Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Stereogenic α-carbons determine the planar chirality of [13]-macrodilactones

Anniefer N. Magpusao, Kelli Rutledge, Brandon Q. Mercado, Mark W. Peczuh*
Department of Chemistry, University of Connecticut, 55 North Eagleville Road, U-3060, Storrs, CT 06269
Department of Chemistry, Yale University, 225 Prospect Street, New Haven, CT 06520

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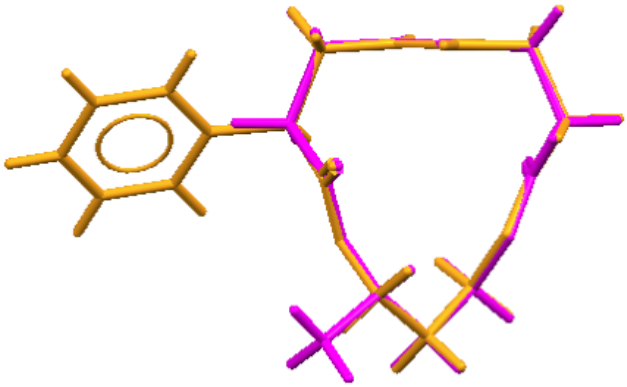
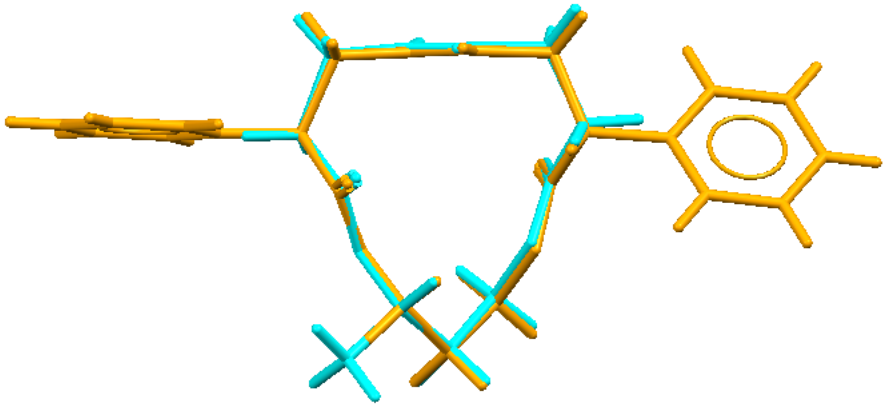
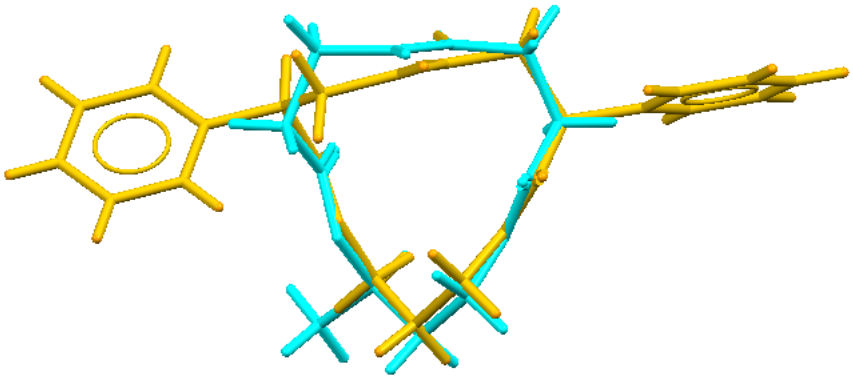


Overlay of *R*,p*R* **1** and *S*, p*R* **4** (RMSD 0.0454) showing common [13]-macro-dilactone structure.



overlay of **1** *and trans - 7R, 12R, pS* – **6;** RMSD = 0.0642



overlay of **1** *and cis – 7S, 12R, pR* – **7** RMSD = 0.49

Figure S1. Overlays.

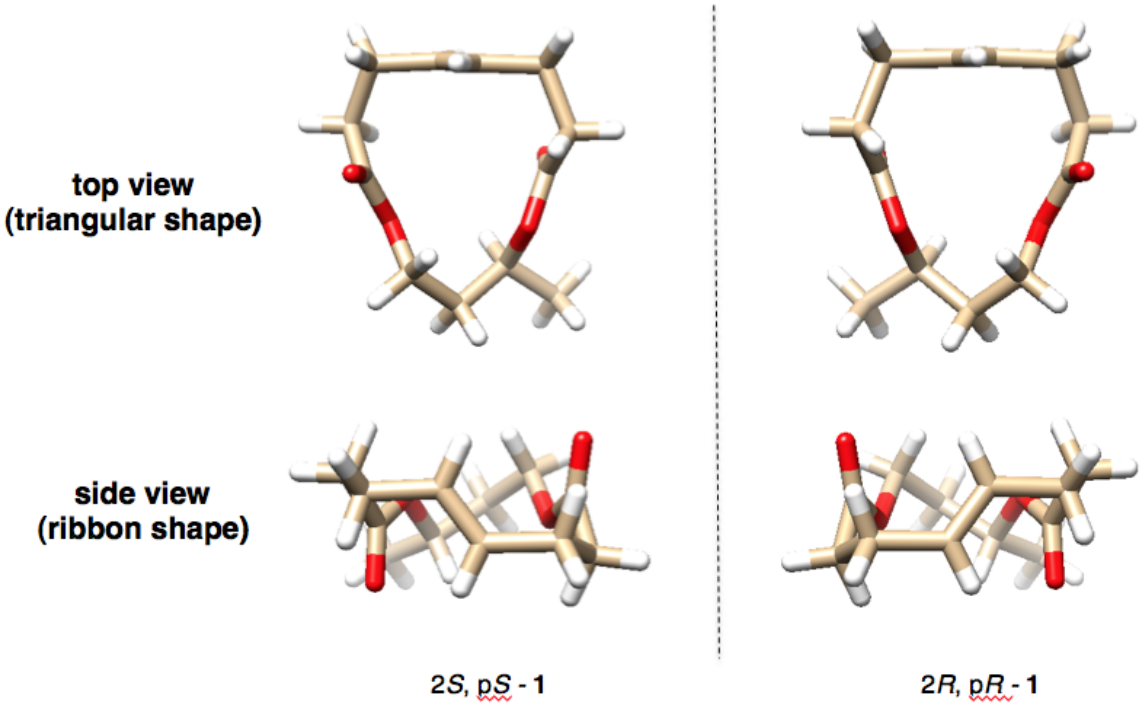


Figure S2. Top (triangular shape) and side (ribbon shape) views of macrocycle **1** planar enantiomers.

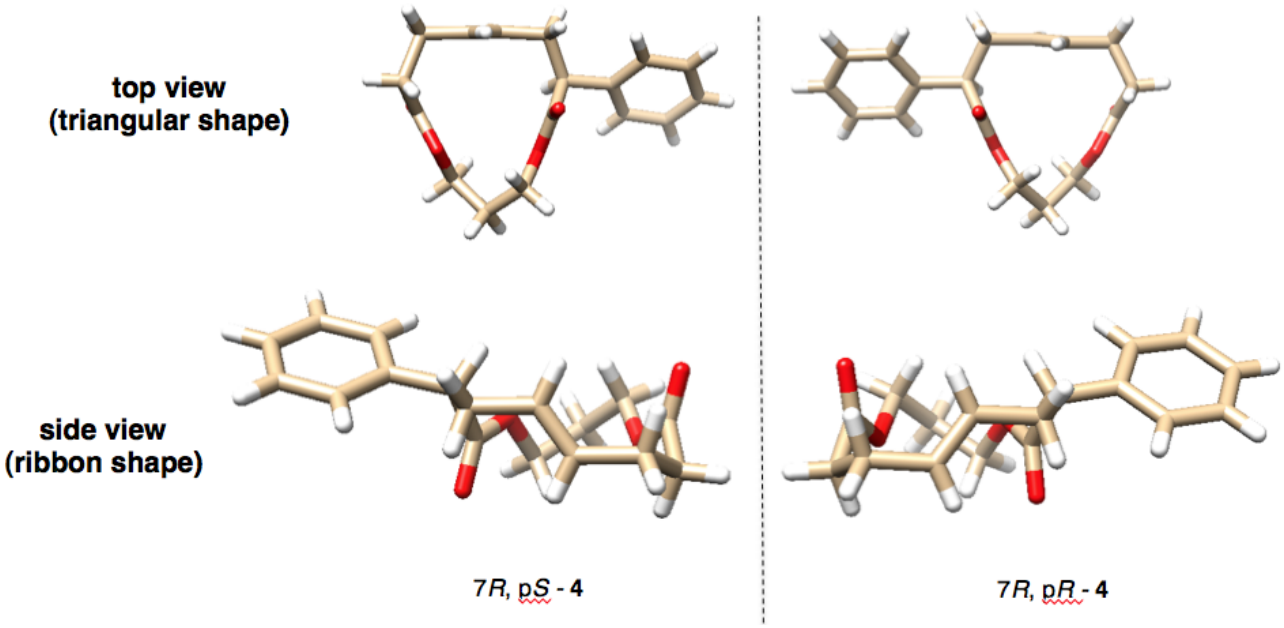


Figure S3. Top (triangular shape) and side (ribbon shape) views of macrocycle **2** planar enantiomers.

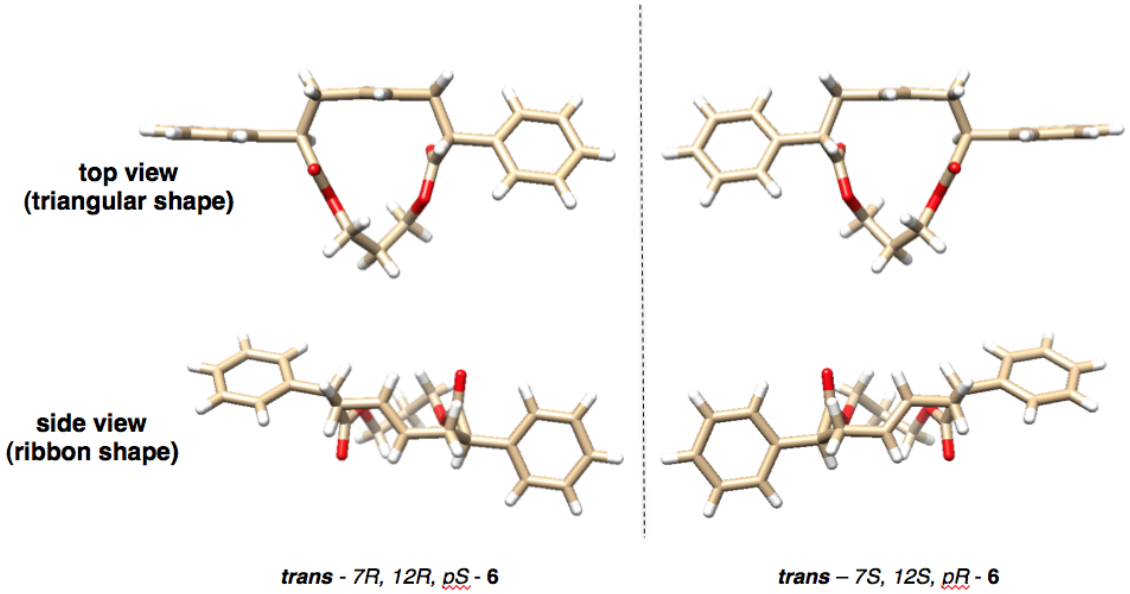


Figure S4. Top (triangular shape) and side (ribbon shape) views of macrocycle **6** planar enantiomers.

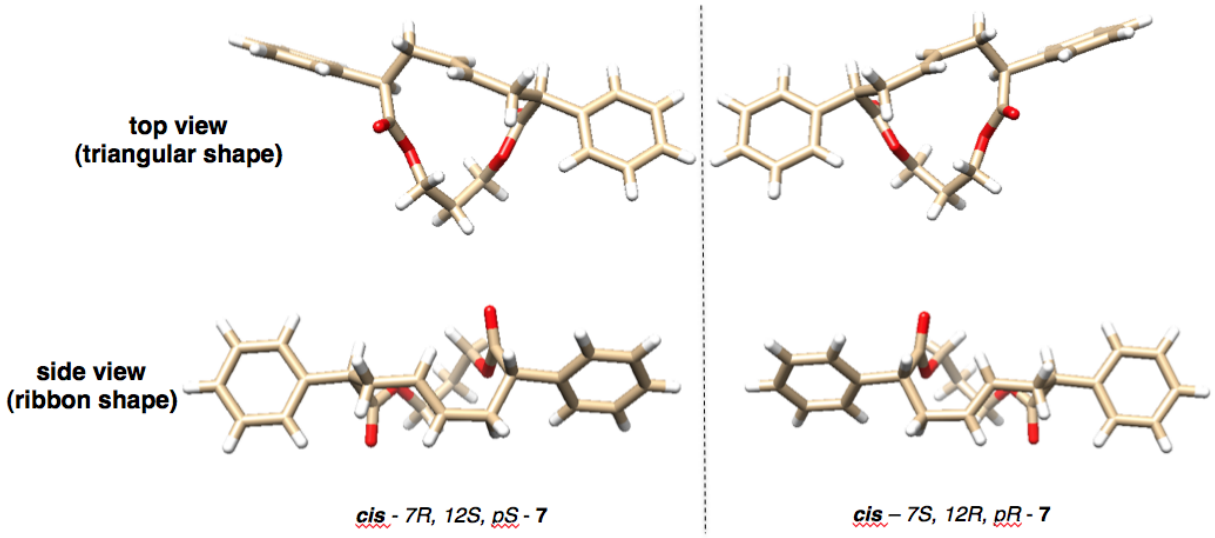


Figure S5. Top (triangular shape) and side (ribbon shape) views of macrocycle **7** planar enantiomers.

Table S1. Chiral HPLC integration data

Compound	Enantiomeric ratio: Area% (Area)	
Rac-4	49.90 (2465392)	50.10 (2475148)
7s, pR-**4**	21.13 (2614785)	78.87 (9762330)
Rac-**5**	47.36 (708771)	52.64 (787739)
7s, pR-**5**	21.77 (675305)	78.23 (2427390)

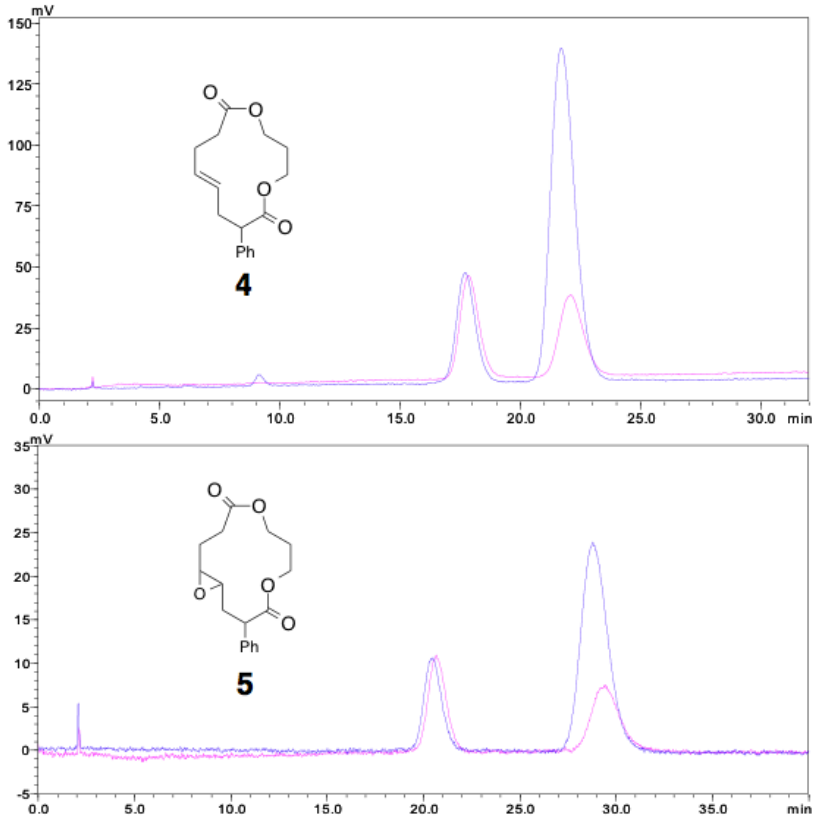


Figure S6. (**Note:** This figure is a the same as Figure 4 in the main text. It is added here for reference.) Chiral HPLC profiles of racemic (pink) and chiral (blue) C12-phenyl [13]-macrodilactone **3** and their corresponding epoxides **4** upon DMDO epoxidation.

Procedure for determination of RMSDs

The root mean square deviations (RMSDs) were produced with the structure overlay feature of the Mercury software package. Pairs of atoms were selected to calculate the square root of the mean square differences between atomic coordinates. Our approach focused on the 13 atoms of the macrocycle in compound **1**. These coordinates were mapped onto the corresponding atom positions of compounds **4**, **6**, and **7**. All of the compounds reported here crystallized as racemic mixtures. The coordinates were carefully inspected to insure the average RMSD between two sets of coordinates reflected corresponding conformations in the alkene and ester functional groups.

Experimental Procedures

General

Reactions were monitored using TLC. UV light, *p*-anisaldehyde, potassium permanganate ($KMnO_4$) or ceric ammonium molybdate (CAM) solutions were used for visualization. Chromatography was performed on silica gel and solvent systems used were based on the R_f values. ^{1}H NMR spectra (400 MHz) were referenced to $CDCl_3$ (δ_H 7.27 ppm) and ^{13}CNMR spectra (100 MHz) were referenced to $CDCl_3$ (δ_C 77.23 ppm).

Sequential Acylations

Method A:

Dicyclohexylcarbodiimide (DCC) (1.09 mmol) and N,N-dimethylaminopyridine (DMAP) (0.3 mmol) in DCM (7 mL) were stirred at 0 °C. 4-pentenoic acid (1 mmol) was added and the mixture was stirred at the same temperature for 30 minutes until a white suspension was observed in the flask. 1,3-propanediol (1 mmol) in DCM (3 mL) was then added to the reaction mixture and stirred overnight at room temperature. The mixture was filtered through a celite and solvent was removed from the filtrate under reduced pressure. The crude residue was purified by silica gel column chromatography (3:1 Hex:EtOAc) to give the monoacylated product.

Method B:

DCC (1.09 mmol) and DMAP (0.3 mmol) were added in DCM (40 mL) and cooled to 0°C. The acid of choice (either rac-**2** or S-**2**, 1 mmol) was added to the solution and stirred at the same temperature for 30 minutes. The monoacylated product (1 mmol) from the first acylation was then added to the mixture and stirred overnight at room temperature. The reaction mixture was filtered through celite and and the DCM of the filtrate was removed under reduced pressure. Crude residue was purified by silica gel column chromatography to give the diene.

