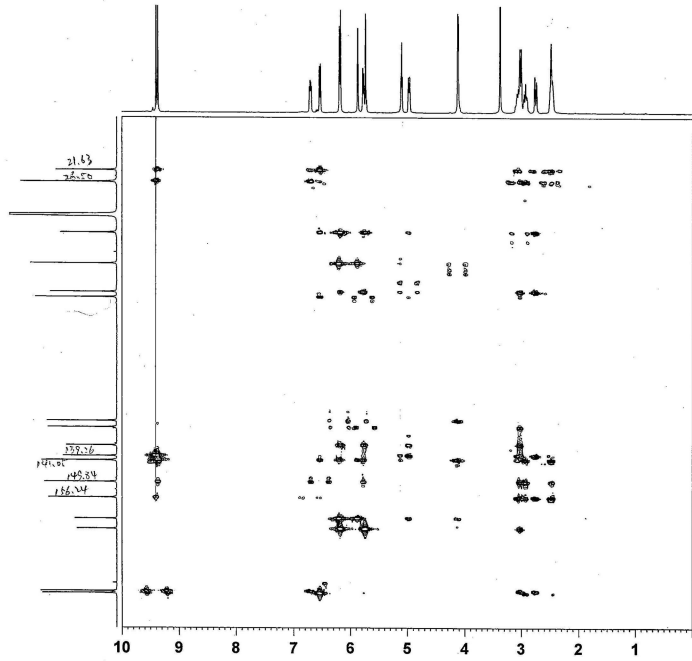
NAME YRT-24  
 EXPNO 7  
 PROCNO 1  
 Date\_ 20191101  
 Time 22.49  
 INSTRUM spect  
 F2PROG 5 mm PABBO BB-  
 PULPROG hmbcsp1pndgf  
 TD 1024  
 SOLVENT DMSO  
 NS 16  
 DS 16  
 SWH 7507.507 Hz  
 FIDRES 7.331550 Hz  
 AQ 0.0683150 sec  
 RG 23100  
 DW 66.600 usec  
 DE 6.00 usec  
 TE 296.1 K  
 CNST2 145.0000000  
 CNST13 10.0000000  
 d0 0.0000000 sec  
 d1 1.5000000 sec  
 d2 0.00344628 sec  
 d6 0.0500000 sec  
 D16 0.0002000 sec  
 INO 0.0001325 sec

----- CHANNEL F1 -----  
 NU1 1H  
 P1 13.50 usec  
 P2 27.00 usec  
 F11 2.20 GB  
 SFO1 500.0330060 MHz

----- CHANNEL F2 -----  
 NU2 13C  
 P3 10.20 usec  
 P4 2.20 GB  
 SFO2 125.7452173 MHz

----- GRADIENT CHANNEL -----  
 GRNAM1 SINE.100  
 GRNAM2 SINE.100  
 GRNAM3 SINE.100  
 GP1 50.00 %  
 GP2 30.00 %  
 GP3 40.10 %  
 P16 1000.00 usec  
 NDO 2  
 TD 512  
 SFO1 125.7452 MHz  
 FIDRES 73.702827 Hz  
 SW 300.098 ppm  
 FMODE QF  
 SF 500.0330000 MHz  
 SINE  
 L8 0.00 Hz  
 L9 0.00 Hz  
 PC 1.40  
 SI 1024  
 MC2 QF  
 SF 125.7326440 MHz  
 SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 FC 1.40  
 SI 1024  
 MC2 QF  
 SF 125.7326440 MHz  
 SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