One-pot acylation

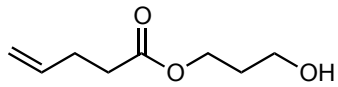
In a round bottom flask, DCC (0.23 g, 1.09 mmol) and DMAP (.037 g, 0.300 mmol) were dissolved in DCM (40mL), and the solution was cooled to 0°C. Rac-**2** (1.00 mmol) was added and stirred at the same temperature for 30 minutes. 1,3-propanediol (0.500 mmol) in DCM (10 mL) was then added to the mixture and stirred overnight at room temperature. The mixture was then filtered through celite. The solvent of the filtrate was removed under reduced pressure and the residue was purified by silica gel column chromatography to get the diene.

Ring Closing Metathesis

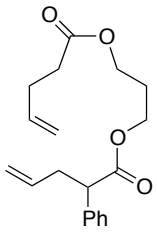
Grubbs' second-generation catalyst (0.050 mmol) was added to a solution of the diene in toluene (100 mL). The mixture was heated to reflux at 110 °C overnight. The toluene was removed under reduced pressure and the crude product was purified by column chromatography.

DMDO Epoxidation (Lee, D.; Sello, J. K.; Schreiber S. L. *J. Am. Chem. Soc.* **1999**, *121*, 10648-10649)

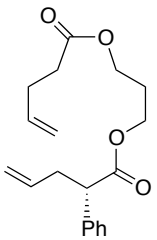
Excess amount of $NaHCO_3$ (0.450 g, 0.94 mmol) and Oxone (0.450 g, 0.19 mmol) was added to a solution of macrocycle **4** (racemic or chiral) (75 mg) in acetone:H_2O:DCM (1:1:1, 15 mL) at 0 °C. The resulting heterogeneous mixture was stirred for 3 h at 0 °C and extracted with DCM. The epoxide was purified using column chromatography.



3-hydroxypropyl 4-pentenoate. The synthesis of this compound followed the general monoacylation procedure (Method A) to give 3-hydroxypropyl 4-pentenoate in 52% yield as a colorless oil (1.0 mmol scale). R_f 0.2 (30% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 5.82 (ddd, 1H, *J*= 10.4, 6.3, 6.3, 6.3 Hz), 5.08 (dd, 1H, *J* = 16.6, 16.6, 0 Hz), 5.02 (dd, 1H, *J*= 10.2, 10.2, 0 Hz), 4.25 (t, 2H, *J* = 6.1 Hz), 3.69 (m 2H), 2.80 (s, 1H), 2.41 (m, 4H), 1.88 (qn, 2H, *J* = 6.1 Hz); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.6, 136.6, 115.6, 61.5, 59.0, 33.6, 31.7, 28.9; TOF HRMS (ESI) *m/z* calcd for $C_8H_{14}O_3$ $(M+Na)^+$ 181.0841, found 181.0838.

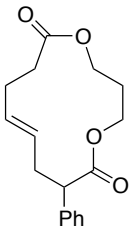


***rac*-3.** The synthesis of this compound followed the general method of dienes through monoacylation (Method B) in 50% yield and as a clear yellowish oil (0.63 mmol). R_f 0.6 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.33 (m, 4H), 7.28 (m, 1H), 5.83 (m, 1H), 5.74 (dddd/ddt, 1H, *J*= 17.0, 10.3, 6.7, 6.7), 5.08 (m, 2H), 5.01 (dd, 2H, *J*= 10.4, 5.0), 4.16 (ddd, 2H, *J*= 17.5, 11.34, 6.3), 4.08 (m, 2H), 3.66 (dd, 1H, *J*= 8.5, 7.1), 2.85 (ddd, 1H, *J*= 14.8, 8.2, 8.2), 2.54 (ddd, 1H, *J*= 13.8, 6.8, 6.8), 2.39 (ddd, 4H, *J*= 15.5, 11.35, 4.17), 1.93 (dddd/dq, 2H, *J*= 6.48, 6.48, 6.48, 6.48); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.5, 173.1, 138.7, 136.8, 135.4, 128.9, 128.1, 127.6, 117.3, 115.8, 61.5, 61.0, 51.7, 37.7, 33.7, 29.1, 28.1; TOF HRMS (DART) *m/z* calcd for $C_{19}H_{24}O_4$ $(M+H)^+$ 317.1753, found 317.1732.

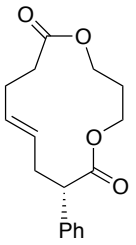


***S*-3.** Followed the general method of dienes through monoacylation (method A and then method B) in 75% yield as a yellowish oil (0.79 mmol). R_f 0.6 (20% EtOAc:Hex); $[\alpha]_D$ +257.4° (c 1.0, CH_2Cl_2);^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.30 (m, 5H), 5.80 (m, 2H), 5.08 (m, 2H), 5.02 (dd, 2H, *J*=10.3, 4.9), 4.16 (ddd, 2H, *J*= 17.57, 11.09, 6.31), 4.07 (m, 2H), 3.66(dd, 1H, *J*= 8.5, 7.0), 2.84 (ddd, 1H, *J*=

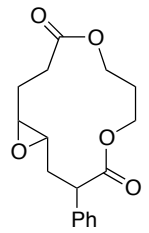
15.01, 8.07, 8.07), 2.54 (ddd, 1H, *J*= 13.64, 6.74, 6.74), 2.38 (ddd, 4H, *J*= 14.71, 11.34, 4.35), 1.92 (dddd/dq, 2H, *J*= 6.37, 6.37, 6.37, 6.37); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.5, 173.1, 138.7, 136.8, 135.4, 128.8, 128.1, 127.6, 117.2, 115.7, 61.5, 61.0, 51.7, 37.6, 33.7, 29.0, 28.1; TOF HRMS (ESI) *m/z* calcd for $C_{19}H_{24}O_4$ $(M+Na)^+$ 339.1572, found 339.1556.



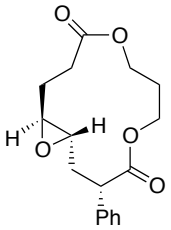
***rac*-4.** Followed the general RCM method to give the product in 54% yield and as a white crystalline solid (0.61 mmol). m.p. 78-79 °C; R_f 0.4 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.37 (d, 2H, *J*= 7.1), 7.31 (dd, 2H, *J*= 7.1, 7.1), 7.26 (dd, 1H, *J*= 3.1, 3.1), 5.55 (m, 2H), 4.54 (m, 1H), 4.44 (m, 1H), 4.01 (ddd/dt, 1H, *J*= 8.2, 4.1, 4.1), 3.83 (ddd/dt, 1H, *J*= 8.2, 4.1, 4.1), 3.60 (dd, 1H, *J*= 12.6, 2.7), 2.77 (ddd/dt, 1H, *J*= 12.9, 12.0, 8.1), 2.35 (m, 5H), 2.03 (m, 2H); ^{13}C NMR ($CDCl_3$) 100 MHz δ 174.2, 173.9, 139.1, 131.1, 129.1, 128.9, 127.9, 127.6, 60.6, 60.4, 52.1, 37.9, 34.3, 28.8, 26.0; TOF HRMS (ESI) *m/z* calcd for $C_{17}H_{20}O_4$ $(M+Na)^+$ 311.1259, found 311.1256; anal. for $C_{17}H_{20}O_4$, C 70.78, H 6.96, O 22.26, found C 70.86, H 6.96.



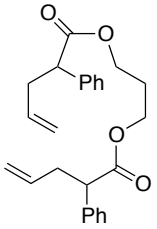
***7S,pR*-4**. Followed the general method of RCM on a (1.14 mmol) scale to give *7S,pR*-**4** in 25% yield as a white solid. m.p. 72-74 °C; $[\alpha]_D$ +2.6° (c 1.0, CH_2Cl_2); R_f 0.4 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.39 (d, 2H, *J*= 7.2), 7.23 (dd, 2H, *J*= 7.2, 7.2), 7.26 (m, 1H), 5.56 (m, 2H), 4.54 (m, 1H), 4.46 (m, 1H), 4.04 (ddd/dt, 1H, *J*= 8.4, 4.0, 4.0), 3.86 (ddd/dt, 1H, *J*= 8.4, 4.0, 4.0), 3.62 (dd, 1H, *J*= 12.6, 2.9), 2.79 (ddd/dt, 1H, *J*= 12.9, 12.9, 8.2), 2.37 (m, 5H), 2.05 (m, 2H);); ^{13}C NMR ($CDCl_3$) 100 MHz δ 174.1, 173.9, 139.0, 131.0, 129.0, 128.8, 127.9, 127.6, 60.6, 60.4, 52.0, 37.9, 34.3, 28.7, 26.0; TOF HRMS (ESI) *m/z* calcd for $C_{17}H_{20}O_4$ $(M+Na)^+$ 311.1259, found 311.1253.



***rac*-5**. Compound *rac*-**4** was epoxidized using a procedure for in situ generation of DMDO as described to give *rac*-**5** in 64% yield (0.26 mmol) as a white solid. m.p. 100-102 °C; R_f 0.2 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.30 (m, 5H), 4.82 (m, 2H), 3.91 (ddd/dt, 1H, *J*= 8.1, 3.7, 3.7), 3.72 (m, 2H), 2.87 (ddd, 2H, *J*= 8.8, 8.8, 2.6), 2.47 (dd, 2H, *J*= 8.24, 5.04), 2.24 (m, 2H), 2.03 (m, 3H), 1.60 (m, 1H); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.4, 172.9, 139.1, 129.0, 127.7, 127.6, 60.2, 59.5, 58.5, 57.6, 47.8, 36.7, 29.6, 26.9, 26.3; TOF HRMS (ESI) *m*/*z* calcd for $C_{17}H_{20}O_5$ $(M+Na)^+$ 327.1208, found 327.1206.

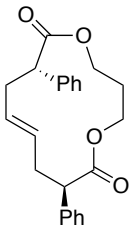


***7S,pR* -5.** Compound *7S,pR*-**4** was epoxidized using a procedure for in situ generation of DMDO as described to give 7*S*,p*R*-**5** in 67% yield and as a white solid (0.25 mmol). mp 114-118 °C; $[\alpha]_D$ +120.3° (c 1.0, CH_2Cl_2); R_f 0.2 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.29 (m, 5H), 4.83 (m, 2H), 3.92 (ddd/dt, 1 H, *J*= 8.2, 4.3, 4.3), 3.73 (m, 2H), 2.87 (ddd, 2H, *J*= 8.8, 8.8, 2.6), 2.47 (dd, 2H, *J*= 8.2, 5.3), 2.25 (m, 2H), 2.06 (m, 2H), 2.00 (ddd/dt, 1H, *J*= 12.9, 9.6, 9.6), 1.61 (m, 1H); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.4, 172.9, 139.1, 129.1, 127.7, 127.6, 60.2, 59.5, 58.5, 57.6, 47.8, 36.7, 29.6, 26.9, 26.3; TOF HRMS (ESI) *m*/*z* calcd for $C_{17}H_{20}O_5$ $(M+Na)^+$ 327.1208, found 327.1216.

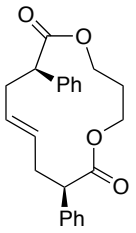


S1. Followed the general procedure of diene through diacylation in 46% yield and clear yellowish oil (2.55 mmol). R_f 0.8 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.22 (m, 10H), 5.63 (dddd/dt, 2H, *J*= 17.3, 10.3, 7.0, 7.0), 5.00 (dd, 2H, *J*= 17.1, 1.3), 4.92 (dd, 2H, *J*= 10.2, 0), 3.96 (m, 4H), 3.54 (dd, 2H, *J*= 7.9, 7.9), 2.73 (ddd, 2H, *J*= 14.58, 8.05, 8.05), 2.43 (ddd, 2H, *J*= 13.93, 6.75, 6.75), 1.77 (dddd/tt, 2H,

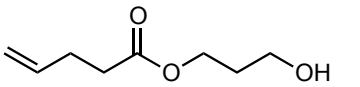
J= 6.13, 6.13, 6.13, 6.13); ^{13}C NMR ($CDCl_3$) 100 MHz δ 173.5, 138.7, 135.4, 128.9, 128.1, 127.6, 117.3, 61.3, 51.7, 37.7, 28.1; TOF HRMS (ESI) *m/z* calcd for $C_{25}H_{28}O_4$ $(M+Na)^+$ 415.1885, found 415.1911.

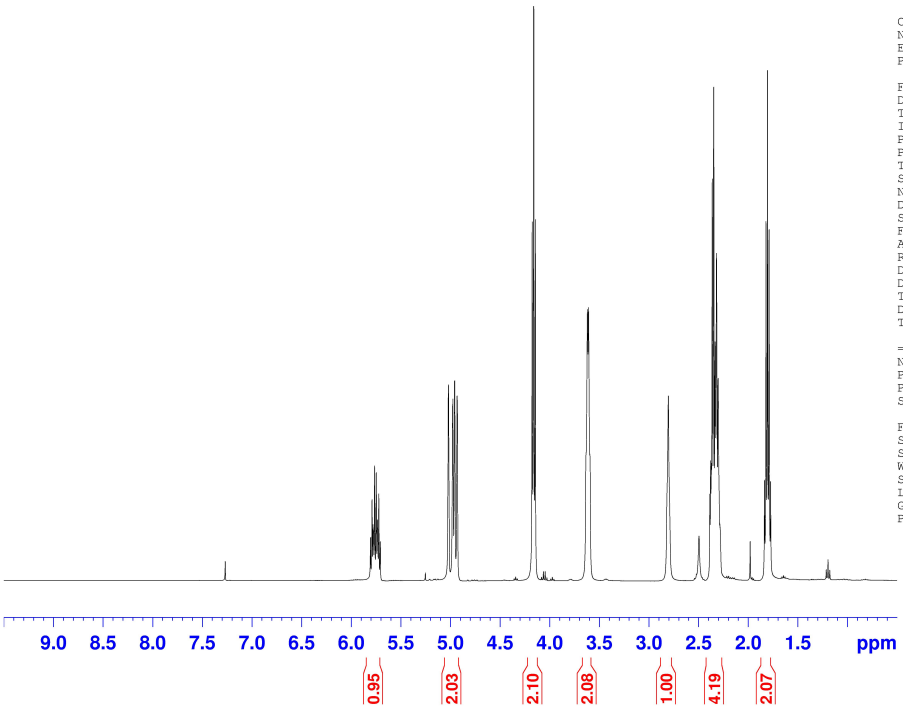


6. Obtained using the general RCM procedure in 47% yield (0.45 mmol) as a white solid. m.p. 172-174 °C; R_f 0.56 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.33 (m, 10H), 5.64 (ddd/dt, 2H, *J*= 3.67, 3.67, 0), 4.67 (m, 2H), 3.80 (ddd/dt, 2H, *J*= 7.09, 3.17, 3.17), 3.62 (dd, 2H, *J*= 12.50, 2.14), 2.82 (m, 2H), 2.28 (dd, 2H, *J*= 12.62, 0), 2.03 (m, 2H); ^{13}C NMR ($CDCl_3$) 100 MHz δ 174.1, 139.0, 130.3, 128.9, 127.8, 127.6, 59.7, 51.8, 38.1, 25.5; TOF HRMS (DART) m/z calcd for $C_{23}H_{24}O_4$ $(M+H)^+$ 365.1753, found 365.1749



7. Obtained in the same RCM reaction as **6** in 20% yield (0.19 mmol) as a white solid. m.p. 147-156 °C; R_f 0.44 (20% EtOAc:Hex); ^{1}HNMR ($CDCl_3$) 400 MHz. δ 7.33 (m, 10 H), 5.74 (ddd, 2H, *J*= 2.84, 2.84, 0), 4.41 (ddd, 2H, *J*= 11.37, 5.71, 5.71), 4.09 (ddd, 2H, *J*= 10.93, 5.15, 5.15), 3.75 (ddd, 2H, *J*= 12.17, 3.31, 0), 2.78 (m, 2H), 2.40 (dd, 2H, *J*= 13.57, 0), 2.08 (dddd/dq, 2H, *J*= 5.20, 5.20, 5.20, 5.20); ^{13}C NMR ($CDCl_3$) 100 MHz δ 174.1, 139.1, 129.7, 128.9, 128.1, 127.7, 63.1, 52.4, 36.9, 27.3; TOF HRMS (DART) m/z calcd for $C_{23}H_{24}O_4$ $(M+H)^+$ 365.1753, found 365.1748.



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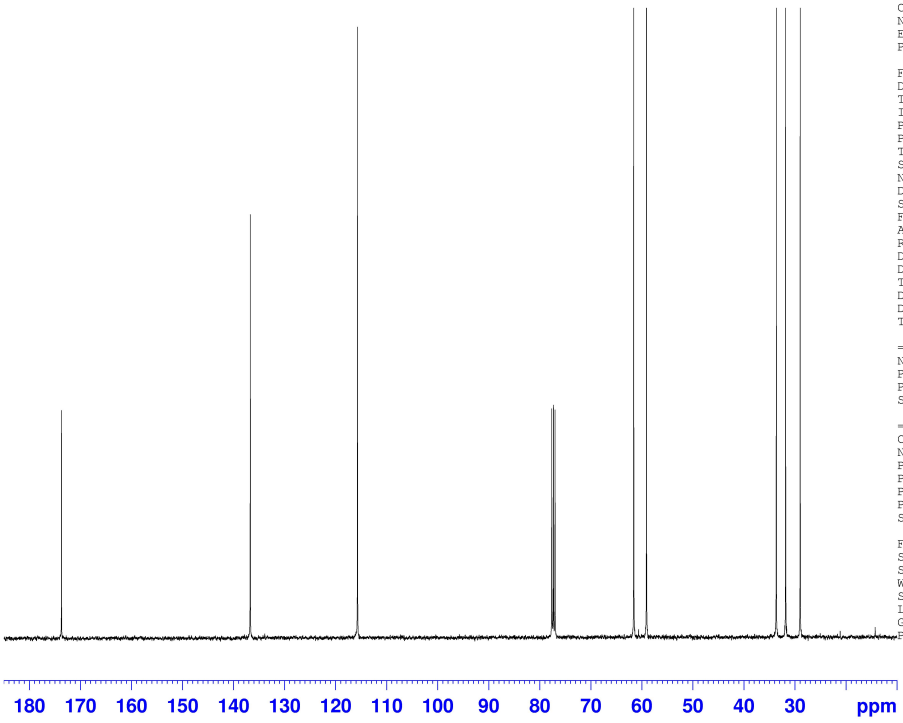
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.25 usec
PLW1           12.00000000 W
SFO1          400.1464009 MHz

F2 - Processing parameters
SI                    131072
SF               400.1440000 MHz
WDW                      EM
SSB          0
LB                    0.50 Hz
GB           0
PC                    1.00
```



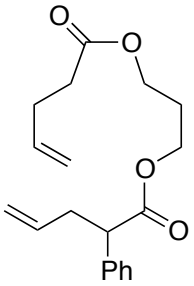

```
Current Data Parameters
NAME      monoacylated-Am-II-59
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_              20141231
Time                   9.58
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                   43698
SOLVENT              CDCl3
NS                     305
DS                       4
SWH              24038.461 Hz
FIDRES               0.550104 Hz
AQ                0.9089684 sec
RG                     203
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                1.50000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1           50.00299835 W
SFO1          100.6263500 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                    1H
PCPD2                90.00 usec
PLW2           12.00000000 W
PLW12           0.33333001 W
PLW13           0.27000001 W
SFO2          400.1456006 MHz

F2 - Processing parameters
SI                    131072
SF               100.6162656 MHz
WDW                      EM
SSB          0
LB                    2.50 Hz
GB           0
PC                    1.40
```

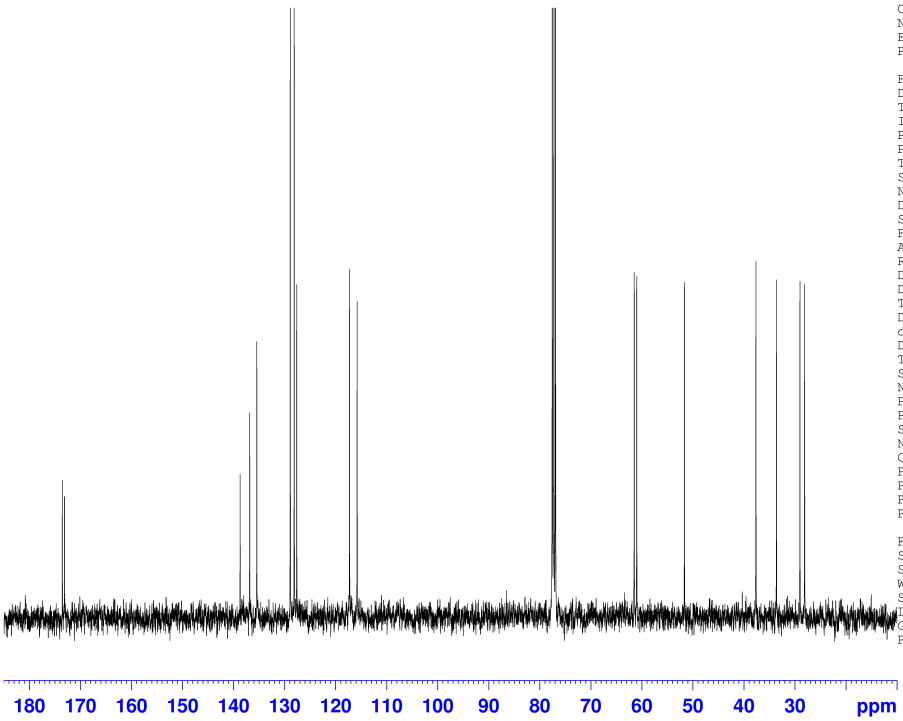



```
Current Data Parameters
NAME         am-II-57-f6
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140717
Time               18.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 48076
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.166670 Hz
AQ              2.9999423 sec
RG                    64
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.25 usec
PLW1         12.00000000 W
SFO1         400.1464009 MHz

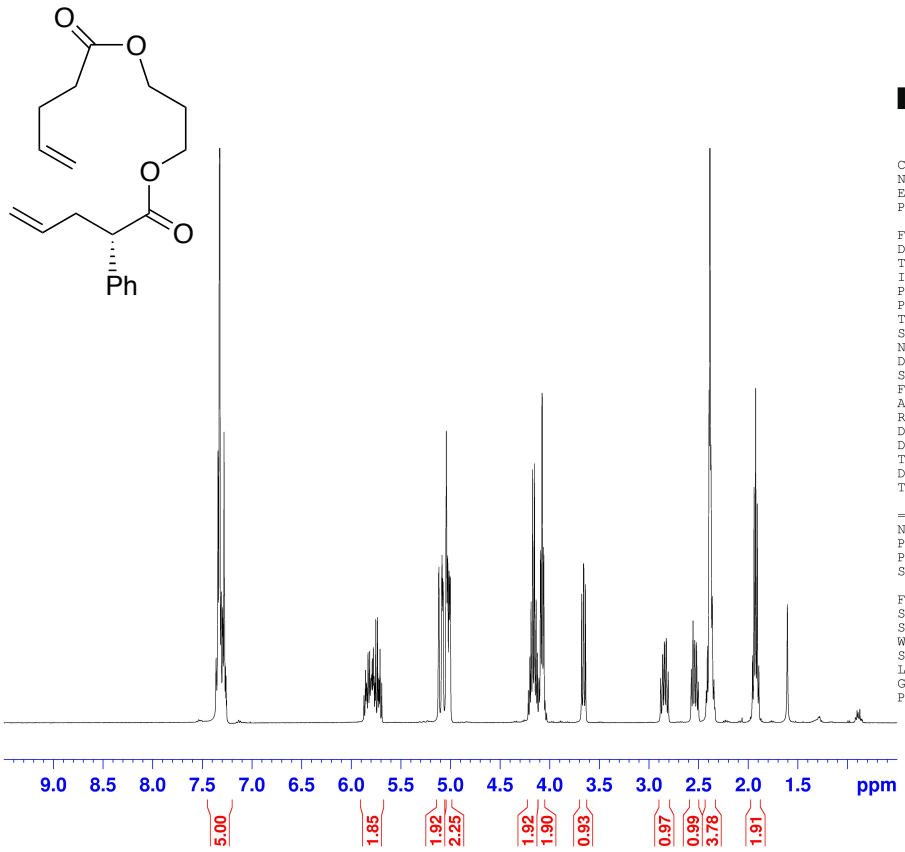
F2 - Processing parameters
SI                131072
SF           400.1440000 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME         am-II-57-f6
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140717
Time               18.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 43698
SOLVENT            CDCl3
NS                   113
DS                     4
SWH            24038.461 Hz
FIDRES          0.550104 Hz
AQ              0.9089184 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             1.50000000 sec
d11            0.03000000 sec
DELTA          1.39999998 sec
TD0                    1
SFO1         100.6263500 MHz
NUC1                  13C
P1                10.00 usec
PLW1         50.00299835 W
SFO2         400.1456006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

F2 - Processing parameters
SI                131072
SF           100.6162656 MHz
WDW                   EM
SSB       0
LB                 2.50 Hz
GB        0
PC                 1.40
```



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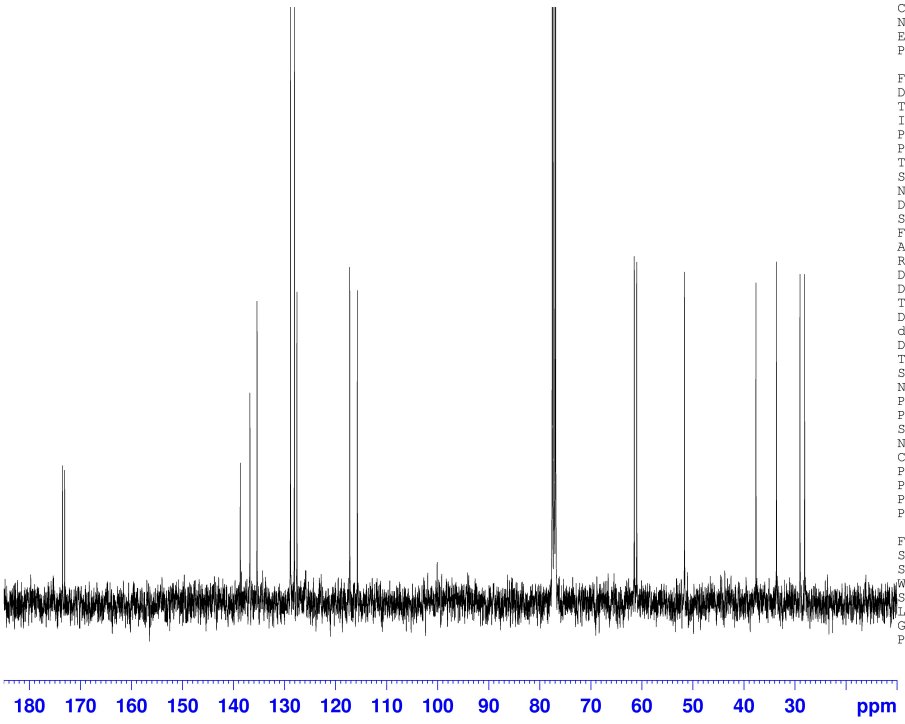
```
Current Data Parameters
NAME         am-II-59-f5
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140717
Time               17.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 48076
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.166670 Hz
AQ              2.9999423 sec
RG                  80.6
DW                62.400 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.25 usec
PLW1         12.00000000 W
SFO1         400.1464009 MHz

F2 - Processing parameters
SI                131072
SF          400.1440000 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```



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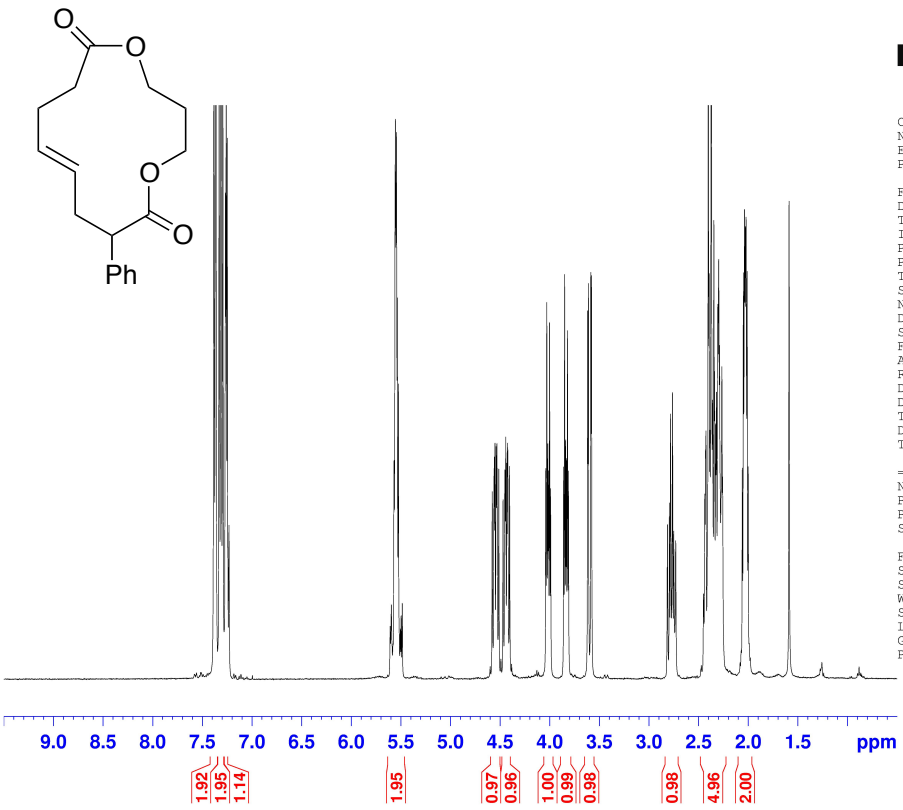
```
Current Data Parameters
NAME         am-II-59-f5
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140717
Time               17.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 43698
SOLVENT            CDCl3
NS                   110
DS                     4
SWH            24038.461 Hz
FIDRES          0.550104 Hz
AQ              0.9089184 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1             1.50000000 sec
d11            0.03000000 sec
DELTA          1.39999998 sec
TD0                    1
SFO1         100.6263500 MHz
NUC1                  13C
P1                10.00 usec
PLW1         50.00299835 W
SFO2         400.1456006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

F2 - Processing parameters
SI                131072
SF          100.6162695 MHz
WDW                   EM
SSB       0
LB                 2.50 Hz
GB        0
PC                 1.40
```

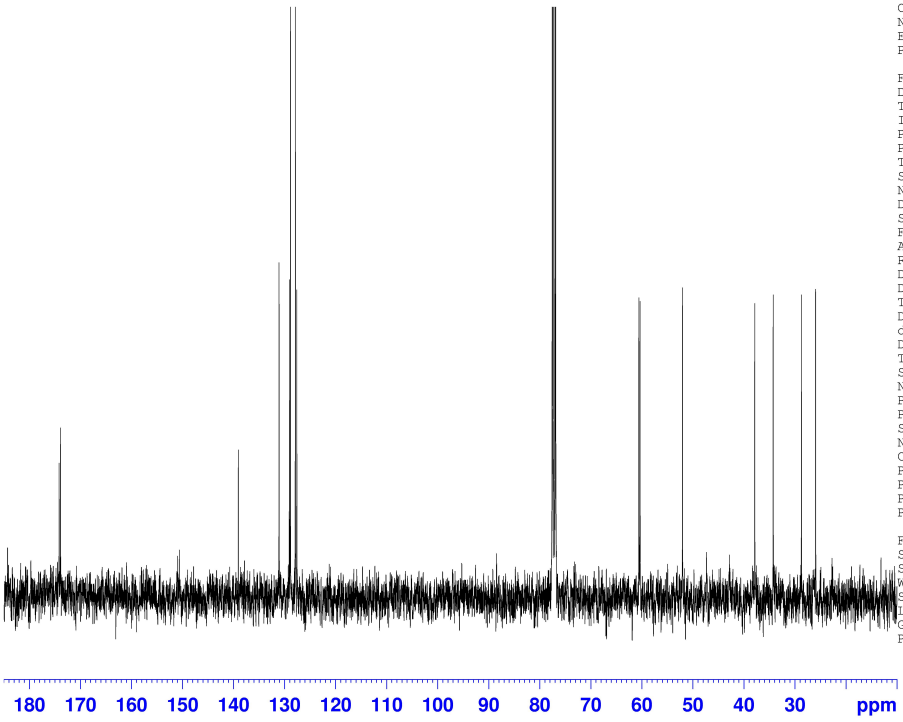



```
Current Data Parameters
NAME                  am-R18-F9
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130523
Time                      10.56
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       48076
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.166670 Hz
AQ                    2.9999423 sec
RG                         128
DW                      62.400 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       15.20 usec
PLW1                12.00000000 W
SFO1                400.1464009 MHz

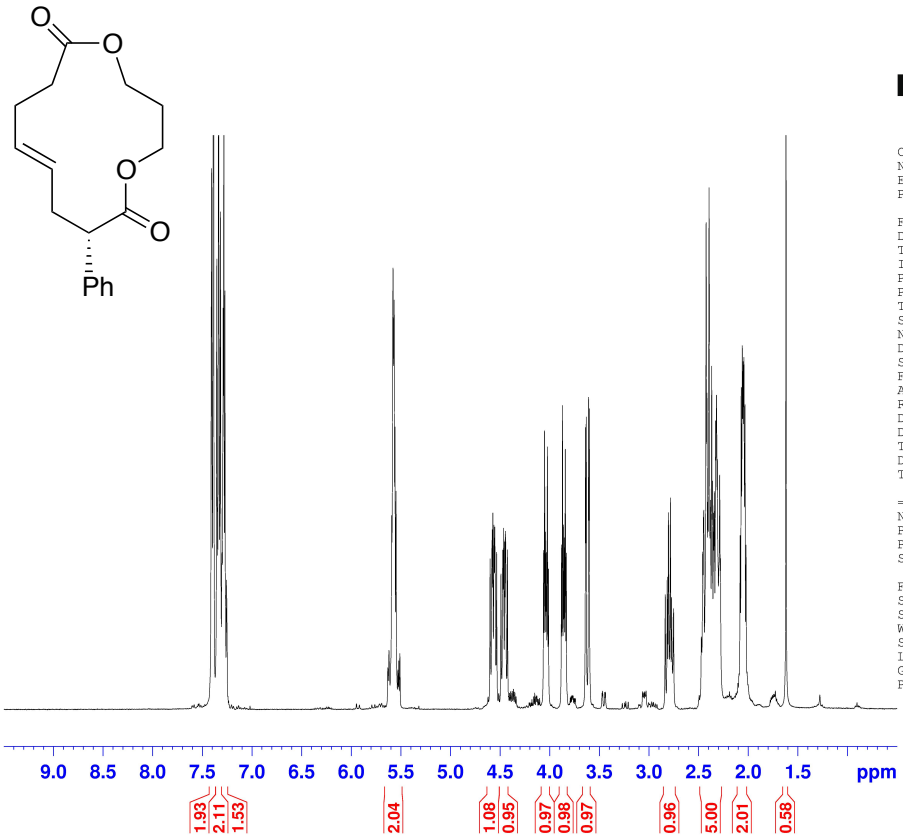
F2 - Processing parameters
SI                       131072
SF                  400.1440100 MHz
WDW                          EM
SSB                 0
LB                        0.50 Hz
GB                  0
PC                        1.00
```




```
Current Data Parameters
NAME                  am-R18-F9
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130523
Time                      11.02
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       43698
SOLVENT                  CDCl3
NS                          86
DS                           4
SWH                  24038.461 Hz
FIDRES                0.550104 Hz
AQ                    0.9089184 sec
RG                         203
DW                      20.800 usec
DE                       6.50 usec
TE                      300.1 K
D1                    1.50000000 sec
d11                   0.03000000 sec
DELTA                 1.39999998 sec
TD0                           1
SFO1                100.6263500 MHz
NUC1                         13C
P1                       10.00 usec
PLW1                50.00299835 W
SFO2                400.1456006 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.00000000 W
PLW12                0.33333001 W
PLW13                0.27000001 W

F2 - Processing parameters
SI                       131072
SF                  100.6162656 MHz
WDW                          EM
SSB                 0
LB                        2.50 Hz
GB                  0
PC                        1.40
```



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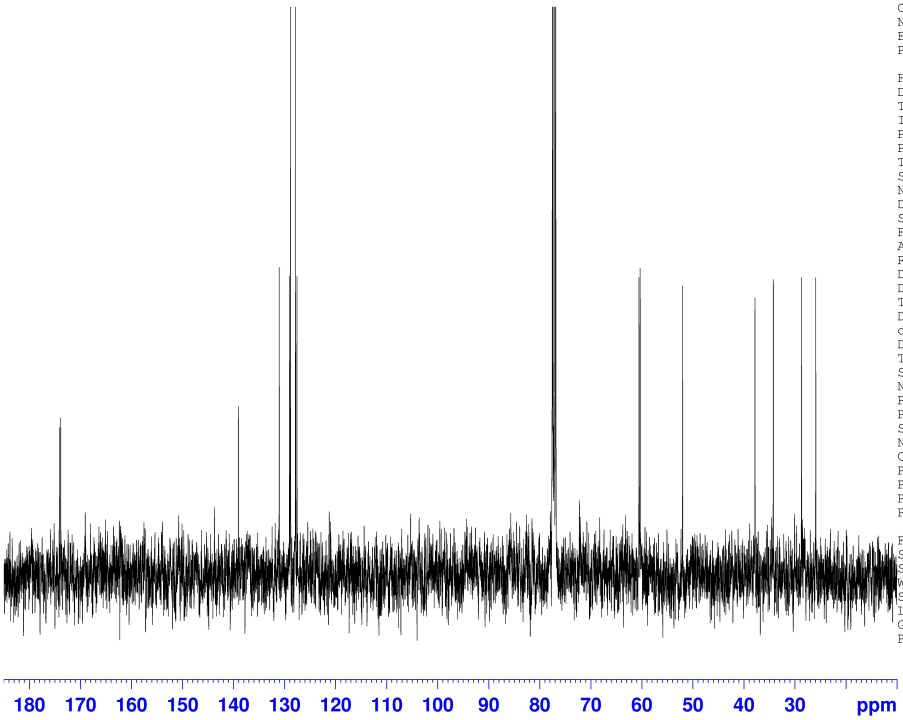
```
Current Data Parameters
NAME      am-II-63-col2-f5
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140729
Time                 23.30
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  48076
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES           0.166670 Hz
AQ               2.9999423 sec
RG                   80.6
DW                 62.400 usec
DE                  6.50 usec
TE                 300.0 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.25 usec
PLW1          12.00000000 W
SFO1          400.1464009 MHz

F2 - Processing parameters
SI                  131072
SF            400.1440000 MHz
WDW                    EM
SSB       0
LB                   0.50 Hz
GB        0
PC                   1.00
```