YRT-24 hmbc 2019 11 01

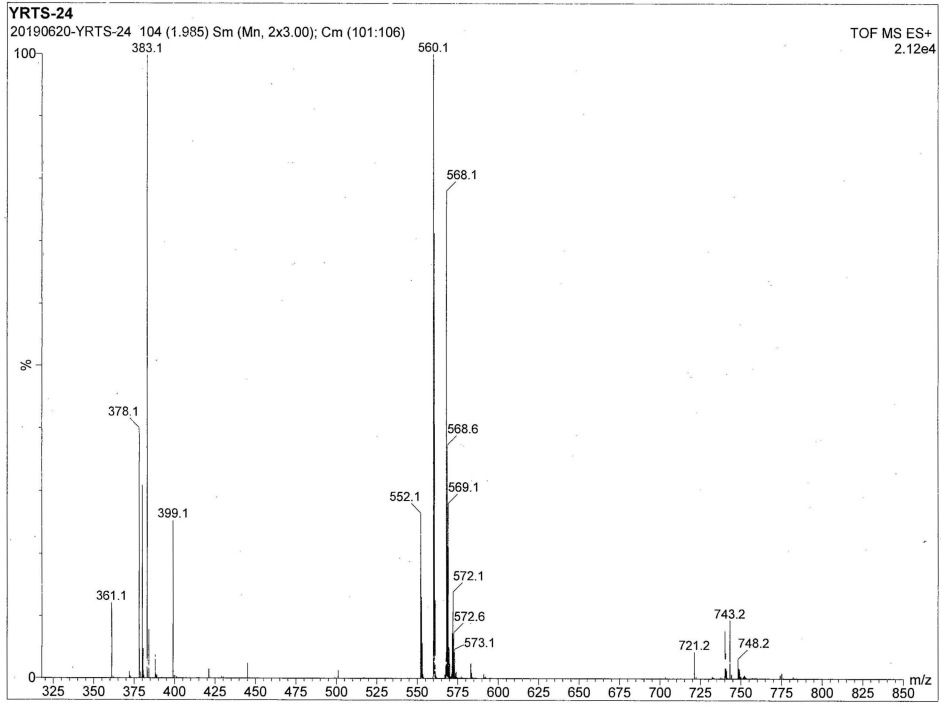


NAME YRT-24  
 EKFO 7  
 F60CND 1  
 Date\_ 20191101  
 Time 22.49  
 INSTRUM spect  
 PROBRD 5 mm PARO BBI-  
 PULPROG hmbcgp1pndgf  
 TD 1024  
 SOLVENT DMSO  
 NS 16  
 DS 16  
 SWH 7507.507 Hz  
 FIDRES 7.331550 Hz  
 AQ 0.0683150 sec  
 RG 23100  
 DW 66.600 usec  
 DE 6.00 usec  
 TE 296.1 K  
 CHST2 145.000000  
 CNST13 10.000000  
 CD 0.000000 sec  
 D1 1.5000000 sec  
 d2 0.0034498 sec  
 d6 0.0500000 sec  
 D16 0.0000000 sec  
 INO 0.00001325 sec

==== CHANNEL F1 =====  
 NU1 13C  
 P1 13.50 usec  
 PL1 2.20 dB  
 SFO1 500.0330060 MHz

==== CHANNEL F2 =====  
 NU2 13C  
 P3 10.20 usec  
 PL3 2.20 dB  
 SFO2 125.7452173 MHz

==== GRADIENT CHANNEL =====  
 GPRM1 SINE.100  
 GPRM2 SINE.100  
 GPRM3 SINE.100  
 GFI1 50.00 A  
 GFI2 30.00 A  
 GFI3 40.10 A  
 P16 1000.00 usec  
 NCO 2  
 TD 512  
 SFO1 125.7452 MHz  
 FIDRES 73.702827 Hz  
 SW 300.098 ppm  
 F8MODE GF  
 ST 2048  
 SF 500.0330000 MHz  
 SSB SINE  
 KSW 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40  
 SI 1024  
 MC2 GF  
 SFO 125.7326440 MHz  
 SSB SINE  
 KSB 0  
 LB 0.00 Hz  
 GB 0



单晶数据

Table 1. Crystal data and structure refinement for 121225f.