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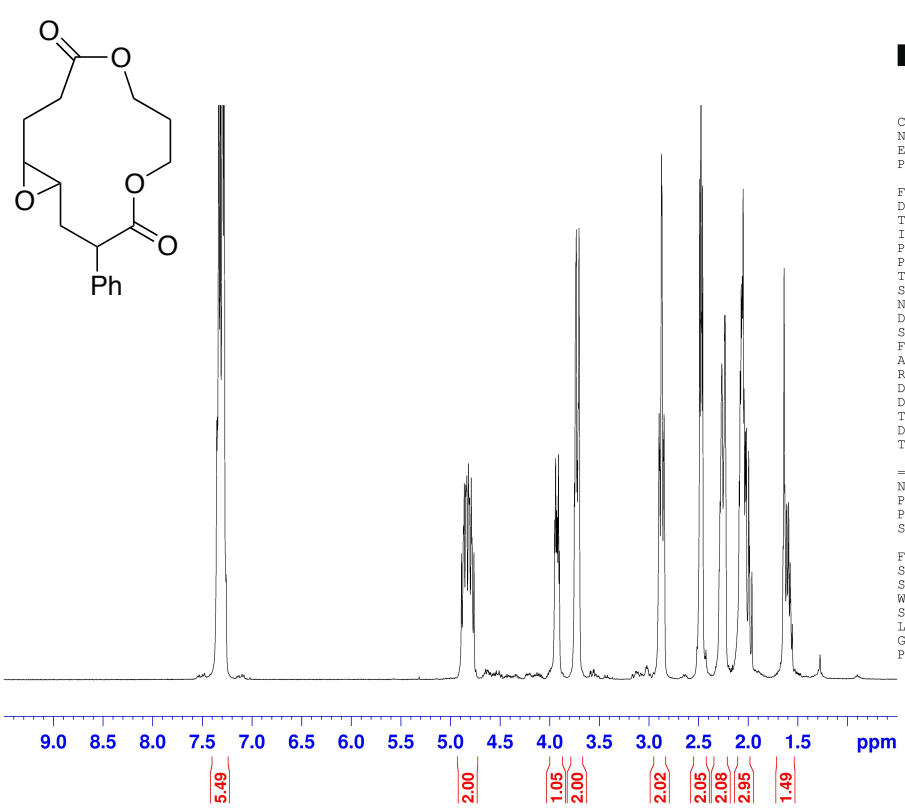
```
Current Data Parameters
NAME      am-II-63-col2-f5
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140729
Time                 23.33
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  43698
SOLVENT             CDCl3
NS                     32
DS                      4
SWH              24038.461 Hz
FIDRES           0.550104 Hz
AQ               0.9089184 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 300.0 K
D1             1.50000000 sec
d11            0.03000000 sec
DELTA          1.39999998 sec
TD0                     1
SFO1          100.6263500 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          50.00299835 W
SFO2          400.1456006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.33333001 W
PLW13          0.27000001 W

F2 - Processing parameters
SI                  131072
SF            100.6162684 MHz
WDW                    EM
SSB       0
LB                   2.50 Hz
GB        0
PC                   1.40
```



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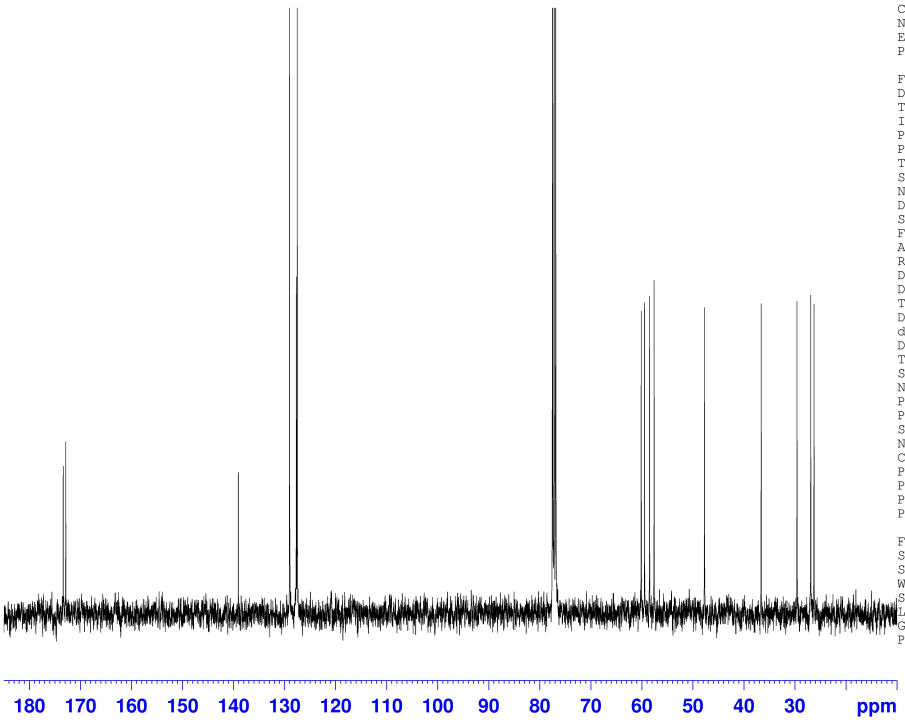
```
Current Data Parameters
NAME      am-II-67-f3-f4
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140729
Time              23.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               48076
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES        0.166670 Hz
AQ            2.9999423 sec
RG                  64
DW               62.400 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               15.25 usec
PLW1        12.00000000 W
SFO1        400.1464009 MHz

F2 - Processing parameters
SI              131072
SF          400.1440000 MHz
WDW                 EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```



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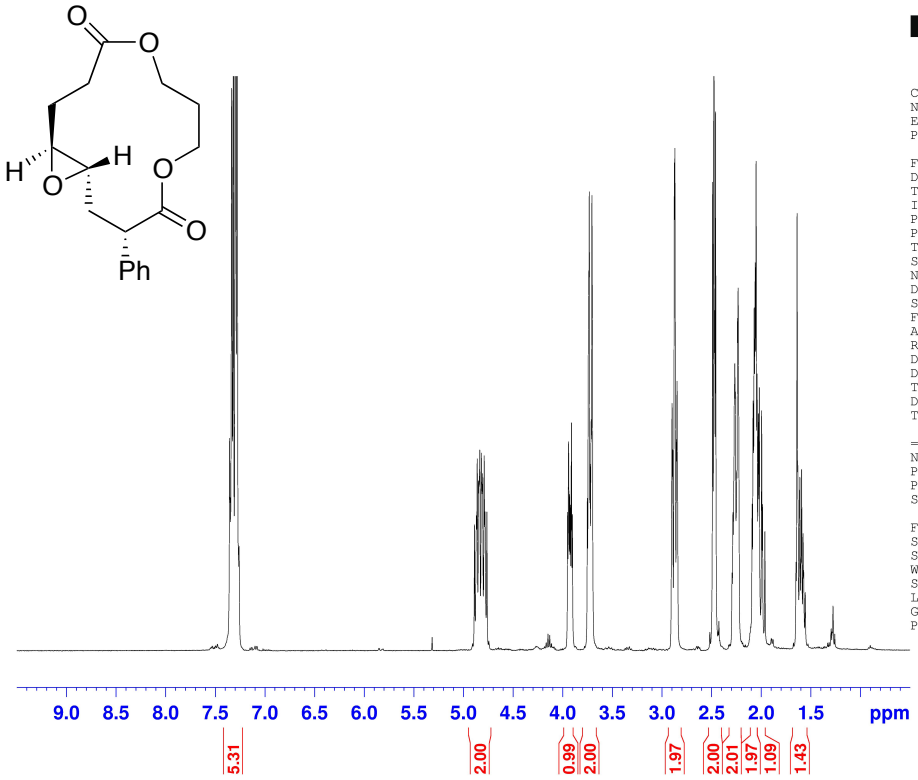
```
Current Data Parameters
NAME      am-II-67-f3-f4
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140729
Time              23.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               43698
SOLVENT          CDCl3
NS                 108
DS                   4
SWH          24038.461 Hz
FIDRES        0.550104 Hz
AQ            0.9089184 sec
RG                 203
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            1.50000000 sec
d11           0.03000000 sec
DELTA         1.39999998 sec
TD0                  1
SFO1        100.6263500 MHz
NUC1                13C
P1               10.00 usec
PLW1        50.00299835 W
SFO2        400.1456006 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.33333001 W
PLW13        0.27000001 W

F2 - Processing parameters
SI              131072
SF          100.6162702 MHz
WDW                 EM
SSB       0
LB                2.50 Hz
GB        0
PC                1.40
```

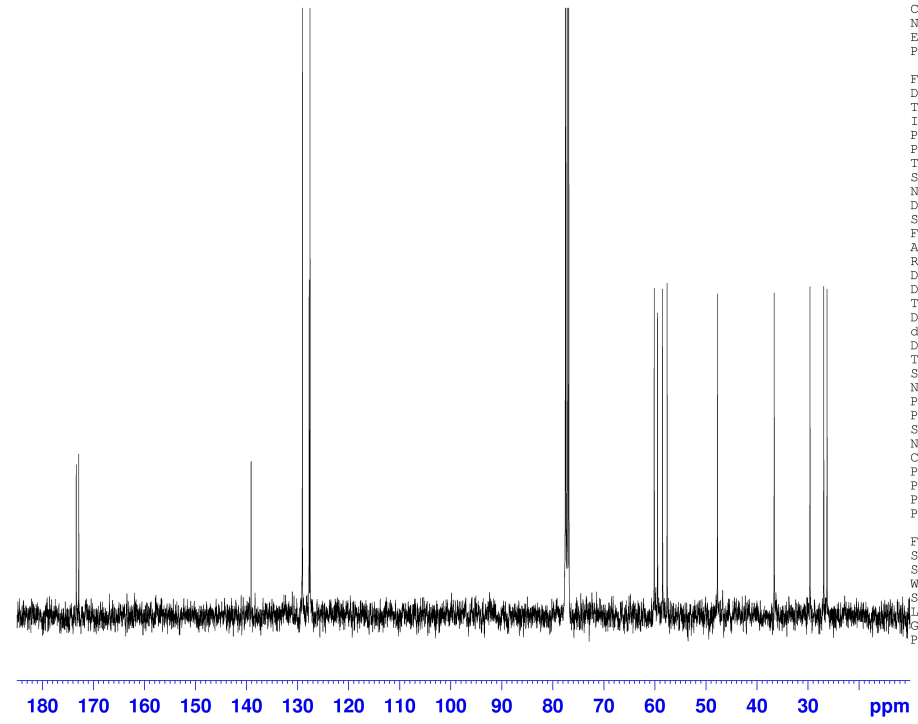



```
Current Data Parameters
NAME      am-II-65-col2-f6-f8
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140729
Time                 23.48
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   48076
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES               0.166670 Hz
AQ                2.9999423 sec
RG                    71.8
DW                   62.400 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.25 usec
PLW1           12.00000000 W
SFO1           400.1464009 MHz

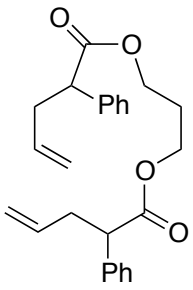
F2 - Processing parameters
SI                    131072
SF             400.1440000 MHz
WDW                     EM
SSB          0
LB                    0.50 Hz
GB           0
PC                    1.00
```




```
Current Data Parameters
NAME      am-II-65-col2-f6-f8
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20140729
Time                 23.52
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   43698
SOLVENT              CDCl3
NS                     115
DS                       4
SWH              24038.461 Hz
FIDRES               0.550104 Hz
AQ                0.9089184 sec
RG                     203
DW                   20.800 usec
DE                    6.50 usec
TE                   300.1 K
D1                1.50000000 sec
d11               0.03000000 sec
DELTA             1.39999998 sec
TD0                      1
SFO1           100.6263500 MHz
NUC1                    13C
P1                   10.00 usec
PLW1           50.00299835 W
SFO2           400.1456006 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                90.00 usec
PLW2           12.00000000 W
PLW12           0.33333001 W
PLW13           0.27000001 W

F2 - Processing parameters
SI                    131072
SF             100.6162701 MHz
WDW                     EM
SSB          0
LB                    2.50 Hz
GB           0
PC                    1.40
```

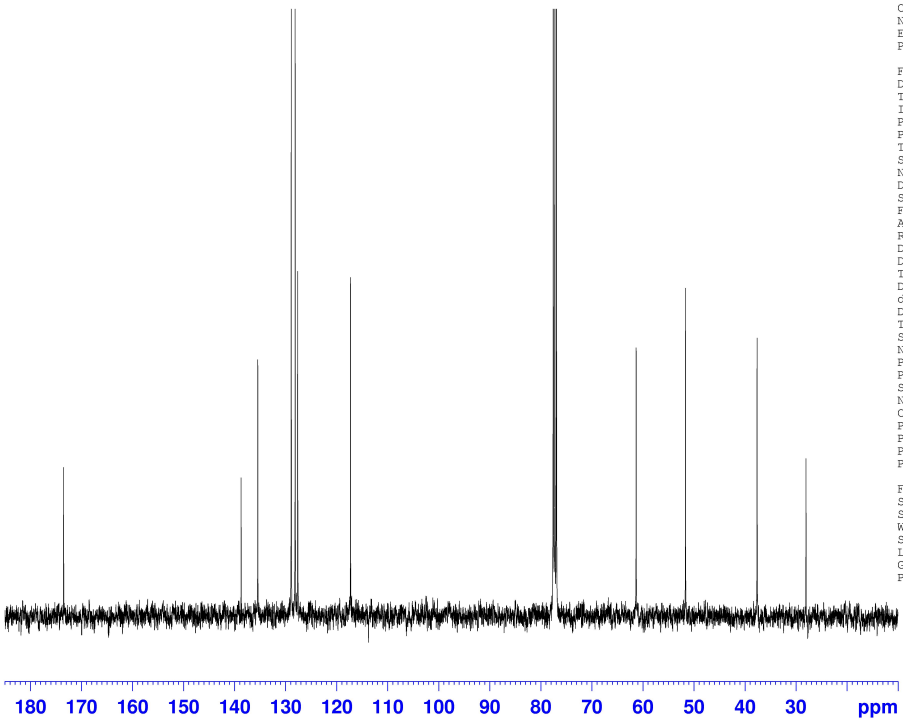



```
Current Data Parameters
NAME      am-R14-col2-bisacyl-f2
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20130513
Time                   15.29
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     48076
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.166670 Hz
AQ                  2.9999423 sec
RG                        64
DW                    62.400 usec
DE                     6.50 usec
TE                    300.0 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.20 usec
PLW1              12.00000000 W
SFO1              400.1464009 MHz

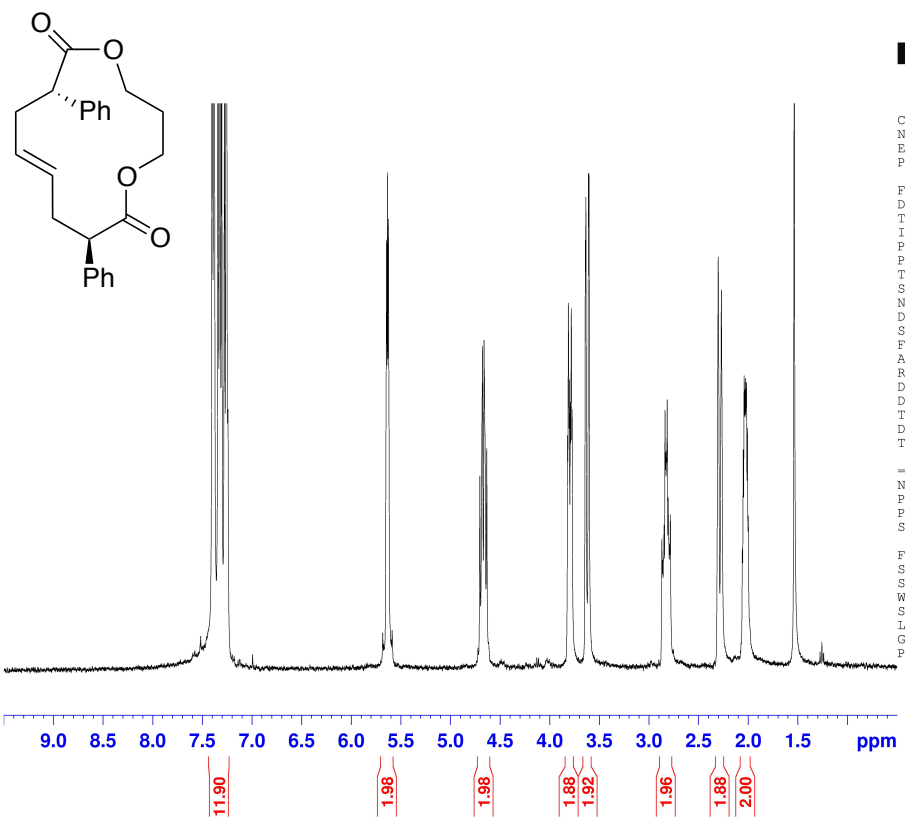
F2 - Processing parameters
SI                       131072
SF                400.1440097 MHz
WDW                         EM
SSB           0
LB                       0.50 Hz
GB            0
PC                       1.40
```




```
Current Data Parameters
NAME      am-R14-col2-bisacyl-f2
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_               20130513
Time                   15.40
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                     43698
SOLVENT                CDCl3
NS                       119
DS                         4
SWH                24038.461 Hz
FIDRES              0.550104 Hz
AQ                  0.9089184 sec
RG                       203
DW                    20.800 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.50000000 sec
d11                0.03000000 sec
DELTA              1.39999998 sec
TD0                        1
SFO1              100.6263500 MHz
NUC1                      13C
P1                      10.00 usec
PLW1              50.00299835 W
SFO2              400.1456006 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2              12.00000000 W
PLW12              0.33333001 W
PLW13              0.27000001 W

F2 - Processing parameters
SI                       131072
SF                100.6162656 MHz
WDW                         EM
SSB           0
LB                       2.50 Hz
GB            0
PC                       1.40
```

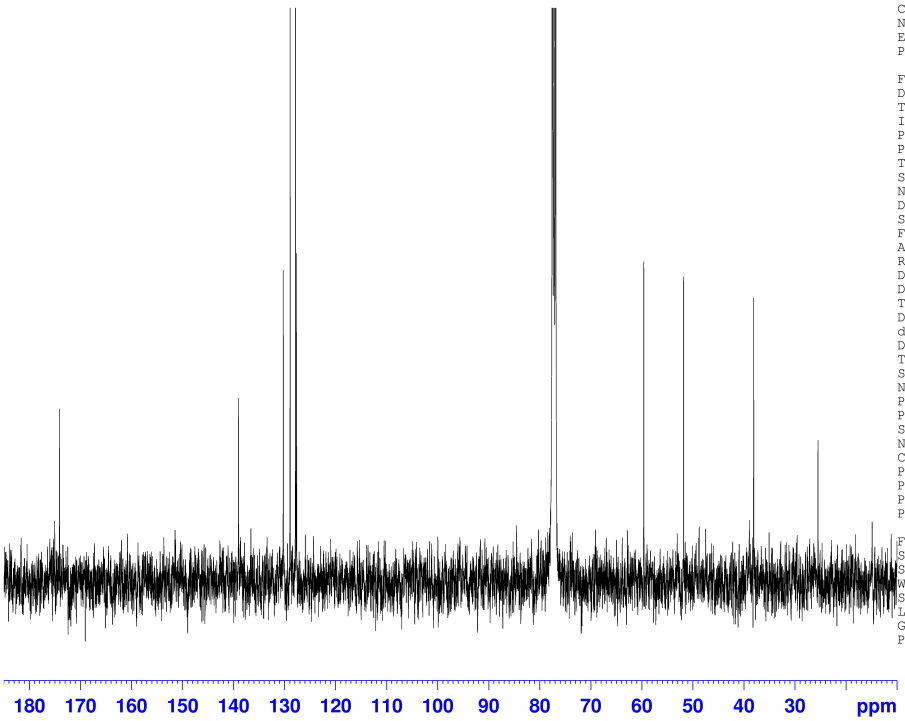



```
Current Data Parameters
NAME       am-37-col2-F1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20130917
Time              18.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                48076
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES        0.166670 Hz
AQ            2.9999423 sec
RG                  203
DW               62.400 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.20 usec
PLW1         12.00000000 W
SFO1         400.1464009 MHz

F2 - Processing parameters
SI                 131072
SF           400.1440094 MHz
WDW                  EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```




```
Current Data Parameters
NAME       am-37-col2-F1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20130917
Time              18.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                43698
SOLVENT           CDCl3
NS                  697
DS                    4
SWH           24038.461 Hz
FIDRES         0.550104 Hz
AQ            0.9089184 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               300.1 K
D1            1.50000000 sec
d11           0.03000000 sec
DELTA         1.39999998 sec
TD0                   1
SFO1         100.6263500 MHz
NUC1                 13C
P1                10.00 usec
PLW1         50.00299835 W
SFO2         400.1456006 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

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WDW                  EM
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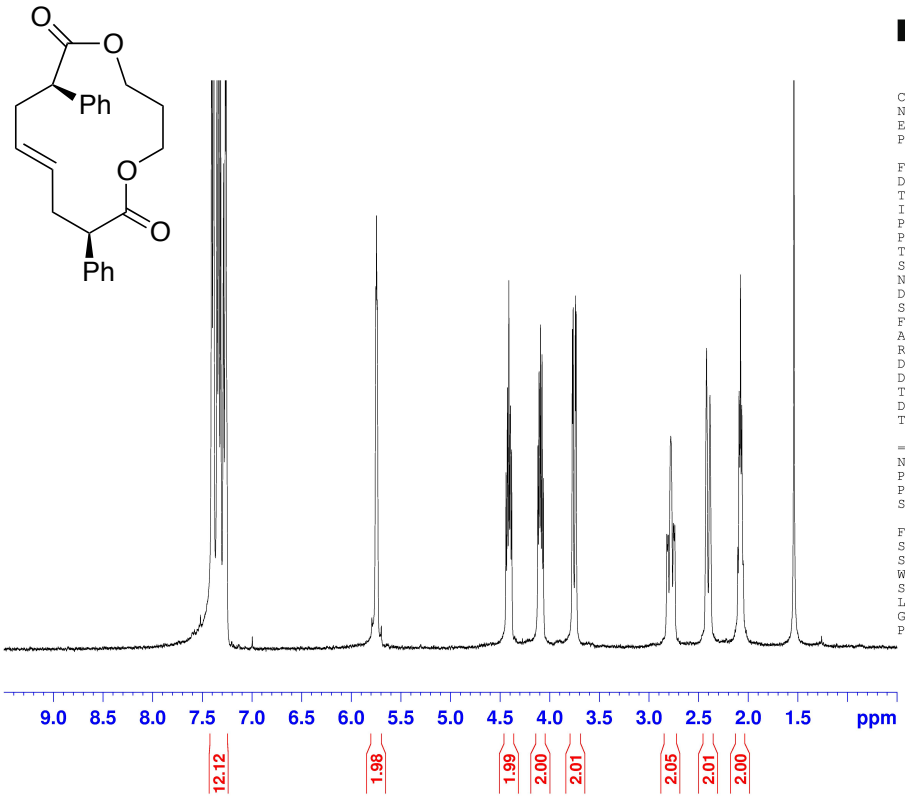


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RG                  203
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DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
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P1                15.20 usec
PLW1         12.00000000 W
SFO1         400.1464009 MHz

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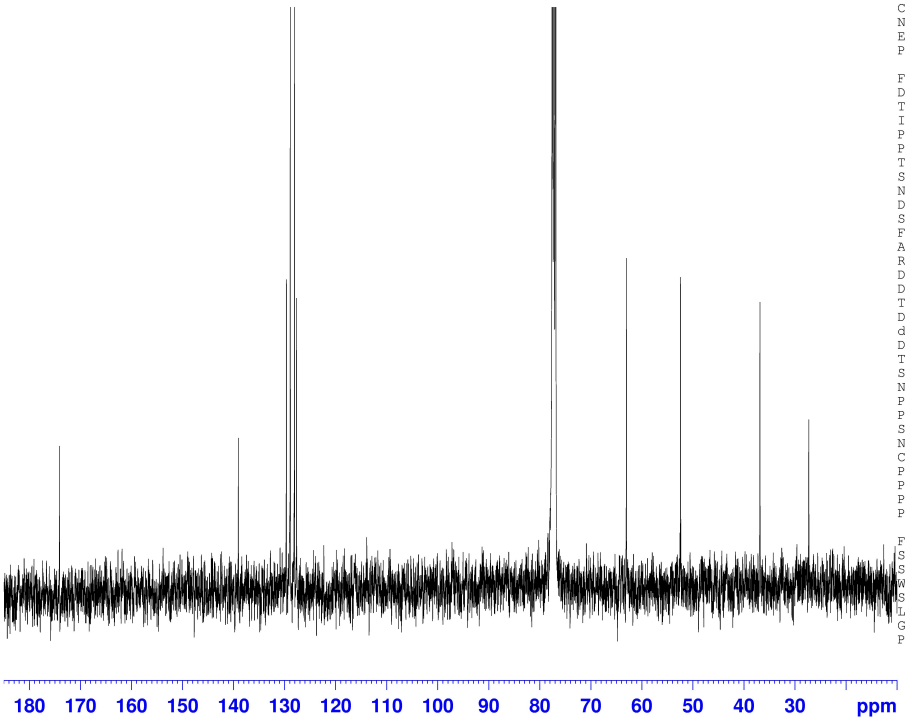


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PROCNO                1

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PULPROG         zgpg30
TD               43698
SOLVENT           CDCl3
NS                  833
DS                    4
SWH           24038.461 Hz
FIDRES         0.550104 Hz
AQ             0.9089184 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                300.1 K
D1             1.50000000 sec
d11            0.03000000 sec
DELTA          1.39999998 sec
TD0                   1
SFO1         100.6263500 MHz
NUC1                13C
P1                10.00 usec
PLW1         50.00299835 W
SFO2         400.1456006 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.33333001 W
PLW13         0.27000001 W

F2 - Processing parameters
SI                131072
SF           100.6162656 MHz
WDW                  EM
SSB       0
LB                2.50 Hz
GB        0
PC                1.40
```

X-ray Crystallography

Experimental and Refinement Details

Low-temperature diffraction data (ω-scans) were collected on a Rigaku R-AXIS RAPID diffractometer coupled to an R-AXIS RAPID imaging plate detector with Mo *K*α radiation (λ = 0.71073 Å) for the structure of **6**, and on a Rigaku MicroMax-007HF diffractometer coupled to a Saturn994+ CCD detector with Cu *K*α (λ = 1.54178 Å) for the structures of **4**, and **7**. All structures were solved by direct methods using SHELXT and refined against F^2 on all data by full-matrix least squares with SHELXL. (Sheldrick, G. M. Acta Cryst. 2008, A64, 112–122) All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms to which they are linked (1.5 times for methyl groups). All root mean square deviations were calculated by mapping the 13 atomic coordinates of the macrocycle contained in CCDC 686767 (mp09) onto the coordinates reported in this manuscript. Full details of the X-ray structure determination are in the CIF included as Supporting Information. CCDC numbers 1041906 (**4**), 1041908 (**6**), and 141907 (**7**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

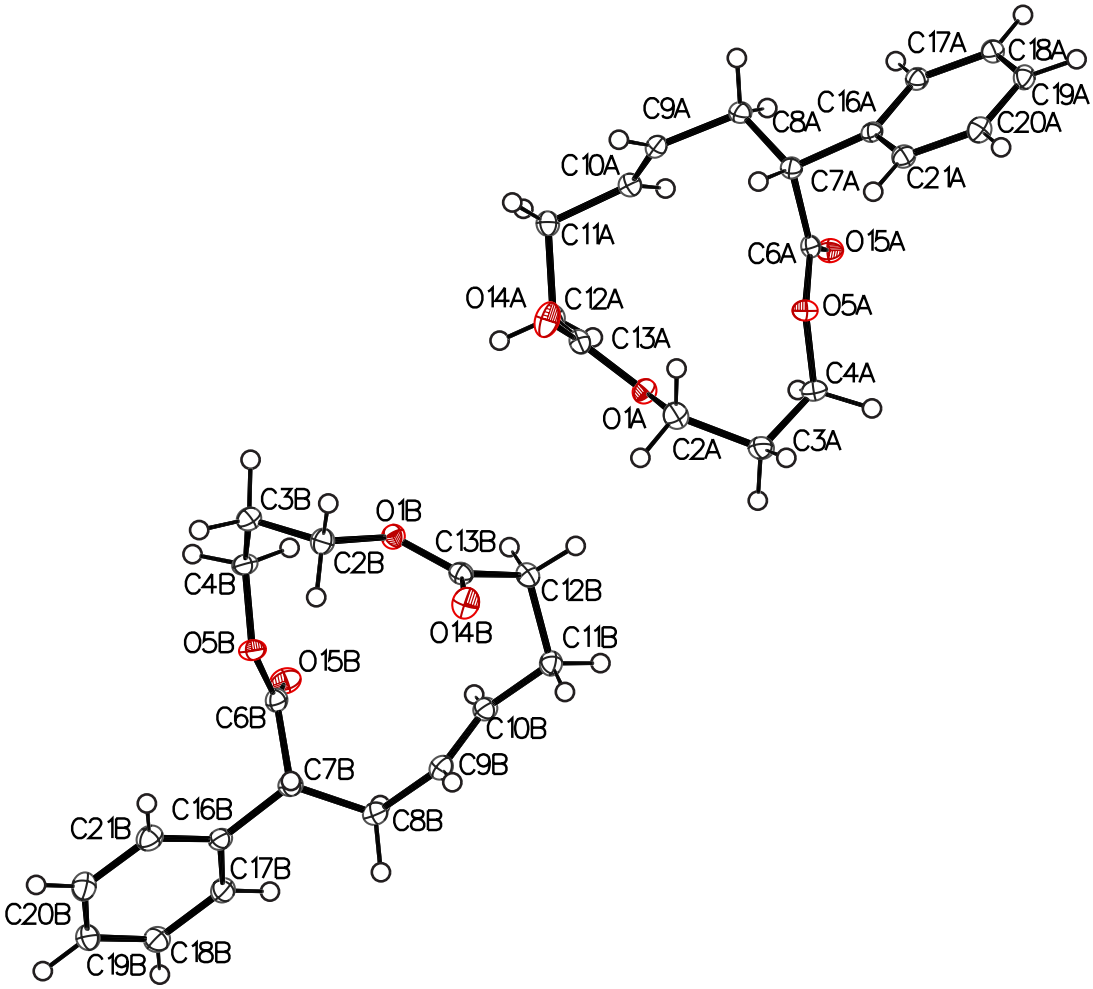

Figure 1. The full numbering scheme of compound **4.** All atoms shown are depicted with 50% thermal contours.

Table 1. Crystal data and structure refinement for compound 4.

Identification code	compound 4	
Empirical formula	$C_{17}H_{20}O_4$	
Formula weight	288.33	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 5.51640(10) Å	α = 94.989(7)°
	b = 11.8803(3) Å	β = 90.739(6)°
	c = 23.3669(16) Å	γ = 98.520(7)°
Volume	1508.23(12) $Å^3$	
Z	4	
Density (calculated)	1.270 Mg/m^3	
Absorption coefficient	0.731 mm^{-1}	
F(000)	616	
Crystal color	Colorless	
Crystal size	0.200 x 0.200 x 0.050 mm^3	
Θ range for data collection	1.899 to 68.240°	
Index ranges	$-6 \leq h \leq 6, -14 \leq k \leq 14, -28 \leq l \leq 28$	
Reflections collected	54047	
Independent reflections	5407 [R(int) = 0.0459]	
Completeness to θ = 67.687°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.964 and 0.802	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5407 / 0 / 379	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2σ(I) = 4987 data]	R1 = 0.0391, wR2 = 0.0948	
R indices (all data)	R1 = 0.0421, wR2 = 0.0973	
Largest diff. peak and hole	0.446 and -0.216 $e.Å^{-3}$	

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

	x	y	z	U(eq)
O(1A)	2890(2)	5630(1)	2852(1)	26(1)
C(2A)	5093(3)	6222(1)	2611(1)	30(1)
C(3A)	4295(3)	7045(1)	2212(1)	31(1)
C(4A)	2579(3)	7802(1)	2492(1)	29(1)
O(5A)	3674(2)	8265(1)	3047(1)	26(1)
C(6A)	2149(3)	8457(1)	3475(1)	22(1)
C(7A)	3569(3)	8830(1)	4040(1)	22(1)
C(8A)	2168(3)	8258(1)	4528(1)	25(1)
C(9A)	2282(3)	6996(1)	4480(1)	26(1)
C(10A)	476(3)	6191(1)	4286(1)	26(1)
C(11A)	690(3)	4945(1)	4201(1)	27(1)
C(12A)	877(3)	4547(1)	3561(1)	26(1)
C(13A)	3239(3)	5098(1)	3325(1)	25(1)
O(14A)	5241(2)	5075(1)	3534(1)	37(1)
O(15A)	-48(2)	8372(1)	3414(1)	28(1)
C(16A)	3984(3)	10129(1)	4108(1)	21(1)
C(17A)	2311(3)	10759(1)	4377(1)	24(1)
C(18A)	2683(3)	11949(1)	4398(1)	25(1)
C(19A)	4718(3)	12516(1)	4145(1)	26(1)
C(20A)	6390(3)	11892(1)	3880(1)	27(1)
C(21A)	6037(3)	10709(1)	3865(1)	24(1)
O(1B)	10678(2)	2699(1)	2376(1)	27(1)
C(2B)	12600(3)	2024(1)	2488(1)	29(1)
C(3B)	11459(3)	1023(1)	2803(1)	29(1)
C(4B)	9120(3)	389(1)	2513(1)	28(1)
O(5B)	9721(2)	118(1)	1918(1)	28(1)
C(6B)	7874(3)	-102(1)	1535(1)	25(1)
C(7B)	8842(3)	-228(1)	929(1)	28(1)
C(8B)	7598(3)	541(1)	561(1)	30(1)
C(9B)	8547(3)	1786(1)	723(1)	30(1)
C(10B)	7354(3)	2499(1)	1030(1)	27(1)

C(11B)	8287(3)	3737(1)	1192(1)	26(1)
C(12B)	8983(3)	4002(1)	1834(1)	25(1)
C(13B)	11170(3)	3455(1)	1979(1)	25(1)
O(14B)	13138(2)	3642(1)	1761(1)	34(1)
O(15B)	5737(2)	-189(1)	1657(1)	35(1)
C(16B)	8471(3)	-1488(1)	715(1)	26(1)
C(17B)	6467(3)	-2013(1)	375(1)	29(1)
C(18B)	6247(3)	-3163(1)	186(1)	32(1)
C(19B)	8010(3)	-3806(1)	340(1)	34(1)
C(20B)	9987(3)	-3298(1)	683(1)	35(1)
C(21B)	10230(3)	-2148(1)	868(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for compound 4.