Identification code	121225f
Empirical formula	C <sub>19</sub> H <sub>20</sub> O <sub>7</sub>
Formula weight	360.35
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 10.1693(7) Å    alpha = 90 deg. b = 7.8196(6) Å    beta = 98.3250(10) deg. c = 11.0028(8) Å    gamma = 90 deg.
Volume	865.72(11) Å <sup>3</sup>
Z, Calculated density	2, 1.382 Mg/m <sup>3</sup>
Absorption coefficient	0.106 mm <sup>-1</sup>
F(000)	380
Crystal size	0.34 x 0.25 x 0.20 mm
Theta range for data collection	2.55 to 25.02 deg.
Limiting indices	-12<=h<=12, -9<=k<=6, -13<=l<=7
Reflections collected / unique	3001 / 2105 [R(int) = 0.0339]
Completeness to theta = 25.02	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9791 and 0.9649
Refinement method	Full-matrix least-squares on F <sup>2</sup>



Data / restraints / parameters	2105 / 1 / 237
Goodness-of-fit on $F^2$	1.025
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0449, wR2 = 0.0875
R indices (all data)	R1 = 0.0677, wR2 = 0.1014
Absolute structure parameter	0.0(17)
Extinction coefficient	0.008(3)
Largest diff. peak and hole	0.172 and -0.168 e. $\text{\AA}^{-3}$

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 121225f.

$U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U(\text{eq})$
O(1)	5079(2)	2584(4)	8995(2)	47(1)
O(2)	7110(3)	1527(4)	9546(2)	58(1)
O(3)	804(3)	1447(5)	5136(3)	91(1)
O(4)	5104(4)	9033(5)	5560(3)	83(1)
O(5)	6730(2)	7515(3)	7843(2)	41(1)
O(6)	7864(3)	7469(4)	9757(2)	52(1)
O(7)	10996(4)	10049(6)	8477(3)	96(1)
C(1)	6394(3)	2528(5)	8924(3)	40(1)
C(2)	6724(4)	3812(5)	8038(3)	36(1)
C(3)	5506(3)	4876(5)	7660(3)	34(1)
C(4)	4394(3)	3798(5)	8110(3)	37(1)
C(5)	3629(3)	2775(5)	7096(3)	42(1)
C(6)	2338(4)	2874(6)	6641(4)	48(1)
C(7)	1283(4)	4005(6)	7002(4)	61(1)
C(8)	1621(4)	5903(6)	7248(4)	57(1)
C(9)	2440(4)	6642(5)	6374(4)	53(1)
C(10)	3609(4)	7457(5)	6612(3)	44(1)
C(11)	4361(4)	7798(5)	7864(3)	44(1)
C(12)	5592(3)	6670(5)	8237(3)	36(1)
C(13)	7898(4)	3857(6)	7671(3)	50(1)
C(14)	1924(5)	1651(6)	5626(4)	64(1)
C(15)	4164(5)	8077(6)	5528(4)	60(1)
C(16)	7776(4)	7878(5)	8698(3)	39(1)
C(17)	8815(4)	8852(5)	8178(3)	40(1)
C(18)	10036(4)	9198(6)	9065(4)	56(1)
C(19)	8648(4)	9359(6)	7018(4)	56(1)

Table 3. Bond lengths [Å] and angles [deg] for 121225f.

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O(1)-C(1)	1.352(4)
O(1)-C(4)	1.462(4)
O(2)-C(1)	1.211(4)
O(3)-C(14)	1.198(5)
O(4)-C(15)	1.210(5)
O(5)-C(16)	1.344(4)
O(5)-C(12)	1.453(4)
O(6)-C(16)	1.200(4)
O(7)-C(18)	1.413(5)
O(7)-H(7)	0.8200
C(1)-C(2)	1.471(5)
C(2)-C(13)	1.316(5)
C(2)-C(3)	1.500(5)
C(3)-C(12)	1.537(5)
C(3)-C(4)	1.548(5)
C(3)-H(3)	0.9800
C(4)-C(5)	1.496(5)
C(4)-H(4)	0.9800
C(5)-C(6)	1.338(5)
C(5)-H(5)	0.9300
C(6)-C(14)	1.485(6)
C(6)-C(7)	1.488(6)
C(7)-C(8)	1.539(6)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.479(6)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.341(5)
C(9)-H(9)	0.9300
C(10)-C(15)	1.473(6)
C(10)-C(11)	1.500(5)
C(11)-C(12)	1.537(5)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-H(12)	0.9800
C(13)-H(13A)	0.9300
C(13)-H(13B)	0.9300
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300

C(16)-C(17)	1.483(5)
C(17)-C(19)	1.323(5)
C(17)-C(18)	1.489(5)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9300
C(19)-H(19B)	0.9300

C(1)-O(1)-C(4)	111.3(3)
C(16)-O(5)-C(12)	118.1(3)
C(18)-O(7)-H(7)	109.5
O(2)-C(1)-O(1)	120.4(4)
O(2)-C(1)-C(2)	129.8(3)
O(1)-C(1)-C(2)	109.8(3)
C(13)-C(2)-C(1)	121.7(4)
C(13)-C(2)-C(3)	130.5(4)
C(1)-C(2)-C(3)	107.7(3)
C(2)-C(3)-C(12)	113.4(3)
C(2)-C(3)-C(4)	102.8(3)
C(12)-C(3)-C(4)	111.4(3)
C(2)-C(3)-H(3)	109.7
C(12)-C(3)-H(3)	109.7
C(4)-C(3)-H(3)	109.7
O(1)-C(4)-C(5)	107.2(3)
O(1)-C(4)-C(3)	105.4(3)
C(5)-C(4)-C(3)	112.2(3)
O(1)-C(4)-H(4)	110.6
C(5)-C(4)-H(4)	110.6
C(3)-C(4)-H(4)	110.6
C(6)-C(5)-C(4)	128.7(4)
C(6)-C(5)-H(5)	115.7
C(4)-C(5)-H(5)	115.7
C(5)-C(6)-C(14)	113.6(4)
C(5)-C(6)-C(7)	129.9(4)
C(14)-C(6)-C(7)	116.5(3)
C(6)-C(7)-C(8)	118.0(3)
C(6)-C(7)-H(7A)	107.8
C(8)-C(7)-H(7A)	107.8
C(6)-C(7)-H(7B)	107.8
C(8)-C(7)-H(7B)	107.8
H(7A)-C(7)-H(7B)	107.2
C(9)-C(8)-C(7)	113.2(4)
C(9)-C(8)-H(8A)	108.9
C(7)-C(8)-H(8A)	108.9

C(9)-C(8)-H(8B)	108.9
C(7)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7
C(10)-C(9)-C(8)	128.7(4)
C(10)-C(9)-H(9)	115.6
C(8)-C(9)-H(9)	115.6
C(9)-C(10)-C(15)	115.5(4)
C(9)-C(10)-C(11)	125.7(4)
C(15)-C(10)-C(11)	118.8(4)
C(10)-C(11)-C(12)	115.5(3)
C(10)-C(11)-H(11A)	108.4
C(12)-C(11)-H(11A)	108.4
C(10)-C(11)-H(11B)	108.4
C(12)-C(11)-H(11B)	108.4
H(11A)-C(11)-H(11B)	107.5
O(5)-C(12)-C(11)	108.2(3)
O(5)-C(12)-C(3)	107.0(3)
C(11)-C(12)-C(3)	114.8(3)
O(5)-C(12)-H(12)	108.9
C(11)-C(12)-H(12)	108.9
C(3)-C(12)-H(12)	108.9
C(2)-C(13)-H(13A)	120.0
C(2)-C(13)-H(13B)	120.0
H(13A)-C(13)-H(13B)	120.0
O(3)-C(14)-C(6)	124.9(5)
O(3)-C(14)-H(14)	117.6
C(6)-C(14)-H(14)	117.6
O(4)-C(15)-C(10)	124.9(4)
O(4)-C(15)-H(15)	117.5
C(10)-C(15)-H(15)	117.5
O(6)-C(16)-O(5)	124.3(3)
O(6)-C(16)-C(17)	123.7(3)
O(5)-C(16)-C(17)	112.0(3)
C(19)-C(17)-C(16)	121.8(4)
C(19)-C(17)-C(18)	123.8(4)
C(16)-C(17)-C(18)	114.4(3)
O(7)-C(18)-C(17)	110.5(3)
O(7)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18A)	109.5
O(7)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	108.1
C(17)-C(19)-H(19A)	120.0
C(17)-C(19)-H(19B)	120.0

H(19A)-C(19)-H(19B) 120.0

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for 121225f.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
O(1)	39(1)	60(2)	42(1)	19(2)	10(1)	8(2)
O(2)	56(2)	68(2)	49(2)	15(2)	5(1)	18(2)
O(3)	78(2)	104(3)	81(2)	6(2)	-26(2)	-29(2)
O(4)	80(3)	106(3)	66(2)	24(2)	17(2)	-5(2)
O(5)	43(2)	48(2)	34(1)	1(1)	4(1)	-12(1)
O(6)	54(2)	60(2)	39(2)	10(2)	-4(1)	-6(2)
O(7)	96(3)	120(3)	73(2)	-17(2)	17(2)	-70(3)
C(1)	38(2)	48(2)	33(2)	0(2)	3(2)	14(2)
C(2)	33(2)	47(2)	27(2)	-2(2)	5(2)	1(2)
C(3)	29(2)	45(2)	28(2)	1(2)	6(1)	0(2)
C(4)	30(2)	43(2)	38(2)	7(2)	4(2)	4(2)
C(5)	39(2)	37(2)	48(2)	8(2)	5(2)	-4(2)
C(6)	37(2)	53(3)	52(2)	11(2)	0(2)	-6(2)
C(7)	32(2)	73(3)	77(3)	8(3)	9(2)	-3(3)
C(8)	39(2)	72(3)	61(3)	-4(3)	11(2)	10(2)
C(9)	57(3)	51(2)	48(2)	5(2)	-3(2)	17(3)
C(10)	46(2)	43(2)	42(2)	5(2)	2(2)	13(2)
C(11)	52(2)	40(2)	42(2)	-3(2)	12(2)	3(2)
C(12)	39(2)	43(2)	25(2)	-2(2)	8(2)	-5(2)
C(13)	39(2)	56(3)	58(2)	-3(2)	13(2)	2(2)
C(14)	62(3)	54(3)	69(3)	10(3)	-11(2)	-14(3)
C(15)	68(3)	66(3)	46(3)	11(2)	8(2)	12(3)
C(16)	43(2)	35(2)	40(2)	-4(2)	3(2)	1(2)
C(17)	42(2)	33(2)	45(2)	-6(2)	6(2)	-4(2)
C(18)	53(3)	60(3)	56(2)	-7(2)	4(2)	-21(2)
C(19)	59(3)	58(3)	54(3)	-3(2)	16(2)	-11(2)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 121225f.

	x	y	z	U(eq)
H(7)	11474	10632	8980	144
H(3)	5341	4973	6763	41
H(4)	3796	4530	8503	44
H(5)	4115	1962	6735	50
H(7A)	1003	3531	7738	73
H(7B)	525	3949	6357	73
H(8A)	800	6549	7202	69
H(8B)	2093	6021	8076	69
H(9)	2099	6525	5547	64
H(11A)	3761	7645	8465	53
H(11B)	4641	8985	7901	53
H(12)	5744	6558	9133	43
H(13A)	8546	3064	7973	60
H(13B)	8081	4682	7110	60
H(14)	2583	993	5350	77
H(15)	3761	7705	4760	72
H(18A)	9813	9898	9734	68
H(18B)	10401	8127	9409	68
H(19A)	7862	9106	6505	67
H(19B)	9316	9968	6716	67



Table 6. Torsion angles [deg] for 121225f.

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C(4)-O(1)-C(1)-O(2)	-176.2(3)
C(4)-O(1)-C(1)-C(2)	4.3(4)
O(2)-C(1)-C(2)-C(13)	10.3(6)
O(1)-C(1)-C(2)-C(13)	-170.3(4)
O(2)-C(1)-C(2)-C(3)	-172.0(4)
O(1)-C(1)-C(2)-C(3)	7.4(4)
C(13)-C(2)-C(3)-C(12)	-77.1(5)
C(1)-C(2)-C(3)-C(12)	105.5(3)
C(13)-C(2)-C(3)-C(4)	162.5(4)
C(1)-C(2)-C(3)-C(4)	-15.0(3)
C(1)-O(1)-C(4)-C(5)	105.9(3)
C(1)-O(1)-C(4)-C(3)	-13.8(4)
C(2)-C(3)-C(4)-O(1)	17.1(3)
C(12)-C(3)-C(4)-O(1)	-104.7(3)
C(2)-C(3)-C(4)-C(5)	-99.3(3)
C(12)-C(3)-C(4)-C(5)	138.9(3)
O(1)-C(4)-C(5)-C(6)	127.1(4)
C(3)-C(4)-C(5)-C(6)	-117.6(4)
C(4)-C(5)-C(6)-C(14)	179.8(3)
C(4)-C(5)-C(6)-C(7)	-0.5(7)
C(5)-C(6)-C(7)-C(8)	43.4(6)
C(14)-C(6)-C(7)-C(8)	-136.9(4)
C(6)-C(7)-C(8)-C(9)	39.9(5)
C(7)-C(8)-C(9)-C(10)	-125.4(5)
C(8)-C(9)-C(10)-C(15)	-178.8(4)
C(8)-C(9)-C(10)-C(11)	0.3(7)
C(9)-C(10)-C(11)-C(12)	105.2(4)
C(15)-C(10)-C(11)-C(12)	-75.8(5)
C(16)-O(5)-C(12)-C(11)	122.4(3)
C(16)-O(5)-C(12)-C(3)	-113.5(3)
C(10)-C(11)-C(12)-O(5)	89.6(4)
C(10)-C(11)-C(12)-C(3)	-29.7(5)
C(2)-C(3)-C(12)-O(5)	59.7(3)
C(4)-C(3)-C(12)-O(5)	175.1(3)
C(2)-C(3)-C(12)-C(11)	179.7(3)
C(4)-C(3)-C(12)-C(11)	-64.8(4)
C(5)-C(6)-C(14)-O(3)	175.2(4)
C(7)-C(6)-C(14)-O(3)	-4.5(6)
C(9)-C(10)-C(15)-O(4)	169.4(4)
C(11)-C(10)-C(15)-O(4)	-9.7(6)

C(12)-O(5)-C(16)-O(6)	4.2(5)
C(12)-O(5)-C(16)-C(17)	-175.7(3)
O(6)-C(16)-C(17)-C(19)	-176.3(4)
O(5)-C(16)-C(17)-C(19)	3.7(5)
O(6)-C(16)-C(17)-C(18)	3.7(5)
O(5)-C(16)-C(17)-C(18)	-176.4(3)
C(19)-C(17)-C(18)-O(7)	-3.1(6)
C(16)-C(17)-C(18)-O(7)	176.9(3)

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Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 121225f [A and deg.].

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D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O7-H7	0.820	2.044	162.60	2.837	O6 [ -x+2, y+1/2, -z+2 ]