O(1A)-C(13A)	1.3441(18)
O(1A)-C(2A)	1.4570(17)
C(2A)-C(3A)	1.515(2)
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(3A)-C(4A)	1.516(2)
C(3A)-H(3AA)	0.9900
C(3A)-H(3AB)	0.9900
C(4A)-O(5A)	1.4526(17)
C(4A)-H(4AA)	0.9900
C(4A)-H(4AB)	0.9900
O(5A)-C(6A)	1.3399(17)
C(6A)-O(15A)	1.2066(17)
C(6A)-C(7A)	1.5242(19)
C(7A)-C(16A)	1.5203(19)
C(7A)-C(8A)	1.5368(19)
C(7A)-H(7A)	1.0000
C(8A)-C(9A)	1.5042(19)
C(8A)-H(8AA)	0.9900
C(8A)-H(8AB)	0.9900
C(9A)-C(10A)	1.321(2)
C(9A)-H(9A)	0.9500
C(10A)-C(11A)	1.499(2)
C(10A)-H(10A)	0.9500
C(11A)-C(12A)	1.538(2)
C(11A)-H(11A)	0.9900
C(11A)-H(11B)	0.9900
C(12A)-C(13A)	1.503(2)
C(12A)-H(12A)	0.9900
C(12A)-H(12B)	0.9900
C(13A)-O(14A)	1.2073(18)
C(16A)-C(21A)	1.390(2)
C(16A)-C(17A)	1.395(2)
C(17A)-C(18A)	1.394(2)

C(17A)-H(17A)	0.9500
C(18A)-C(19A)	1.388(2)
C(18A)-H(18A)	0.9500
C(19A)-C(20A)	1.385(2)
C(19A)-H(19A)	0.9500
C(20A)-C(21A)	1.387(2)
C(20A)-H(20A)	0.9500
C(21A)-H(21A)	0.9500
O(1B)-C(13B)	1.3477(18)
O(1B)-C(2B)	1.4550(17)
C(2B)-C(3B)	1.515(2)
C(2B)-H(2BA)	0.9900
C(2B)-H(2BB)	0.9900
C(3B)-C(4B)	1.514(2)
C(3B)-H(3BA)	0.9900
C(3B)-H(3BB)	0.9900
C(4B)-O(5B)	1.4524(17)
C(4B)-H(4BA)	0.9900
C(4B)-H(4BB)	0.9900
O(5B)-C(6B)	1.3279(18)
C(6B)-O(15B)	1.2077(18)
C(6B)-C(7B)	1.523(2)
C(7B)-C(16B)	1.519(2)
C(7B)-C(8B)	1.534(2)
C(7B)-H(7B)	1.0000
C(8B)-C(9B)	1.508(2)
C(8B)-H(8BA)	0.9900
C(8B)-H(8BB)	0.9900
C(9B)-C(10B)	1.318(2)
C(9B)-H(9B)	0.9500
C(10B)-C(11B)	1.498(2)
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.538(2)
C(11B)-H(11C)	0.9900
C(11B)-H(11D)	0.9900
C(12B)-C(13B)	1.5007(19)

C(12B)-H(12C)	0.9900
C(12B)-H(12D)	0.9900
C(13B)-O(14B)	1.2047(18)
C(16B)-C(17B)	1.390(2)
C(16B)-C(21B)	1.397(2)
C(17B)-C(18B)	1.386(2)
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.385(2)
C(18B)-H(18B)	0.9500
C(19B)-C(20B)	1.376(2)
C(19B)-H(19B)	0.9500
C(20B)-C(21B)	1.382(2)
C(20B)-H(20B)	0.9500
C(21B)-H(21B)	0.9500

C(13A)-O(1A)-C(2A)	115.83(11)
O(1A)-C(2A)-C(3A)	107.49(12)
O(1A)-C(2A)-H(2AA)	110.2
C(3A)-C(2A)-H(2AA)	110.2
O(1A)-C(2A)-H(2AB)	110.2
C(3A)-C(2A)-H(2AB)	110.2
H(2AA)-C(2A)-H(2AB)	108.5
C(2A)-C(3A)-C(4A)	112.86(12)
C(2A)-C(3A)-H(3AA)	109.0
C(4A)-C(3A)-H(3AA)	109.0
C(2A)-C(3A)-H(3AB)	109.0
C(4A)-C(3A)-H(3AB)	109.0
H(3AA)-C(3A)-H(3AB)	107.8
O(5A)-C(4A)-C(3A)	107.07(12)
O(5A)-C(4A)-H(4AA)	110.3
C(3A)-C(4A)-H(4AA)	110.3
O(5A)-C(4A)-H(4AB)	110.3
C(3A)-C(4A)-H(4AB)	110.3
H(4AA)-C(4A)-H(4AB)	108.6
C(6A)-O(5A)-C(4A)	117.36(11)
O(15A)-C(6A)-O(5A)	124.24(13)

O(15A)-C(6A)-C(7A)	124.81(13)
O(5A)-C(6A)-C(7A)	110.93(12)
C(16A)-C(7A)-C(6A)	107.31(11)
C(16A)-C(7A)-C(8A)	115.09(11)
C(6A)-C(7A)-C(8A)	109.07(11)
C(16A)-C(7A)-H(7A)	108.4
C(6A)-C(7A)-H(7A)	108.4
C(8A)-C(7A)-H(7A)	108.4
C(9A)-C(8A)-C(7A)	110.71(12)
C(9A)-C(8A)-H(8AA)	109.5
C(7A)-C(8A)-H(8AA)	109.5
C(9A)-C(8A)-H(8AB)	109.5
C(7A)-C(8A)-H(8AB)	109.5
H(8AA)-C(8A)-H(8AB)	108.1
C(10A)-C(9A)-C(8A)	124.99(14)
C(10A)-C(9A)-H(9A)	117.5
C(8A)-C(9A)-H(9A)	117.5
C(9A)-C(10A)-C(11A)	124.11(14)
C(9A)-C(10A)-H(10A)	117.9
C(11A)-C(10A)-H(10A)	117.9
C(10A)-C(11A)-C(12A)	111.43(12)
C(10A)-C(11A)-H(11A)	109.3
C(12A)-C(11A)-H(11A)	109.3
C(10A)-C(11A)-H(11B)	109.3
C(12A)-C(11A)-H(11B)	109.3
H(11A)-C(11A)-H(11B)	108.0
C(13A)-C(12A)-C(11A)	110.75(12)
C(13A)-C(12A)-H(12A)	109.5
C(11A)-C(12A)-H(12A)	109.5
C(13A)-C(12A)-H(12B)	109.5
C(11A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	108.1
O(14A)-C(13A)-O(1A)	123.11(14)
O(14A)-C(13A)-C(12A)	124.20(13)
O(1A)-C(13A)-C(12A)	112.69(12)
C(21A)-C(16A)-C(17A)	118.81(13)

C(21A)-C(16A)-C(7A)	118.73(12)
C(17A)-C(16A)-C(7A)	122.36(12)
C(18A)-C(17A)-C(16A)	120.55(13)
C(18A)-C(17A)-H(17A)	119.7
C(16A)-C(17A)-H(17A)	119.7
C(19A)-C(18A)-C(17A)	120.04(13)
C(19A)-C(18A)-H(18A)	120.0
C(17A)-C(18A)-H(18A)	120.0
C(20A)-C(19A)-C(18A)	119.51(13)
C(20A)-C(19A)-H(19A)	120.2
C(18A)-C(19A)-H(19A)	120.2
C(19A)-C(20A)-C(21A)	120.54(13)
C(19A)-C(20A)-H(20A)	119.7
C(21A)-C(20A)-H(20A)	119.7
C(20A)-C(21A)-C(16A)	120.55(13)
C(20A)-C(21A)-H(21A)	119.7
C(16A)-C(21A)-H(21A)	119.7
C(13B)-O(1B)-C(2B)	115.93(11)
O(1B)-C(2B)-C(3B)	107.47(12)
O(1B)-C(2B)-H(2BA)	110.2
C(3B)-C(2B)-H(2BA)	110.2
O(1B)-C(2B)-H(2BB)	110.2
C(3B)-C(2B)-H(2BB)	110.2
H(2BA)-C(2B)-H(2BB)	108.5
C(4B)-C(3B)-C(2B)	113.01(12)
C(4B)-C(3B)-H(3BA)	109.0
C(2B)-C(3B)-H(3BA)	109.0
C(4B)-C(3B)-H(3BB)	109.0
C(2B)-C(3B)-H(3BB)	109.0
H(3BA)-C(3B)-H(3BB)	107.8
O(5B)-C(4B)-C(3B)	105.89(12)
O(5B)-C(4B)-H(4BA)	110.6
C(3B)-C(4B)-H(4BA)	110.6
O(5B)-C(4B)-H(4BB)	110.6
C(3B)-C(4B)-H(4BB)	110.6
H(4BA)-C(4B)-H(4BB)	108.7

C(6B)-O(5B)-C(4B)	117.25(11)
O(15B)-C(6B)-O(5B)	124.16(13)
O(15B)-C(6B)-C(7B)	125.45(13)
O(5B)-C(6B)-C(7B)	110.38(12)
C(16B)-C(7B)-C(6B)	108.82(12)
C(16B)-C(7B)-C(8B)	115.43(12)
C(6B)-C(7B)-C(8B)	108.01(12)
C(16B)-C(7B)-H(7B)	108.1
C(6B)-C(7B)-H(7B)	108.1
C(8B)-C(7B)-H(7B)	108.1
C(9B)-C(8B)-C(7B)	111.16(12)
C(9B)-C(8B)-H(8BA)	109.4
C(7B)-C(8B)-H(8BA)	109.4
C(9B)-C(8B)-H(8BB)	109.4
C(7B)-C(8B)-H(8BB)	109.4
H(8BA)-C(8B)-H(8BB)	108.0
C(10B)-C(9B)-C(8B)	124.89(15)
C(10B)-C(9B)-H(9B)	117.6
C(8B)-C(9B)-H(9B)	117.6
C(9B)-C(10B)-C(11B)	125.12(14)
C(9B)-C(10B)-H(10B)	117.4
C(11B)-C(10B)-H(10B)	117.4
C(10B)-C(11B)-C(12B)	113.18(12)
C(10B)-C(11B)-H(11C)	108.9
C(12B)-C(11B)-H(11C)	108.9
C(10B)-C(11B)-H(11D)	108.9
C(12B)-C(11B)-H(11D)	108.9
H(11C)-C(11B)-H(11D)	107.8
C(13B)-C(12B)-C(11B)	110.24(12)
C(13B)-C(12B)-H(12C)	109.6
C(11B)-C(12B)-H(12C)	109.6
C(13B)-C(12B)-H(12D)	109.6
C(11B)-C(12B)-H(12D)	109.6
H(12C)-C(12B)-H(12D)	108.1
O(14B)-C(13B)-O(1B)	123.09(13)
O(14B)-C(13B)-C(12B)	124.51(13)

O(1B)-C(13B)-C(12B)	112.38(12)
C(17B)-C(16B)-C(21B)	118.49(14)
C(17B)-C(16B)-C(7B)	123.13(13)
C(21B)-C(16B)-C(7B)	118.38(13)
C(18B)-C(17B)-C(16B)	120.47(14)
C(18B)-C(17B)-H(17B)	119.8
C(16B)-C(17B)-H(17B)	119.8
C(19B)-C(18B)-C(17B)	120.33(15)
C(19B)-C(18B)-H(18B)	119.8
C(17B)-C(18B)-H(18B)	119.8
C(20B)-C(19B)-C(18B)	119.70(15)
C(20B)-C(19B)-H(19B)	120.1
C(18B)-C(19B)-H(19B)	120.1
C(19B)-C(20B)-C(21B)	120.27(15)
C(19B)-C(20B)-H(20B)	119.9
C(21B)-C(20B)-H(20B)	119.9
C(20B)-C(21B)-C(16B)	120.72(14)
C(20B)-C(21B)-H(21B)	119.6
C(16B)-C(21B)-H(21B)	119.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 4. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1A)	25(1)	27(1)	27(1)	5(1)	2(1)	1(1)
C(2A)	27(1)	27(1)	35(1)	5(1)	10(1)	2(1)
C(3A)	40(1)	28(1)	24(1)	1(1)	6(1)	4(1)
C(4A)	37(1)	29(1)	19(1)	-1(1)	-3(1)	5(1)
O(5A)	27(1)	28(1)	20(1)	-1(1)	1(1)	3(1)
C(6A)	26(1)	16(1)	23(1)	3(1)	0(1)	2(1)
C(7A)	24(1)	21(1)	21(1)	2(1)	-1(1)	2(1)
C(8A)	31(1)	22(1)	21(1)	1(1)	0(1)	1(1)
C(9A)	33(1)	24(1)	21(1)	5(1)	-1(1)	4(1)
C(10A)	30(1)	24(1)	25(1)	2(1)	1(1)	4(1)
C(11A)	29(1)	22(1)	29(1)	4(1)	2(1)	1(1)
C(12A)	24(1)	22(1)	30(1)	1(1)	1(1)	0(1)
C(13A)	27(1)	20(1)	28(1)	2(1)	1(1)	5(1)
O(14A)	23(1)	42(1)	50(1)	19(1)	-2(1)	4(1)
O(15A)	26(1)	32(1)	26(1)	1(1)	-1(1)	4(1)
C(16A)	24(1)	21(1)	17(1)	1(1)	-4(1)	2(1)
C(17A)	25(1)	23(1)	22(1)	3(1)	1(1)	1(1)
C(18A)	28(1)	24(1)	25(1)	1(1)	-1(1)	6(1)
C(19A)	29(1)	20(1)	27(1)	4(1)	-6(1)	0(1)
C(20A)	23(1)	27(1)	29(1)	5(1)	0(1)	-1(1)
C(21A)	24(1)	26(1)	24(1)	2(1)	0(1)	3(1)
O(1B)	26(1)	29(1)	27(1)	4(1)	2(1)	8(1)
C(2B)	26(1)	31(1)	30(1)	4(1)	-3(1)	9(1)
C(3B)	33(1)	31(1)	24(1)	2(1)	-4(1)	7(1)
C(4B)	32(1)	32(1)	19(1)	1(1)	1(1)	6(1)
O(5B)	30(1)	36(1)	19(1)	-1(1)	-1(1)	7(1)
C(6B)	29(1)	21(1)	24(1)	4(1)	-1(1)	1(1)
C(7B)	32(1)	27(1)	23(1)	2(1)	0(1)	2(1)
C(8B)	37(1)	30(1)	23(1)	2(1)	-1(1)	5(1)
C(9B)	36(1)	28(1)	25(1)	6(1)	3(1)	3(1)
C(10B)	30(1)	27(1)	24(1)	3(1)	1(1)	2(1)

C(11B)	27(1)	25(1)	27(1)	4(1)	-1(1)	5(1)
C(12B)	24(1)	24(1)	28(1)	0(1)	-1(1)	4(1)
C(13B)	24(1)	25(1)	24(1)	-1(1)	-1(1)	3(1)
O(14B)	23(1)	40(1)	42(1)	11(1)	5(1)	6(1)
O(15B)	32(1)	43(1)	29(1)	2(1)	-2(1)	0(1)
C(16B)	33(1)	25(1)	20(1)	3(1)	1(1)	0(1)
C(17B)	31(1)	28(1)	27(1)	4(1)	-2(1)	3(1)
C(18B)	36(1)	28(1)	30(1)	2(1)	-4(1)	-4(1)
C(19B)	46(1)	23(1)	31(1)	3(1)	3(1)	2(1)
C(20B)	39(1)	33(1)	35(1)	8(1)	0(1)	10(1)
C(21B)	32(1)	33(1)	28(1)	4(1)	-4(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for compound 4.

	x	y	z	U(eq)
H(2AA)	5992	5666	2396	35
H(2AB)	6190	6644	2922	35
H(3AA)	3462	6603	1867	37
H(3AB)	5765	7532	2084	37
H(4AA)	2377	8428	2250	34
H(4AB)	947	7351	2541	34
H(7A)	5202	8562	4012	27
H(8AA)	2891	8610	4903	30
H(8AB)	435	8383	4510	30
H(9A)	3767	6760	4599	31
H(10A)	-1054	6416	4194	32
H(11A)	-763	4496	4360	32
H(11B)	2163	4802	4413	32
H(12A)	794	3706	3514	31
H(12B)	-524	4748	3342	31
H(17A)	906	10375	4547	28
H(18A)	1542	12372	4585	31
H(19A)	4964	13325	4153	31
H(20A)	7789	12277	3708	32
H(21A)	7208	10291	3687	29
H(2BA)	13940	2494	2726	35
H(2BB)	13289	1747	2122	35
H(3BA)	12657	485	2829	35
H(3BB)	11099	1306	3199	35
H(4BA)	8560	-318	2698	33
H(4BB)	7806	874	2536	33
H(7B)	10643	56	948	33
H(8BA)	7909	348	150	36
H(8BB)	5804	400	614	36
H(9B)	10123	2078	595	35

H(10B)	5779	2205	1159	33
H(11C)	7009	4196	1093	32
H(11D)	9744	3970	963	32
H(12C)	9365	4839	1927	30
H(12D)	7582	3710	2068	30
H(17B)	5239	-1580	271	34
H(18B)	4880	-3512	-50	38
H(19B)	7855	-4594	210	40
H(20B)	11189	-3739	793	42
H(21B)	11609	-1804	1102	38

Table 6. Torsion angles [°] for compound 4.

C(13A)-O(1A)-C(2A)-C(3A)	-162.90(12)
O(1A)-C(2A)-C(3A)-C(4A)	51.04(17)
C(2A)-C(3A)-C(4A)-O(5A)	48.17(17)
C(3A)-C(4A)-O(5A)-C(6A)	-147.38(12)
C(4A)-O(5A)-C(6A)-O(15A)	-7.25(19)
C(4A)-O(5A)-C(6A)-C(7A)	174.49(11)
O(15A)-C(6A)-C(7A)-C(16A)	-83.58(16)
O(5A)-C(6A)-C(7A)-C(16A)	94.67(13)
O(15A)-C(6A)-C(7A)-C(8A)	41.71(18)
O(5A)-C(6A)-C(7A)-C(8A)	-140.04(12)
C(16A)-C(7A)-C(8A)-C(9A)	-169.00(12)
C(6A)-C(7A)-C(8A)-C(9A)	70.38(15)
C(7A)-C(8A)-C(9A)-C(10A)	-103.31(17)
C(8A)-C(9A)-C(10A)-C(11A)	175.26(13)
C(9A)-C(10A)-C(11A)-C(12A)	-104.66(17)
C(10A)-C(11A)-C(12A)-C(13A)	66.58(16)
C(2A)-O(1A)-C(13A)-O(14A)	-1.9(2)
C(2A)-O(1A)-C(13A)-C(12A)	177.78(12)
C(11A)-C(12A)-C(13A)-O(14A)	53.22(19)
C(11A)-C(12A)-C(13A)-O(1A)	-126.50(13)
C(6A)-C(7A)-C(16A)-C(21A)	-87.24(15)
C(8A)-C(7A)-C(16A)-C(21A)	151.18(13)
C(6A)-C(7A)-C(16A)-C(17A)	89.13(15)
C(8A)-C(7A)-C(16A)-C(17A)	-32.46(18)
C(21A)-C(16A)-C(17A)-C(18A)	0.5(2)
C(7A)-C(16A)-C(17A)-C(18A)	-175.87(12)
C(16A)-C(17A)-C(18A)-C(19A)	0.6(2)
C(17A)-C(18A)-C(19A)-C(20A)	-1.0(2)
C(18A)-C(19A)-C(20A)-C(21A)	0.3(2)
C(19A)-C(20A)-C(21A)-C(16A)	0.9(2)
C(17A)-C(16A)-C(21A)-C(20A)	-1.2(2)
C(7A)-C(16A)-C(21A)-C(20A)	175.28(12)
C(13B)-O(1B)-C(2B)-C(3B)	-164.10(12)
O(1B)-C(2B)-C(3B)-C(4B)	49.65(16)

C(2B)-C(3B)-C(4B)-O(5B)	52.24(16)
C(3B)-C(4B)-O(5B)-C(6B)	-158.93(12)
C(4B)-O(5B)-C(6B)-O(15B)	-6.8(2)
C(4B)-O(5B)-C(6B)-C(7B)	173.30(12)
O(15B)-C(6B)-C(7B)-C(16B)	-75.32(18)
O(5B)-C(6B)-C(7B)-C(16B)	104.54(14)
O(15B)-C(6B)-C(7B)-C(8B)	50.67(19)
O(5B)-C(6B)-C(7B)-C(8B)	-129.46(13)
C(16B)-C(7B)-C(8B)-C(9B)	-166.53(13)
C(6B)-C(7B)-C(8B)-C(9B)	71.46(16)
C(7B)-C(8B)-C(9B)-C(10B)	-103.89(18)
C(8B)-C(9B)-C(10B)-C(11B)	-179.92(14)
C(9B)-C(10B)-C(11B)-C(12B)	-108.87(17)
C(10B)-C(11B)-C(12B)-C(13B)	67.05(16)
C(2B)-O(1B)-C(13B)-O(14B)	-5.9(2)
C(2B)-O(1B)-C(13B)-C(12B)	172.54(12)
C(11B)-C(12B)-C(13B)-O(14B)	58.94(19)
C(11B)-C(12B)-C(13B)-O(1B)	-119.47(13)
C(6B)-C(7B)-C(16B)-C(17B)	96.17(16)
C(8B)-C(7B)-C(16B)-C(17B)	-25.4(2)
C(6B)-C(7B)-C(16B)-C(21B)	-83.85(16)
C(8B)-C(7B)-C(16B)-C(21B)	154.58(14)
C(21B)-C(16B)-C(17B)-C(18B)	-0.9(2)
C(7B)-C(16B)-C(17B)-C(18B)	179.09(14)
C(16B)-C(17B)-C(18B)-C(19B)	0.8(2)
C(17B)-C(18B)-C(19B)-C(20B)	0.1(2)
C(18B)-C(19B)-C(20B)-C(21B)	-0.7(2)
C(19B)-C(20B)-C(21B)-C(16B)	0.5(2)
C(17B)-C(16B)-C(21B)-C(20B)	0.3(2)
C(7B)-C(16B)-C(21B)-C(20B)	-179.72(14)

Symmetry transformations used to generate equivalent atoms:

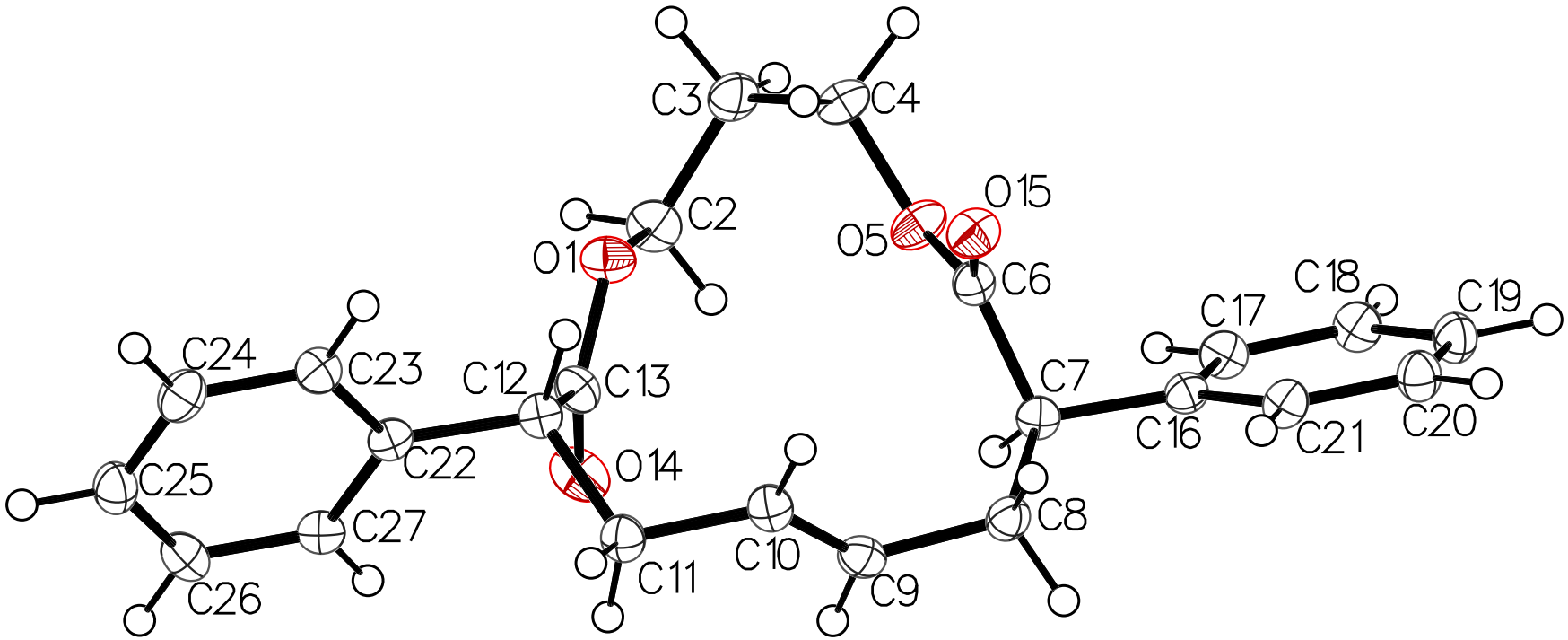

Figure 1. The full numbering scheme of compound **6.** All atoms shown are depicted with 50% thermal contours.

Table 1. Crystal data and structure refinement for compound 6.

Identification code	compound 6	
Empirical formula	$C_{23}H_{24}O_4$	
Formula weight	364.42	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 5.5848(4) Å	α = 69.615(5)°.
	b = 11.7915(8) Å	β = 84.229(6)°.
	c = 15.6064(11) Å	γ = 81.837(6)°.
Volume	952.16(12) $Å^3$	
Z	2	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	388	
Crystal color	Colorless	
Crystal size	0.220 x 0.210 x 0.190 mm^3	
Theta range for data collection	3.494 to 27.468°	
Index ranges	$-7 \leq h \leq 7, -15 \leq k \leq 15, -20 \leq l \leq 20$	
Reflections collected	16756	
Independent reflections	4345 [R(int) = 0.0758]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.984 and 0.795	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4345 / 0 / 245	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I) = 2226 data]	R1 = 0.0510, wR2 = 0.1119	
R indices (all data, ? Å)	R1 = 0.1232, wR2 = 0.1695	
Extinction coefficient	0.033(5)	
Largest diff. peak and hole	0.294 and -0.298 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5977(3)	870(2)	3798(1)	40(1)
C(2)	3635(5)	1442(3)	4031(2)	42(1)
C(3)	4086(5)	2264(3)	4535(2)	44(1)
C(4)	5900(6)	3139(3)	4028(2)	46(1)
O(5)	5166(3)	3714(2)	3097(1)	43(1)
C(6)	6933(5)	4052(2)	2442(2)	31(1)
C(7)	5895(5)	4532(2)	1497(2)	31(1)
C(8)	7677(5)	4057(2)	847(2)	35(1)
C(9)	7640(5)	2716(2)	1074(2)	36(1)
C(10)	9293(5)	1865(2)	1535(2)	34(1)
C(11)	9174(5)	527(2)	1821(2)	35(1)
C(12)	8588(4)	-46(2)	2868(2)	31(1)
C(13)	6054(5)	450(2)	3098(2)	34(1)
O(14)	4275(3)	475(2)	2707(1)	48(1)
O(15)	9019(3)	3988(2)	2591(1)	43(1)
C(16)	5379(5)	5906(2)	1224(2)	30(1)
C(17)	3146(5)	6401(2)	1504(2)	36(1)
C(18)	2631(5)	7650(2)	1295(2)	38(1)
C(19)	4312(5)	8417(3)	797(2)	39(1)
C(20)	6527(5)	7937(2)	513(2)	38(1)
C(21)	7047(5)	6688(2)	725(2)	35(1)
C(22)	8855(4)	-1421(2)	3173(2)	30(1)
C(23)	10826(5)	-2094(2)	3672(2)	35(1)
C(24)	11176(5)	-3355(3)	3921(2)	41(1)
C(25)	9574(5)	-3962(3)	3684(2)	41(1)
C(26)	7601(5)	-3306(3)	3194(2)	40(1)
C(27)	7252(5)	-2052(2)	2941(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for compound 6.

O(1)-C(13)	1.342(3)
O(1)-C(2)	1.457(3)
C(2)-C(3)	1.504(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.511(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-O(5)	1.447(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
O(5)-C(6)	1.343(3)
C(6)-O(15)	1.198(3)
C(6)-C(7)	1.526(3)
C(7)-C(16)	1.516(3)
C(7)-C(8)	1.539(3)
C(7)-H(7)	1.0000
C(8)-C(9)	1.497(4)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.321(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.492(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.555(3)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.511(4)
C(12)-C(22)	1.511(3)
C(12)-H(12)	1.0000
C(13)-O(14)	1.209(3)
C(16)-C(21)	1.387(3)
C(16)-C(17)	1.396(4)
C(17)-C(18)	1.386(4)

C(17)-H(17)	0.9500
C(18)-C(19)	1.381(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.383(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.386(4)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.389(3)
C(22)-C(23)	1.394(4)
C(23)-C(24)	1.390(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.372(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.383(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.381(4)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500

C(13)-O(1)-C(2)	116.3(2)
O(1)-C(2)-C(3)	107.8(2)
O(1)-C(2)-H(2A)	110.2
C(3)-C(2)-H(2A)	110.2
O(1)-C(2)-H(2B)	110.2
C(3)-C(2)-H(2B)	110.2
H(2A)-C(2)-H(2B)	108.5
C(2)-C(3)-C(4)	112.9(2)
C(2)-C(3)-H(3A)	109.0
C(4)-C(3)-H(3A)	109.0
C(2)-C(3)-H(3B)	109.0
C(4)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
O(5)-C(4)-C(3)	107.2(2)
O(5)-C(4)-H(4A)	110.3
C(3)-C(4)-H(4A)	110.3

O(5)-C(4)-H(4B)	110.3
C(3)-C(4)-H(4B)	110.3
H(4A)-C(4)-H(4B)	108.5
C(6)-O(5)-C(4)	116.9(2)
O(15)-C(6)-O(5)	124.0(2)
O(15)-C(6)-C(7)	125.6(2)
O(5)-C(6)-C(7)	110.4(2)
C(16)-C(7)-C(6)	107.9(2)
C(16)-C(7)-C(8)	115.72(19)
C(6)-C(7)-C(8)	108.1(2)
C(16)-C(7)-H(7)	108.3
C(6)-C(7)-H(7)	108.3
C(8)-C(7)-H(7)	108.3
C(9)-C(8)-C(7)	110.6(2)
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(10)-C(9)-C(8)	124.8(3)
C(10)-C(9)-H(9)	117.6
C(8)-C(9)-H(9)	117.6
C(9)-C(10)-C(11)	125.0(3)
C(9)-C(10)-H(10)	117.5
C(11)-C(10)-H(10)	117.5
C(10)-C(11)-C(12)	112.0(2)
C(10)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11B)	109.2
C(12)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
C(13)-C(12)-C(22)	111.0(2)
C(13)-C(12)-C(11)	109.1(2)
C(22)-C(12)-C(11)	111.4(2)
C(13)-C(12)-H(12)	108.4
C(22)-C(12)-H(12)	108.4

C(11)-C(12)-H(12)	108.4
O(14)-C(13)-O(1)	122.8(2)
O(14)-C(13)-C(12)	125.0(2)
O(1)-C(13)-C(12)	112.2(2)
C(21)-C(16)-C(17)	118.7(2)
C(21)-C(16)-C(7)	122.8(2)
C(17)-C(16)-C(7)	118.5(2)
C(18)-C(17)-C(16)	120.4(2)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	120.2(3)
C(19)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(18)-C(19)-C(20)	119.9(3)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(19)-C(20)-C(21)	119.8(2)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	121.0(2)
C(20)-C(21)-H(21)	119.5
C(16)-C(21)-H(21)	119.5
C(27)-C(22)-C(23)	117.8(2)
C(27)-C(22)-C(12)	122.4(2)
C(23)-C(22)-C(12)	119.7(2)
C(24)-C(23)-C(22)	120.8(3)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	120.5(3)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.3(3)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(27)-C(26)-C(25)	120.4(3)
C(27)-C(26)-H(26)	119.8

C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(22)	121.1(2)
C(26)-C(27)-H(27)	119.4
C(22)-C(27)-H(27)	119.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 6. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	50(1)	39(1)	-22(1)	3(1)	1(1)
C(2)	33(2)	49(2)	44(2)	-20(1)	9(1)	2(1)
C(3)	51(2)	44(2)	32(1)	-13(1)	9(1)	-2(1)
C(4)	58(2)	50(2)	26(1)	-8(1)	0(1)	-8(2)
O(5)	37(1)	56(1)	30(1)	-7(1)	4(1)	-7(1)
C(6)	31(2)	31(1)	32(1)	-10(1)	2(1)	-5(1)
C(7)	29(1)	32(1)	31(1)	-11(1)	0(1)	-3(1)
C(8)	40(2)	33(2)	29(1)	-9(1)	1(1)	1(1)
C(9)	38(2)	39(2)	33(1)	-17(1)	2(1)	-4(1)
C(10)	32(2)	34(2)	37(1)	-14(1)	4(1)	-3(1)
C(11)	34(2)	33(2)	37(1)	-13(1)	3(1)	-2(1)
C(12)	26(1)	32(1)	33(1)	-12(1)	0(1)	-3(1)
C(13)	29(2)	34(2)	41(2)	-16(1)	0(1)	-6(1)
O(14)	29(1)	56(1)	68(1)	-34(1)	-8(1)	0(1)
O(15)	34(1)	51(1)	42(1)	-12(1)	-5(1)	-9(1)
C(16)	29(1)	33(1)	28(1)	-10(1)	0(1)	-4(1)
C(17)	31(2)	40(2)	38(1)	-14(1)	4(1)	-7(1)
C(18)	33(2)	39(2)	40(2)	-15(1)	2(1)	3(1)
C(19)	42(2)	32(2)	41(2)	-11(1)	-1(1)	0(1)
C(20)	37(2)	34(2)	40(2)	-10(1)	4(1)	-6(1)
C(21)	29(1)	35(2)	35(1)	-9(1)	2(1)	2(1)
C(22)	25(1)	35(1)	28(1)	-11(1)	4(1)	-4(1)
C(23)	31(1)	37(2)	36(1)	-12(1)	-2(1)	-5(1)
C(24)	36(2)	41(2)	40(2)	-7(1)	-4(1)	1(1)
C(25)	46(2)	33(2)	42(2)	-12(1)	5(1)	-2(1)
C(26)	39(2)	39(2)	47(2)	-22(1)	4(1)	-10(1)
C(27)	31(1)	38(2)	33(1)	-14(1)	-2(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for compound 6.

	x	y	z	U(eq)
H(2A)	2618	813	4422	51
H(2B)	2781	1920	3468	51
H(3A)	4687	1758	5143	53
H(3B)	2535	2735	4636	53
H(4A)	5917	3760	4321	55
H(4B)	7546	2696	4036	55
H(7)	4327	4192	1544	37
H(8A)	7226	4490	207	42
H(8B)	9334	4223	900	42
H(9)	6332	2459	872	43
H(10)	10662	2125	1698	41
H(11A)	10746	128	1656	42
H(11B)	7911	376	1485	42
H(12)	9752	201	3199	37
H(17)	1974	5880	1839	43
H(18)	1116	7979	1494	46
H(19)	3948	9273	650	47
H(20)	7690	8462	173	46
H(21)	8569	6363	526	42
H(23)	11943	-1685	3844	42
H(24)	12535	-3800	4258	49
H(25)	9817	-4824	3855	50
H(26)	6479	-3721	3031	48
H(27)	5891	-1614	2603	41

Table 6. Torsion angles [°] for compound 6.

C(13)-O(1)-C(2)-C(3)	-157.9(2)
O(1)-C(2)-C(3)-C(4)	52.1(3)
C(2)-C(3)-C(4)-O(5)	49.4(3)
C(3)-C(4)-O(5)-C(6)	-149.5(2)
C(4)-O(5)-C(6)-O(15)	-5.9(4)
C(4)-O(5)-C(6)-C(7)	174.8(2)
O(15)-C(6)-C(7)-C(16)	-84.9(3)
O(5)-C(6)-C(7)-C(16)	94.4(2)
O(15)-C(6)-C(7)-C(8)	40.9(3)
O(5)-C(6)-C(7)-C(8)	-139.8(2)
C(16)-C(7)-C(8)-C(9)	-168.1(2)
C(6)-C(7)-C(8)-C(9)	70.9(3)
C(7)-C(8)-C(9)-C(10)	-101.7(3)
C(8)-C(9)-C(10)-C(11)	175.4(2)
C(9)-C(10)-C(11)-C(12)	-107.0(3)
C(10)-C(11)-C(12)-C(13)	66.0(3)
C(10)-C(11)-C(12)-C(22)	-171.1(2)
C(2)-O(1)-C(13)-O(14)	-3.9(4)
C(2)-O(1)-C(13)-C(12)	176.1(2)
C(22)-C(12)-C(13)-O(14)	-72.9(3)
C(11)-C(12)-C(13)-O(14)	50.2(3)
C(22)-C(12)-C(13)-O(1)	107.1(2)
C(11)-C(12)-C(13)-O(1)	-129.8(2)
C(6)-C(7)-C(16)-C(21)	91.9(3)
C(8)-C(7)-C(16)-C(21)	-29.2(3)
C(6)-C(7)-C(16)-C(17)	-86.6(3)
C(8)-C(7)-C(16)-C(17)	152.3(2)
C(21)-C(16)-C(17)-C(18)	-0.8(4)
C(7)-C(16)-C(17)-C(18)	177.9(2)
C(16)-C(17)-C(18)-C(19)	0.8(4)
C(17)-C(18)-C(19)-C(20)	-0.6(4)
C(18)-C(19)-C(20)-C(21)	0.3(4)
C(19)-C(20)-C(21)-C(16)	-0.3(4)
C(17)-C(16)-C(21)-C(20)	0.5(4)

C(7)-C(16)-C(21)-C(20)	-178.1(2)
C(13)-C(12)-C(22)-C(27)	51.4(3)
C(11)-C(12)-C(22)-C(27)	-70.4(3)
C(13)-C(12)-C(22)-C(23)	-131.4(2)
C(11)-C(12)-C(22)-C(23)	106.9(3)
C(27)-C(22)-C(23)-C(24)	0.6(4)
C(12)-C(22)-C(23)-C(24)	-176.8(2)
C(22)-C(23)-C(24)-C(25)	-0.4(4)
C(23)-C(24)-C(25)-C(26)	0.0(4)
C(24)-C(25)-C(26)-C(27)	0.4(4)
C(25)-C(26)-C(27)-C(22)	-0.2(4)
C(23)-C(22)-C(27)-C(26)	-0.2(4)
C(12)-C(22)-C(27)-C(26)	177.1(2)

Symmetry transformations used to generate equivalent atoms:

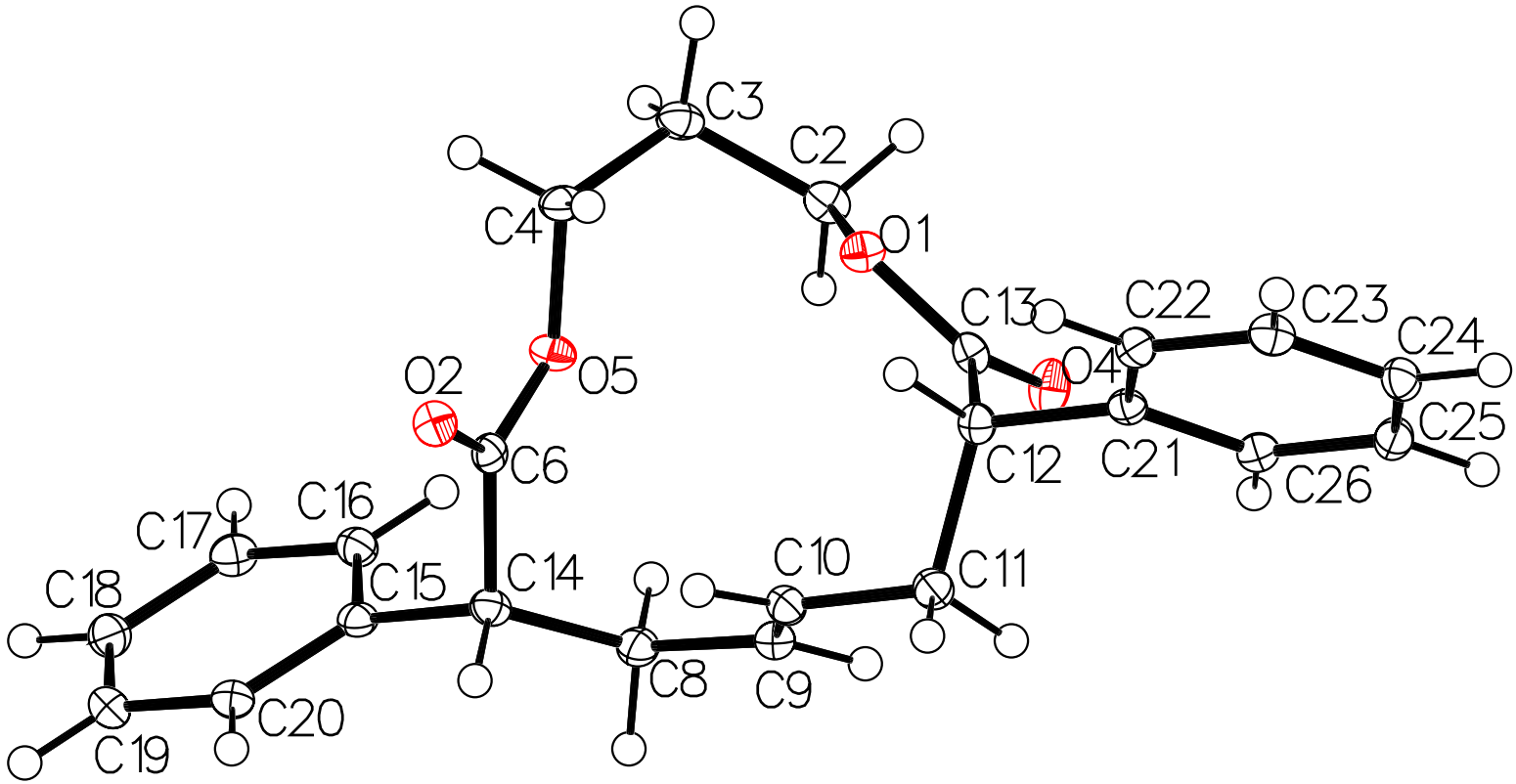

Figure 1. The full numbering scheme of compound **7.** All atoms shown are depicted with 50% thermal contours.

Table 1. Crystal data and structure refinement for compound 7.

Identification code	compound 7	
Empirical formula	$C_{23}H_{24}O_4$	
Formula weight	364.42	
Temperature	93(2) K	
Wavelength	1.54187 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 5.59160(10) Å	α = 70.326(5)°.
	b = 11.9281(2) Å	β = 80.097(6)°.
	c = 15.3677(11) Å	γ = 79.031(6)°.
Volume	941.04(8) $Å^3$	
Z	2	
Density (calculated)	1.286 Mg/m^3	
Absorption coefficient	0.701 mm^{-1}	
F(000)	388	
Crystal color	Colorless	
Crystal size	0.270 x 0.140 x 0.050 mm^3	
Θ range for data collection	3.075 to 66.499°	
Index ranges	$-6 \le h \le 6, -14 \le k \le 14, -18 \le l \le 18$	
Reflections collected	28626	
Independent reflections	3254 [R(int) = 0.0430]	
Completeness to θ = 66.499 °	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.966 and 0.850	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3254 / 0 / 244	
Goodness-of-fit on F^2	1.073	
Final R indices [I>2σ(I) = 3006 data]	R1 = 0.0294, wR2 = 0.0735	
R indices (all data)	R1 = 0.0317, wR2 = 0.0749	
Largest diff. peak and hole	0.208 and -0.153 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound 7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-1076(1)	-5894(1)	-8875(1)	23(1)
O(2)	-5050(1)	-8845(1)	-7662(1)	25(1)
O(4)	723(1)	-5118(1)	-8055(1)	30(1)
O(5)	-1043(1)	-8659(1)	-7995(1)	23(1)
C(2)	1261(2)	-6616(1)	-9041(1)	24(1)
C(3)	784(2)	-7503(1)	-9478(1)	26(1)
C(4)	-1368(2)	-8156(1)	-8973(1)	25(1)
C(6)	-3074(2)	-8933(1)	-7411(1)	20(1)
C(8)	-884(2)	-8701(1)	-6170(1)	24(1)
C(9)	-1701(2)	-7376(1)	-6360(1)	25(1)
C(10)	-3728(2)	-6725(1)	-6697(1)	24(1)
C(11)	-4215(2)	-5377(1)	-6940(1)	25(1)
C(12)	-3702(2)	-4756(1)	-8001(1)	21(1)
C(13)	-1103(2)	-5246(1)	-8309(1)	21(1)
C(14)	-2582(2)	-9403(1)	-6400(1)	21(1)
C(15)	-1595(2)	-10743(1)	-6172(1)	21(1)
C(16)	784(2)	-11137(1)	-6508(1)	23(1)
C(17)	1624(2)	-12356(1)	-6320(1)	26(1)
C(18)	105(2)	-13199(1)	-5793(1)	27(1)
C(19)	-2256(2)	-12815(1)	-5456(1)	27(1)
C(20)	-3102(2)	-11594(1)	-5646(1)	23(1)
C(21)	-4102(2)	-3397(1)	-8244(1)	20(1)
C(22)	-6057(2)	-2729(1)	-8731(1)	22(1)
C(23)	-6505(2)	-1487(1)	-8941(1)	25(1)
C(24)	-5004(2)	-895(1)	-8672(1)	25(1)
C(25)	-3054(2)	-1553(1)	-8186(1)	25(1)
C(26)	-2605(2)	-2794(1)	-7971(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for compound 7.

O(1)-C(13)	1.3413(13)
O(1)-C(2)	1.4555(12)
O(2)-C(6)	1.2074(13)
O(4)-C(13)	1.2060(13)
O(5)-C(6)	1.3399(13)
O(5)-C(4)	1.4489(13)
C(2)-C(3)	1.5127(16)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.5119(16)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(6)-C(14)	1.5183(15)
C(8)-C(9)	1.5002(15)
C(8)-C(14)	1.5316(15)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.3235(17)
C(9)-H(9)	0.9500
C(10)-C(11)	1.5046(15)
C(10)-H(10)	0.9500
C(11)-C(12)	1.5482(16)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(21)	1.5171(15)
C(12)-C(13)	1.5178(14)
C(12)-H(12)	1.0000
C(14)-C(15)	1.5281(15)
C(14)-H(14)	1.0000
C(15)-C(20)	1.3902(16)
C(15)-C(16)	1.3958(15)
C(16)-C(17)	1.3863(16)

C(16)-H(16)	0.9500
C(17)-C(18)	1.3885(17)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3841(17)
C(18)-H(18)	0.9500
C(19)-C(20)	1.3883(16)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.3921(15)
C(21)-C(26)	1.3949(15)
C(22)-C(23)	1.3877(16)
C(22)-H(22)	0.9500
C(23)-C(24)	1.3847(16)
C(23)-H(23)	0.9500
C(24)-C(25)	1.3862(17)
C(24)-H(24)	0.9500
C(25)-C(26)	1.3867(16)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500

C(13)-O(1)-C(2)	115.30(8)
C(6)-O(5)-C(4)	115.79(8)
O(1)-C(2)-C(3)	107.43(9)
O(1)-C(2)-H(2A)	110.2
C(3)-C(2)-H(2A)	110.2
O(1)-C(2)-H(2B)	110.2
C(3)-C(2)-H(2B)	110.2
H(2A)-C(2)-H(2B)	108.5
C(4)-C(3)-C(2)	113.47(9)
C(4)-C(3)-H(3A)	108.9
C(2)-C(3)-H(3A)	108.9
C(4)-C(3)-H(3B)	108.9
C(2)-C(3)-H(3B)	108.9
H(3A)-C(3)-H(3B)	107.7
O(5)-C(4)-C(3)	108.24(9)
O(5)-C(4)-H(4A)	110.1

C(3)-C(4)-H(4A)	110.1
O(5)-C(4)-H(4B)	110.1
C(3)-C(4)-H(4B)	110.1
H(4A)-C(4)-H(4B)	108.4
O(2)-C(6)-O(5)	123.76(10)
O(2)-C(6)-C(14)	124.03(10)
O(5)-C(6)-C(14)	112.19(9)
C(9)-C(8)-C(14)	116.62(9)
C(9)-C(8)-H(8A)	108.1
C(14)-C(8)-H(8A)	108.1
C(9)-C(8)-H(8B)	108.1
C(14)-C(8)-H(8B)	108.1
H(8A)-C(8)-H(8B)	107.3
C(10)-C(9)-C(8)	128.41(11)
C(10)-C(9)-H(9)	115.8
C(8)-C(9)-H(9)	115.8
C(9)-C(10)-C(11)	122.96(11)
C(9)-C(10)-H(10)	118.5
C(11)-C(10)-H(10)	118.5
C(10)-C(11)-C(12)	111.47(9)
C(10)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11A)	109.3
C(10)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(21)-C(12)-C(13)	112.53(9)
C(21)-C(12)-C(11)	111.54(9)
C(13)-C(12)-C(11)	107.36(9)
C(21)-C(12)-H(12)	108.4
C(13)-C(12)-H(12)	108.4
C(11)-C(12)-H(12)	108.4
O(4)-C(13)-O(1)	123.40(10)
O(4)-C(13)-C(12)	125.07(10)
O(1)-C(13)-C(12)	111.47(9)
C(6)-C(14)-C(15)	107.89(8)
C(6)-C(14)-C(8)	113.39(9)

C(15)-C(14)-C(8)	112.41(9)
C(6)-C(14)-H(14)	107.6
C(15)-C(14)-H(14)	107.6
C(8)-C(14)-H(14)	107.6
C(20)-C(15)-C(16)	118.76(10)
C(20)-C(15)-C(14)	120.00(10)
C(16)-C(15)-C(14)	121.20(10)
C(17)-C(16)-C(15)	120.46(11)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	120.31(11)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	119.56(11)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	120.20(11)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(15)	120.71(10)
C(19)-C(20)-H(20)	119.6
C(15)-C(20)-H(20)	119.6
C(22)-C(21)-C(26)	118.76(10)
C(22)-C(21)-C(12)	119.33(9)
C(26)-C(21)-C(12)	121.89(10)
C(23)-C(22)-C(21)	120.58(10)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	120.34(10)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	119.46(10)
C(23)-C(24)-H(24)	120.3
C(25)-C(24)-H(24)	120.3
C(24)-C(25)-C(26)	120.42(10)
C(24)-C(25)-H(25)	119.8

C(26)-C(25)-H(25)	119.8
C(25)-C(26)-C(21)	120.45(10)
C(25)-C(26)-H(26)	119.8
C(21)-C(26)-H(26)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound 7. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	19(1)	24(1)	24(1)	-9(1)	-2(1)	2(1)
O(2)	22(1)	26(1)	28(1)	-7(1)	-6(1)	-2(1)
O(4)	19(1)	28(1)	46(1)	-16(1)	-6(1)	-3(1)
O(5)	21(1)	28(1)	18(1)	-3(1)	-3(1)	-3(1)
C(2)	18(1)	24(1)	26(1)	-6(1)	1(1)	2(1)
C(3)	27(1)	25(1)	20(1)	-6(1)	1(1)	2(1)
C(4)	30(1)	28(1)	17(1)	-6(1)	-4(1)	-2(1)
C(6)	21(1)	16(1)	23(1)	-7(1)	-2(1)	-1(1)
C(8)	28(1)	23(1)	21(1)	-5(1)	-6(1)	-2(1)
C(9)	32(1)	24(1)	20(1)	-6(1)	-3(1)	-6(1)
C(10)	26(1)	22(1)	23(1)	-6(1)	1(1)	-6(1)
C(11)	26(1)	22(1)	24(1)	-8(1)	1(1)	-3(1)
C(12)	18(1)	20(1)	24(1)	-7(1)	-2(1)	-3(1)
C(13)	20(1)	17(1)	23(1)	-3(1)	-2(1)	-3(1)
C(14)	22(1)	21(1)	19(1)	-5(1)	0(1)	-1(1)
C(15)	23(1)	22(1)	16(1)	-5(1)	-4(1)	-2(1)
C(16)	23(1)	25(1)	22(1)	-6(1)	-1(1)	-5(1)
C(17)	24(1)	29(1)	26(1)	-10(1)	-3(1)	1(1)
C(18)	33(1)	21(1)	26(1)	-6(1)	-5(1)	0(1)
C(19)	31(1)	24(1)	24(1)	-4(1)	0(1)	-8(1)
C(20)	23(1)	26(1)	21(1)	-7(1)	-1(1)	-4(1)
C(21)	18(1)	21(1)	19(1)	-7(1)	2(1)	-3(1)
C(22)	20(1)	25(1)	23(1)	-9(1)	-2(1)	-4(1)
C(23)	23(1)	25(1)	24(1)	-6(1)	-4(1)	1(1)
C(24)	28(1)	19(1)	26(1)	-7(1)	0(1)	-2(1)
C(25)	24(1)	25(1)	27(1)	-12(1)	0(1)	-6(1)
C(26)	20(1)	24(1)	22(1)	-8(1)	-2(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for compound 7.

	x	y	z	U(eq)
H(2A)	1959	-7049	-8447	29
H(2B)	2441	-6095	-9463	29
H(3A)	475	-7068	-10130	31
H(3B)	2272	-8102	-9487	31
H(4A)	-2919	-7591	-9056	30
H(4B)	-1447	-8806	-9228	30
H(8A)	-664	-9063	-5502	29
H(8B)	743	-8812	-6529	29
H(9)	-624	-6949	-6221	30
H(10)	-4929	-7127	-6790	29
H(11A)	-3162	-5113	-6612	30
H(11B)	-5947	-5129	-6727	30
H(12)	-4857	-4987	-8320	25
H(14)	-4191	-9324	-6008	26
H(16)	1836	-10567	-6869	28
H(17)	3245	-12616	-6553	32
H(18)	684	-14034	-5664	33
H(19)	-3301	-13388	-5094	32
H(20)	-4728	-11338	-5415	28
H(22)	-7095	-3127	-8920	27
H(23)	-7848	-1041	-9272	30
H(24)	-5308	-44	-8818	30
H(25)	-2018	-1151	-8000	30
H(26)	-1269	-3238	-7635	26

Table 6. Torsion angles [°] for compound 7.

C(13)-O(1)-C(2)-C(3)	165.89(9)
O(1)-C(2)-C(3)-C(4)	-48.00(12)
C(6)-O(5)-C(4)-C(3)	159.85(9)
C(2)-C(3)-C(4)-O(5)	-51.31(12)
C(4)-O(5)-C(6)-O(2)	4.28(15)
C(4)-O(5)-C(6)-C(14)	-177.59(8)
C(14)-C(8)-C(9)-C(10)	0.61(18)
C(8)-C(9)-C(10)-C(11)	-174.03(11)
C(9)-C(10)-C(11)-C(12)	101.01(13)
C(10)-C(11)-C(12)-C(21)	-177.89(9)
C(10)-C(11)-C(12)-C(13)	-54.18(12)
C(2)-O(1)-C(13)-O(4)	10.34(15)
C(2)-O(1)-C(13)-C(12)	-166.94(9)
C(21)-C(12)-C(13)-O(4)	59.67(14)
C(11)-C(12)-C(13)-O(4)	-63.43(14)
C(21)-C(12)-C(13)-O(1)	-123.10(10)
C(11)-C(12)-C(13)-O(1)	113.80(10)
O(2)-C(6)-C(14)-C(15)	95.18(12)
O(5)-C(6)-C(14)-C(15)	-82.93(11)
O(2)-C(6)-C(14)-C(8)	-139.63(11)
O(5)-C(6)-C(14)-C(8)	42.25(12)
C(9)-C(8)-C(14)-C(6)	57.85(13)
C(9)-C(8)-C(14)-C(15)	-179.43(9)
C(6)-C(14)-C(15)-C(20)	-104.45(11)
C(8)-C(14)-C(15)-C(20)	129.79(11)
C(6)-C(14)-C(15)-C(16)	73.31(12)
C(8)-C(14)-C(15)-C(16)	-52.45(13)
C(20)-C(15)-C(16)-C(17)	-0.08(16)
C(14)-C(15)-C(16)-C(17)	-177.87(10)
C(15)-C(16)-C(17)-C(18)	-0.09(17)
C(16)-C(17)-C(18)-C(19)	0.05(17)
C(17)-C(18)-C(19)-C(20)	0.15(17)
C(18)-C(19)-C(20)-C(15)	-0.32(17)
C(16)-C(15)-C(20)-C(19)	0.29(16)

C(14)-C(15)-C(20)-C(19)	178.10(10)
C(13)-C(12)-C(21)-C(22)	127.68(11)
C(11)-C(12)-C(21)-C(22)	-111.59(11)
C(13)-C(12)-C(21)-C(26)	-54.15(14)
C(11)-C(12)-C(21)-C(26)	66.58(13)
C(26)-C(21)-C(22)-C(23)	0.11(16)
C(12)-C(21)-C(22)-C(23)	178.34(10)
C(21)-C(22)-C(23)-C(24)	0.21(17)
C(22)-C(23)-C(24)-C(25)	-0.26(17)
C(23)-C(24)-C(25)-C(26)	-0.01(17)
C(24)-C(25)-C(26)-C(21)	0.33(17)
C(22)-C(21)-C(26)-C(25)	-0.38(16)
C(12)-C(21)-C(26)-C(25)	-178.56(10)

Symmetry transformations used to generate equivalent atoms: