Supplementary material (ESI) for Perkin Transactions 2

Supplementary data

Twisting and planarization in push-pull ethylenes

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Tables S1-S12: X-ray crystallographic bond lengths and angles of compounds **8**-**19**

(including selected torsional angles and hydrogen bonds)

Figures S1-S5: X-ray structures of compounds **10, 11, 13, 16,** and **18**.

Figures S6-S7: Packing diagrams for **17•H_2O** and **19•H_2O**.

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Table S1. Bond lengths [Å] and angles [°] for compound **8**

Code number 1091dm9.

O(1)-C(6)	1.368(3)
O(1)-C(2)	1.429(3)
C(2)-O(3)	1.430(3)
C(2)-C(22)	1.505(4)
C(2)-C(21)	1.505(3)
O(3)-C(4)	1.363(3)
C(4)-O(4)	1.220(3)
C(4)-C(5)	1.425(3)
C(5)-C(7)	1.420(3)
C(5)-C(6)	1.426(3)
C(6)-O(6)	1.218(3)
C(7)-N(1)	1.322(3)
C(7)-N(2)	1.326(3)
N(2)-C(9)	1.440(3)
C(9)-C(10)	1.512(4)
C(10)-N(1)	1.443(3)

C(6)-O(1)-C(2)	117.79(18)
O(1)-C(2)-O(3)	110.68(19)
O(1)-C(2)-C(22)	110.3(2)
O(3)-C(2)-C(22)	109.8(2)
O(1)-C(2)-C(21)	106.8(2)
O(3)-C(2)-C(21)	106.2(2)
C(22)-C(2)-C(21)	113.0(2)
C(4)-O(3)-C(2)	117.76(18)
O(4)-C(4)-O(3)	116.2(2)
O(4)-C(4)-C(5)	126.8(2)
O(3)-C(4)-C(5)	116.9(2)
C(7)-C(5)-C(4)	119.6(2)
C(7)-C(5)-C(6)	119.1(2)
C(4)-C(5)-C(6)	121.1(2)
O(6)-C(6)-O(1)	116.4(2)
O(6)-C(6)-C(5)	127.3(2)
O(1)-C(6)-C(5)	116.3(2)
N(1)-C(7)-N(2)	108.9(2)
N(1)-C(7)-C(5)	125.8(2)

N(2)-C(7)-C(5)	125.3(2)
C(7)-N(2)-C(9)	112.4(2)
N(2)-C(9)-C(10)	102.8(2)
N(1)-C(10)-C(9)	102.6(2)
C(7)-N(1)-C(10)	112.6(2)

Torsion angles [°] for **8** (1091dm9).

C(6)-O(1)-C(2)-O(3)	48.8(3)
C(6)-O(1)-C(2)-C(22)	-72.9(3)
C(6)-O(1)-C(2)-C(21)	164.0(2)
O(1)-C(2)-O(3)-C(4)	-47.5(3)
C(22)-C(2)-O(3)-C(4)	74.5(3)
C(21)-C(2)-O(3)-C(4)	-163.0(2)
C(2)-O(3)-C(4)-O(4)	-159.8(2)
C(2)-O(3)-C(4)-C(5)	21.2(3)
O(4)-C(4)-C(5)-C(7)	1.4(4)
O(3)-C(4)-C(5)-C(7)	-179.7(2)
O(4)-C(4)-C(5)-C(6)	-172.7(3)
O(3)-C(4)-C(5)-C(6)	6.1(4)
C(2)-O(1)-C(6)-O(6)	158.4(2)
C(2)-O(1)-C(6)-C(5)	-23.5(3)
C(7)-C(5)-C(6)-O(6)	-1.4(4)
C(4)-C(5)-C(6)-O(6)	172.8(3)
C(7)-C(5)-C(6)-O(1)	-179.2(2)
C(4)-C(5)-C(6)-O(1)	-5.0(4)
C(4)-C(5)-C(7)-N(1)	-177.2(3)
C(6)-C(5)-C(7)-N(1)	-2.9(4)
C(4)-C(5)-C(7)-N(2)	3.3(4)
C(6)-C(5)-C(7)-N(2)	177.5(3)
N(1)-C(7)-N(2)-C(9)	3.5(3)
C(5)-C(7)-N(2)-C(9)	-176.9(3)
C(7)-N(2)-C(9)-C(10)	-8.0(3)
N(2)-C(9)-C(10)-N(1)	8.8(3)
N(2)-C(7)-N(1)-C(10)	3.0(3)
C(5)-C(7)-N(1)-C(10)	-176.6(3)
C(9)-C(10)-N(1)-C(7)	-7.7(3)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N2-H2	0.840	2.114	128.91	2.721	O4
N2-H2	0.840	2.334	125.92	2.907	O4 [-x, -y+1, -z+2]
N1-H1	0.855	2.135	125.83	2.725	O6
N1-H1	0.855	2.311	125.44	2.892	O6 [-x+2, -y+2, -z+2]

Table S2. Bond lengths [≈] and angles [∞] for compound **9**

Code number 1074dm8.

O(1)-C(6)	1.375(4)
O(1)-C(2)	1.427(4)
C(2)-O(3)	1.441(4)
C(2)-C(12)	1.499(5)
C(2)-C(13)	1.511(5)
O(3)-C(4)	1.373(4)
C(4)-O(4)	1.220(4)
C(4)-C(5)	1.418(4)
C(5)-C(6)	1.428(4)
C(5)-C(7)	1.441(4)
C(6)-O(6)	1.219(4)
C(7)-N(72)	1.324(4)
C(7)-N(71)	1.328(4)
N(71)-C(10)	1.443(4)
N(71)-C(9)	1.465(4)
N(72)-C(11)	1.437(4)
N(72)-C(8)	1.458(4)
C(8)-C(9)	1.499(5)

C(6)-O(1)-C(2)	117.5(2)
O(1)-C(2)-O(3)	109.8(2)
O(1)-C(2)-C(12)	107.2(3)
O(3)-C(2)-C(12)	105.8(3)
O(1)-C(2)-C(13)	110.2(3)
O(3)-C(2)-C(13)	110.5(3)
C(12)-C(2)-C(13)	113.2(3)

C(4)-O(3)-C(2)	118.2(2)
O(4)-C(4)-O(3)	116.8(2)
O(4)-C(4)-C(5)	126.6(3)
O(3)-C(4)-C(5)	116.5(2)
C(4)-C(5)-C(6)	121.6(3)
C(4)-C(5)-C(7)	118.4(2)
C(6)-C(5)-C(7)	119.9(2)
O(6)-C(6)-O(1)	116.9(2)
O(6)-C(6)-C(5)	127.3(3)
O(1)-C(6)-C(5)	115.8(2)
N(72)-C(7)-N(71)	110.8(3)
N(72)-C(7)-C(5)	123.5(3)
N(71)-C(7)-C(5)	125.7(3)
C(7)-N(71)-C(10)	127.5(3)
C(7)-N(71)-C(9)	110.7(3)
C(10)-N(71)-C(9)	121.6(3)
C(7)-N(72)-C(11)	127.0(2)
C(7)-N(72)-C(8)	110.8(2)
C(11)-N(72)-C(8)	122.1(2)
N(72)-C(8)-C(9)	103.4(2)
N(71)-C(9)-C(8)	103.1(2)

Selected torsion angles

51.17 (0.35)	C6 - O1 - C2 - O3
165.72 (0.27)	C6 - O1 - C2 - C21
-70.71 (0.32)	C6 - O1 - C2 - C22
-47.14 (0.35)	O1 - C2 - O3 - C4
-162.59 (0.27)	C21 - C2 - O3 - C4
74.56 (0.31)	C22 - C2 - O3 - C4
-163.63 (0.28)	C2 - O3 - C4 - O4
18.92 (0.38)	C2 - O3 - C4 - C5
-169.08 (0.31)	O4 - C4 - C5 - C6
8.09 (0.43)	O3 - C4 - C5 - C6
7.32 (0.49)	O4 - C4 - C5 - C7
-175.52 (0.25)	O3 - C4 - C5 - C7
154.75 (0.30)	C2 - O1 - C6 - O6
-26.61 (0.39)	C2 - O1 - C6 - C5
174.13 (0.32)	C4 - C5 - C6 - O6

-2.22 (0.52) C7 - C5 - C6 - O6
-4.35 (0.43) C4 - C5 - C6 - O1
179.31 (0.26) C7 - C5 - C6 - O1
54.58 (0.41) C4 - C5 - C7 - N2
-128.96 (0.32) C6 - C5 - C7 - N2
-124.11 (0.32) C4 - C5 - C7 - N1
52.35 (0.44) C6 - C5 - C7 - N1
-173.12 (0.30) N2 - C7 - N1 - C10
5.72 (0.49) C5 - C7 - N1 - C10
1.99 (0.37) N2 - C7 - N1 - C9
-179.18 (0.29) C5 - C7 - N1 - C9
-176.06 (0.30) N1 - C7 - N2 - C11
5.07 (0.48) C5 - C7 - N2 - C11
5.67 (0.36) N1 - C7 - N2 - C8
-173.19 (0.28) C5 - C7 - N2 - C8
-10.51 (0.38) C7 - N2 - C8 - C9
171.13 (0.31) C11 - N2 - C8 - C9
-8.31 (0.38) C7 - N1 - C9 - C8
167.13 (0.30) C10 - N1 - C9 - C8
10.72 (0.37) N2 - C8 - C9 - N1

Table S3. Bond lengths [Å] and angles [°] for compound **10** Code number CW3.

O(1)-C(6)	1.365(3)
O(1)-C(2)	1.442(3)
O(4)-C(4)	1.225(3)
O(3)-C(4)	1.364(3)
O(3)-C(2)	1.432(3)
O(6)-C(6)	1.219(3)
C(4)-C(5)	1.425(4)
N(1)-C(7)	1.322(3)
N(1)-C(8)	1.445(3)
N(2)-C(7)	1.337(3)
N(2)-C(9)	1.452(3)

C(6)-C(5)	1.426(4)
C(5)-C(7)	1.444(4)
C(2)-C(22)	1.498(4)
C(2)-C(21)	1.502(4)

C(6)-O(1)-C(2)	118.0(2)
C(4)-O(3)-C(2)	117.7(2)
O(4)-C(4)-O(3)	115.9(2)
O(4)-C(4)-C(5)	127.1(3)
O(3)-C(4)-C(5)	116.8(2)
C(7)-N(1)-C(8)	124.8(3)
C(7)-N(2)-C(9)	125.9(2)
O(6)-C(6)-O(1)	116.0(2)
O(6)-C(6)-C(5)	127.2(3)
O(1)-C(6)-C(5)	116.8(2)
C(4)-C(5)-C(6)	118.9(2)
C(4)-C(5)-C(7)	119.5(2)
C(6)-C(5)-C(7)	120.3(2)
O(3)-C(2)-O(1)	108.3(2)
O(3)-C(2)-C(22)	106.7(2)
O(1)-C(2)-C(22)	106.4(2)
O(3)-C(2)-C(21)	111.2(2)
O(1)-C(2)-C(21)	111.1(2)
C(22)-C(2)-C(21)	112.9(3)
N(1)-C(7)-N(2)	117.6(2)
N(1)-C(7)-C(5)	120.5(2)
N(2)-C(7)-C(5)	121.8(2)

Selected torsion angles

-164.15 (0.24)	C2 - O3 - C4 - O4
20.49 (0.35)	C2 - O3 - C4 - C5
165.56 (0.24)	C2 - O1 - C6 - O6
-16.24 (0.36)	C2 - O1 - C6 - C5
-159.22 (0.28)	O4 - C4 - C5 - C6

15.55 (0.36) O3 - C4 - C5 - C6
7.85 (0.44) O4 - C4 - C5 - C7
-177.39 (0.24) O3 - C4 - C5 - C7
160.39 (0.28) O6 - C6 - C5 - C4
-17.58 (0.37) O1 - C6 - C5 - C4
-6.57 (0.44) O6 - C6 - C5 - C7
175.46 (0.23) O1 - C6 - C5 - C7
-51.13 (0.32) C4 - O3 - C2 - O1
-165.28 (0.24) C4 - O3 - C2 - C22
71.18 (0.30) C4 - O3 - C2 - C21
48.93 (0.32) C6 - O1 - C2 - O3
163.29 (0.26) C6 - O1 - C2 - C22
-73.41 (0.30) C6 - O1 - C2 - C21
6.41 (0.40) C8 - N1 - C7 - N2
-171.96 (0.26) C8 - N1 - C7 - C5
-165.53 (0.27) C9 - N2 - C7 - N1
12.81 (0.41) C9 - N2 - C7 - C5
-135.65 (0.27) C4 - C5 - C7 - N1
31.24 (0.38) C6 - C5 - C7 - N1
46.06 (0.37) C4 - C5 - C7 - N2
-147.06 (0.26) C6 - C5 - C7 - N2

Table S4. Bond lengths [Å] and angles [°] for compound **11**
Code number1738cw5.

C(2)-O(1)	1.426(2)
C(2)-O(3)	1.446(2)
C(2)-C(22)	1.500(3)
C(2)-C(21)	1.502(3)
C(4)-O(4)	1.221(2)
C(4)-O(3)	1.358(2)
C(4)-C(5)	1.432(3)
C(5)-C(7)	1.425(3)
C(5)-C(6)	1.447(3)

C(6)-O(6)	1.213(2)
C(6)-O(1)	1.364(3)
C(7)-N(1)	1.307(3)
C(7)-S(2)	1.750(2)
C(8)-N(1)	1.454(3)
C(9)-S(2)	1.787(3)

O(1)-C(2)-O(3)	108.55(15)
O(1)-C(2)-C(22)	107.29(18)
O(3)-C(2)-C(22)	105.98(17)
O(1)-C(2)-C(21)	110.90(18)
O(3)-C(2)-C(21)	111.18(17)
C(22)-C(2)-C(21)	112.70(19)
O(4)-C(4)-O(3)	116.02(18)
O(4)-C(4)-C(5)	126.46(19)
O(3)-C(4)-C(5)	117.51(17)
C(7)-C(5)-C(4)	119.17(18)
C(7)-C(5)-C(6)	121.32(18)
C(4)-C(5)-C(6)	118.10(18)
O(6)-C(6)-O(1)	116.82(18)
O(6)-C(6)-C(5)	127.0(2)
O(1)-C(6)-C(5)	115.98(17)
N(1)-C(7)-C(5)	121.54(18)
N(1)-C(7)-S(2)	114.68(16)
C(5)-C(7)-S(2)	123.76(15)
C(7)-N(1)-C(8)	126.58(19)
C(6)-O(1)-C(2)	117.95(15)
C(4)-O(3)-C(2)	118.30(15)
C(7)-S(2)-C(9)	103.34(11)

Selected torsion angles

8.24 (0.35)	O4 - C4 - C5 - C7
-172.96 (0.18)	O3 - C4 - C5 - C7
-158.36 (0.22)	O4 - C4 - C5 - C6

20.44 (0.29) O3 - C4 - C5 - C6
-6.59 (0.33) C7 - C5 - C6 - O6
159.71 (0.21) C4 - C5 - C6 - O6
179.04 (0.17) C7 - C5 - C6 - O1
-14.66 (0.27) C4 - C5 - C6 - O1
-21.20 (0.30) C4 - C5 - C7 - N1
144.96 (0.21) C6 - C5 - C7 - N1
157.07 (0.16) C4 - C5 - C7 - S2
-36.78 (0.27) C6 - C5 - C7 - S2
173.74 (0.20) C5 - C7 - N1 - C8
-4.67 (0.30) S2 - C7 - N1 - C8
161.71 (0.18) O6 - C6 - O1 - C2
-23.33 (0.25) C5 - C6 - O1 - C2
52.71 (0.22) O3 - C2 - O1 - C6
166.83 (0.17) C22 - C2 - O1 - C6
-69.70 (0.21) C21 - C2 - O1 - C6
-169.49 (0.20) O4 - C4 - O3 - C2
11.59 (0.28) C5 - C4 - O3 - C2
-46.37 (0.24) O1 - C2 - O3 - C4
-161.34 (0.19) C22 - C2 - O3 - C4
75.87 (0.23) C21 - C2 - O3 - C4
147.74 (0.18) N1 - C7 - S2 - C9
-30.64 (0.21) C5 - C7 - S2 - C9

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.860	2.069	126.73	2.674	O4
N1-H1	0.860	2.287	139.38	2.992	O4 [-x+1, -y, -z+1]

Table S5. Bond lengths [Å] and angles [°] for compound **12**

Code number1005dm4.

C(2)-O(3)	1.431(2)
C(2)-O(1)	1.439(2)
C(2)-C(22)	1.505(3)

C(2)-C(21)	1.509(3)
C(4)-O(4)	1.213(2)
C(4)-O(3)	1.360(2)
C(4)-C(5)	1.441(3)
C(5)-C(7)	1.410(2)
C(5)-C(6)	1.445(3)
C(6)-O(6)	1.220(2)
C(6)-O(1)	1.354(2)
C(7)-N(1)	1.326(2)
C(7)-S(2)	1.7488(19)
C(9)-S(2)	1.797(2)
C(11)-C(16)	1.366(3)
C(11)-C(12)	1.372(3)
C(11)-N(1)	1.434(2)
C(12)-C(13)	1.381(3)
C(13)-C(14)	1.362(4)
C(14)-C(15)	1.369(4)
C(15)-C(16)	1.370(3)

O(3)-C(2)-O(1)	109.09(15)
O(3)-C(2)-C(22)	106.38(17)
O(1)-C(2)-C(22)	106.40(16)
O(3)-C(2)-C(21)	110.74(17)
O(1)-C(2)-C(21)	110.94(18)
C(22)-C(2)-C(21)	113.06(18)
O(4)-C(4)-O(3)	116.68(17)
O(4)-C(4)-C(5)	126.82(18)
O(3)-C(4)-C(5)	116.35(16)
C(7)-C(5)-C(4)	121.56(16)
C(7)-C(5)-C(6)	119.39(17)
C(4)-C(5)-C(6)	118.53(16)
O(6)-C(6)-O(1)	116.51(17)
O(6)-C(6)-C(5)	126.79(18)
O(1)-C(6)-C(5)	116.68(17)
N(1)-C(7)-C(5)	121.62(16)
N(1)-C(7)-S(2)	113.75(14)
C(5)-C(7)-S(2)	124.60(14)
C(16)-C(11)-C(12)	120.9(2)

C(16)-C(11)-N(1)	119.36(18)
C(12)-C(11)-N(1)	119.77(19)
C(11)-C(12)-C(13)	119.0(2)
C(14)-C(13)-C(12)	120.3(2)
C(13)-C(14)-C(15)	119.9(2)
C(14)-C(15)-C(16)	120.5(3)
C(11)-C(16)-C(15)	119.4(2)
C(7)-N(1)-C(11)	125.29(16)
C(6)-O(1)-C(2)	118.50(14)
C(4)-O(3)-C(2)	118.24(15)
C(7)-S(2)-C(9)	105.02(10)

Torsion angles [°] for **12** (1005dm4).

O(4)-C(4)-C(5)-C(7)	12.8(3)
O(3)-C(4)-C(5)-C(7)	-172.00(17)
O(4)-C(4)-C(5)-C(6)	-158.9(2)
O(3)-C(4)-C(5)-C(6)	16.3(3)
C(7)-C(5)-C(6)-O(6)	-11.4(3)
C(4)-C(5)-C(6)-O(6)	160.5(2)
C(7)-C(5)-C(6)-O(1)	169.88(17)
C(4)-C(5)-C(6)-O(1)	-18.2(3)
C(4)-C(5)-C(7)-N(1)	-147.02(19)
C(6)-C(5)-C(7)-N(1)	24.6(3)
C(4)-C(5)-C(7)-S(2)	34.6(3)
C(6)-C(5)-C(7)-S(2)	-153.74(15)
C(16)-C(11)-C(12)-C(13)	-0.6(3)
N(1)-C(11)-C(12)-C(13)	179.5(2)
C(11)-C(12)-C(13)-C(14)	1.2(4)
C(12)-C(13)-C(14)-C(15)	-0.8(4)
C(13)-C(14)-C(15)-C(16)	-0.2(4)
C(12)-C(11)-C(16)-C(15)	-0.3(3)
N(1)-C(11)-C(16)-C(15)	179.6(2)
C(14)-C(15)-C(16)-C(11)	0.7(4)
C(5)-C(7)-N(1)-C(11)	-169.82(19)
S(2)-C(7)-N(1)-C(11)	8.7(3)
C(16)-C(11)-N(1)-C(7)	87.8(3)
C(12)-C(11)-N(1)-C(7)	-92.3(3)
O(6)-C(6)-O(1)-C(2)	165.81(17)

C(5)-C(6)-O(1)-C(2)	-15.3(2)
O(3)-C(2)-O(1)-C(6)	48.0(2)
C(22)-C(2)-O(1)-C(6)	162.40(18)
C(21)-C(2)-O(1)-C(6)	-74.2(2)
O(4)-C(4)-O(3)-C(2)	-165.04(17)
C(5)-C(4)-O(3)-C(2)	19.2(2)
O(1)-C(2)-O(3)-C(4)	-50.1(2)
C(22)-C(2)-O(3)-C(4)	-164.50(17)
C(21)-C(2)-O(3)-C(4)	72.3(2)
N(1)-C(7)-S(2)-C(9)	-152.39(16)
C(5)-C(7)-S(2)-C(9)	26.1(2)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.888	2.068	128.31	2.710	O6
N1-H1	0.888	2.450	144.13	3.212	O6 [-x+1/2, y+1/2, -z+1/2]

Table S6. Bond lengths [Å] and angles [°] for compound **13**

Code number CW9187.

C(2)-O(3)	1.425(3)
C(2)-O(1)	1.439(3)
C(2)-C(22)	1.502(5)
C(2)-C(21)	1.506(5)
C(4)-O(4)	1.207(3)
C(4)-O(3)	1.372(3)
C(4)-C(5)	1.445(4)
C(5)-C(7)	1.415(4)
C(5)-C(6)	1.437(4)
C(6)-O(6)	1.212(3)
C(6)-O(1)	1.358(3)
C(7)-N(1)	1.320(4)
C(7)-S(1)	1.747(3)

C(8)-S(1)	1.785(3)
C(9)-C(14)	1.397(4)
C(9)-C(10)	1.399(5)
C(9)-N(1)	1.437(4)
C(10)-C(11)	1.380(5)
C(10)-C(15)	1.509(5)
C(11)-C(12)	1.372(5)
C(12)-C(13)	1.366(6)
C(13)-C(14)	1.377(4)
C(14)-C(17)	1.518(5)
C(15)-C(16)	1.429(6)
C(17)-C(18)	1.512(5)

O(3)-C(2)-O(1)	109.2(2)
O(3)-C(2)-C(22)	106.6(3)
O(1)-C(2)-C(22)	105.7(3)
O(3)-C(2)-C(21)	110.7(3)
O(1)-C(2)-C(21)	111.0(3)
C(22)-C(2)-C(21)	113.4(3)
O(4)-C(4)-O(3)	116.4(2)
O(4)-C(4)-C(5)	127.9(2)
O(3)-C(4)-C(5)	115.7(2)
C(7)-C(5)-C(6)	121.7(3)
C(7)-C(5)-C(4)	118.9(2)
C(6)-C(5)-C(4)	118.7(2)
O(6)-C(6)-O(1)	116.5(2)
O(6)-C(6)-C(5)	126.3(2)
O(1)-C(6)-C(5)	117.1(2)
N(1)-C(7)-C(5)	121.0(3)
N(1)-C(7)-S(1)	114.2(2)
C(5)-C(7)-S(1)	124.8(2)
C(14)-C(9)-C(10)	122.5(3)
C(14)-C(9)-N(1)	118.8(3)
C(10)-C(9)-N(1)	118.7(3)

C(11)-C(10)-C(9)	117.2(3)
C(11)-C(10)-C(15)	121.9(3)
C(9)-C(10)-C(15)	120.9(3)
C(12)-C(11)-C(10)	121.5(3)
C(13)-C(12)-C(11)	119.9(3)
C(12)-C(13)-C(14)	122.0(3)
C(13)-C(14)-C(9)	117.0(3)
C(13)-C(14)-C(17)	123.4(3)
C(9)-C(14)-C(17)	119.6(3)
C(16)-C(15)-C(10)	116.7(4)
C(18)-C(17)-C(14)	116.0(3)
C(7)-N(1)-C(9)	126.7(3)
C(6)-O(1)-C(2)	118.4(2)
C(4)-O(3)-C(2)	118.5(2)
C(7)-S(1)-C(8)	105.28(15)

Torsion angles [°] for **13** (CW9187).

O(4)-C(4)-C(5)-C(7)	-7.1(4)
O(3)-C(4)-C(5)-C(7)	173.3(2)
O(4)-C(4)-C(5)-C(6)	163.9(3)
O(3)-C(4)-C(5)-C(6)	-15.7(4)
C(7)-C(5)-C(6)-O(6)	13.3(5)
C(4)-C(5)-C(6)-O(6)	-157.4(3)
C(7)-C(5)-C(6)-O(1)	-170.8(3)
C(4)-C(5)-C(6)-O(1)	18.5(4)
C(6)-C(5)-C(7)-N(1)	-146.2(3)
C(4)-C(5)-C(7)-N(1)	24.5(4)
C(6)-C(5)-C(7)-S(1)	35.8(4)
C(4)-C(5)-C(7)-S(1)	-153.5(2)
C(14)-C(9)-C(10)-C(11)	0.9(5)
N(1)-C(9)-C(10)-C(11)	178.7(3)
C(14)-C(9)-C(10)-C(15)	179.9(3)
N(1)-C(9)-C(10)-C(15)	-2.4(5)
C(9)-C(10)-C(11)-C(12)	-0.5(6)

C(15)-C(10)-C(11)-C(12)	-179.5(4)
C(10)-C(11)-C(12)-C(13)	0.2(7)
C(11)-C(12)-C(13)-C(14)	-0.2(7)
C(12)-C(13)-C(14)-C(9)	0.6(6)
C(12)-C(13)-C(14)-C(17)	179.6(4)
C(10)-C(9)-C(14)-C(13)	-1.0(5)
N(1)-C(9)-C(14)-C(13)	-178.7(3)
C(10)-C(9)-C(14)-C(17)	180.0(3)
N(1)-C(9)-C(14)-C(17)	2.3(5)
C(11)-C(10)-C(15)-C(16)	-30.2(7)
C(9)-C(10)-C(15)-C(16)	150.9(5)
C(13)-C(14)-C(17)-C(18)	9.4(6)
C(9)-C(14)-C(17)-C(18)	-171.6(4)
C(5)-C(7)-N(1)-C(9)	-166.1(3)
S(1)-C(7)-N(1)-C(9)	12.1(4)
C(14)-C(9)-N(1)-C(7)	-102.8(4)
C(10)-C(9)-N(1)-C(7)	79.4(4)
O(6)-C(6)-O(1)-C(2)	-169.3(2)
C(5)-C(6)-O(1)-C(2)	14.4(4)
O(3)-C(2)-O(1)-C(6)	-47.3(3)
C(22)-C(2)-O(1)-C(6)	-161.7(3)
C(21)-C(2)-O(1)-C(6)	75.0(3)
O(4)-C(4)-O(3)-C(2)	160.2(2)
C(5)-C(4)-O(3)-C(2)	-20.1(3)
O(1)-C(2)-O(3)-C(4)	50.4(3)
C(22)-C(2)-O(3)-C(4)	164.2(2)
C(21)-C(2)-O(3)-C(4)	-72.1(3)
N(1)-C(7)-S(1)-C(8)	-153.6(2)
C(5)-C(7)-S(1)-C(8)	24.5(3)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	(D-H)	d(H..A)	<DHA	d(D..A)	A

N1-H1	0.860	2.191	118.25	2.707	O4
N1-H1	0.860	2.278	142.19	3.004	O6 [-x+1, y+1/2, -z+3/2]

Table S7. Bond lengths [Å] and angles [°] for compound **14**
Code number 989dm3.

C(2)-O(3)	1.428(3)
C(2)-O(1)	1.442(3)
C(2)-C(22)	1.500(4)
C(2)-C(21)	1.504(4)
C(4)-O(4)	1.209(3)
C(4)-O(3)	1.372(3)
C(4)-C(5)	1.443(4)
C(5)-C(7)	1.413(4)
C(5)-C(6)	1.437(4)
C(6)-O(6)	1.224(3)
C(6)-O(1)	1.363(3)
C(7)-N(1)	1.321(3)
C(7)-O(2)	1.325(3)
C(10)-O(2)	1.462(4)
C(11)-C(12)	1.374(4)
C(11)-C(16)	1.374(4)
C(11)-N(1)	1.433(3)
C(12)-C(13)	1.385(4)
C(13)-C(14)	1.366(4)
C(14)-C(15)	1.367(5)
C(15)-C(16)	1.386(4)

O(3)-C(2)-O(1)	109.4(2)
O(3)-C(2)-C(22)	106.6(2)
O(1)-C(2)-C(22)	105.5(2)
O(3)-C(2)-C(21)	111.1(2)
O(1)-C(2)-C(21)	110.4(2)
C(22)-C(2)-C(21)	113.7(3)
O(4)-C(4)-O(3)	116.3(3)
O(4)-C(4)-C(5)	127.4(3)
O(3)-C(4)-C(5)	116.2(2)

C(7)-C(5)-C(6)	119.1(2)
C(7)-C(5)-C(4)	120.7(3)
C(6)-C(5)-C(4)	118.8(2)
O(6)-C(6)-O(1)	115.7(3)
O(6)-C(6)-C(5)	126.9(3)
O(1)-C(6)-C(5)	117.4(2)
N(1)-C(7)-O(2)	113.9(3)
N(1)-C(7)-C(5)	121.9(3)
O(2)-C(7)-C(5)	124.2(2)
C(12)-C(11)-C(16)	119.6(3)
C(12)-C(11)-N(1)	116.1(3)
C(16)-C(11)-N(1)	124.2(3)
C(11)-C(12)-C(13)	120.6(3)
C(14)-C(13)-C(12)	119.3(3)
C(13)-C(14)-C(15)	120.6(3)
C(14)-C(15)-C(16)	120.0(3)
C(11)-C(16)-C(15)	119.8(3)
C(7)-N(1)-C(11)	129.7(3)
C(6)-O(1)-C(2)	118.3(2)
C(7)-O(2)-C(10)	120.7(2)
C(4)-O(3)-C(2)	118.0(2)

Torsion angles [°] for **7** (989dm3).

O(4)-C(4)-C(5)-C(7)	2.9(5)
O(3)-C(4)-C(5)-C(7)	179.1(2)
O(4)-C(4)-C(5)-C(6)	-163.4(3)
O(3)-C(4)-C(5)-C(6)	12.8(4)
C(7)-C(5)-C(6)-O(6)	-4.9(4)
C(4)-C(5)-C(6)-O(6)	161.6(3)
C(7)-C(5)-C(6)-O(1)	176.7(2)
C(4)-C(5)-C(6)-O(1)	-16.8(4)
C(6)-C(5)-C(7)-N(1)	15.6(4)
C(4)-C(5)-C(7)-N(1)	-150.7(3)
C(6)-C(5)-C(7)-O(2)	-165.6(3)
C(4)-C(5)-C(7)-O(2)	28.1(4)
C(16)-C(11)-C(12)-C(13)	2.4(4)
N(1)-C(11)-C(12)-C(13)	-179.8(3)
C(11)-C(12)-C(13)-C(14)	-1.0(5)

C(12)-C(13)-C(14)-C(15)	-0.9(5)
C(13)-C(14)-C(15)-C(16)	1.3(5)
C(12)-C(11)-C(16)-C(15)	-2.0(4)
N(1)-C(11)-C(16)-C(15)	-179.5(3)
C(14)-C(15)-C(16)-C(11)	0.2(5)
O(2)-C(7)-N(1)-C(11)	9.3(4)
C(5)-C(7)-N(1)-C(11)	-171.8(3)
C(12)-C(11)-N(1)-C(7)	148.1(3)
C(16)-C(11)-N(1)-C(7)	-34.3(4)
O(6)-C(6)-O(1)-C(2)	167.1(2)
C(5)-C(6)-O(1)-C(2)	-14.3(4)
O(3)-C(2)-O(1)-C(6)	46.7(3)
C(22)-C(2)-O(1)-C(6)	161.0(2)
C(21)-C(2)-O(1)-C(6)	-75.8(3)
N(1)-C(7)-O(2)-C(10)	-142.1(3)
C(5)-C(7)-O(2)-C(10)	39.0(4)
O(4)-C(4)-O(3)-C(2)	-160.9(3)
C(5)-C(4)-O(3)-C(2)	22.4(3)
O(1)-C(2)-O(3)-C(4)	-51.1(3)
C(22)-C(2)-O(3)-C(4)	-164.6(2)
C(21)-C(2)-O(3)-C(4)	71.0(3)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.933	1.895	137.68	2.660	O6

Table S8. Bond lengths [Å] and angles [°] for compound **15**

Code number cw1168.

C(2)-O(3)	1.428(5)
C(2)-O(1)	1.440(4)
C(2)-C(22)	1.489(5)
C(2)-C(21)	1.499(5)
C(4)-O(4)	1.233(5)
C(4)-O(3)	1.351(5)

C(4)-C(5)	1.440(5)
C(5)-C(6)	1.421(5)
C(5)-C(7)	1.438(5)
C(6)-O(6)	1.233(4)
C(6)-O(1)	1.352(4)
C(7)-N(2)	1.326(4)
C(7)-N(1)	1.343(5)
C(8)-C(13)	1.369(5)
C(8)-C(9)	1.386(6)
C(8)-N(1)	1.424(5)
C(9)-C(10)	1.365(6)
C(10)-C(11)	1.377(6)
C(11)-C(12)	1.363(6)
C(12)-C(13)	1.362(6)
C(14)-N(2)	1.450(5)

O(3)-C(2)-O(1)	108.5(3)
O(3)-C(2)-C(22)	106.4(3)
O(1)-C(2)-C(22)	106.6(3)
O(3)-C(2)-C(21)	110.8(3)
O(1)-C(2)-C(21)	109.9(3)
C(22)-C(2)-C(21)	114.4(4)
O(4)-C(4)-O(3)	116.0(4)
O(4)-C(4)-C(5)	126.6(5)
O(3)-C(4)-C(5)	117.3(4)
C(6)-C(5)-C(7)	120.5(3)
C(6)-C(5)-C(4)	118.7(4)
C(7)-C(5)-C(4)	120.6(4)
O(6)-C(6)-O(1)	116.0(4)
O(6)-C(6)-C(5)	126.2(4)
O(1)-C(6)-C(5)	117.8(3)
N(2)-C(7)-N(1)	120.7(4)
N(2)-C(7)-C(5)	120.1(4)
N(1)-C(7)-C(5)	119.1(3)

C(13)-C(8)-C(9)	119.4(4)
C(13)-C(8)-N(1)	123.2(4)
C(9)-C(8)-N(1)	117.2(4)
C(10)-C(9)-C(8)	119.5(4)
C(9)-C(10)-C(11)	121.0(4)
C(12)-C(11)-C(10)	118.9(5)
C(13)-C(12)-C(11)	121.0(5)
C(12)-C(13)-C(8)	120.4(4)
C(7)-N(1)-C(8)	128.1(3)
C(7)-N(2)-C(14)	126.6(3)
C(6)-O(1)-C(2)	118.1(3)
C(4)-O(3)-C(2)	117.7(3)

Selected torsion angles

170.38 (0.42)	O4 - C4 - C5 - C6
-7.69 (0.51)	O3 - C4 - C5 - C6
-4.79 (0.62)	O4 - C4 - C5 - C7
177.14 (0.33)	O3 - C4 - C5 - C7
8.33 (0.58)	C7 - C5 - C6 - O6
-166.85 (0.35)	C4 - C5 - C6 - O6
-175.18 (0.31)	C7 - C5 - C6 - O1
9.64 (0.50)	C4 - C5 - C6 - O1
5.75 (0.54)	C6 - C5 - C7 - N2
-179.17 (0.34)	C4 - C5 - C7 - N2
-177.96 (0.35)	C6 - C5 - C7 - N1
-2.88 (0.53)	C4 - C5 - C7 - N1
1.48 (0.61)	C13 - C8 - C9 - C10
176.54 (0.38)	N1 - C8 - C9 - C10
-0.10 (0.71)	C8 - C9 - C10 - C11
-0.56 (0.75)	C9 - C10 - C11 - C12
-0.15 (0.74)	C10 - C11 - C12 - C13
1.54 (0.70)	C11 - C12 - C13 - C8
-2.19 (0.61)	C9 - C8 - C13 - C12
-176.94 (0.38)	N1 - C8 - C13 - C12

-32.55 (0.60) N2 - C7 - N1 - C8
151.18 (0.37) C5 - C7 - N1 - C8
-31.83 (0.62) C13 - C8 - N1 - C7
153.31 (0.40) C9 - C8 - N1 - C7
-19.39 (0.62) N1 - C7 - N2 - C14
156.84 (0.41) C5 - C7 - N2 - C14
-162.95 (0.32) O6 - C6 - O1 - C2
20.20 (0.47) C5 - C6 - O1 - C2
-49.10 (0.41) O3 - C2 - O1 - C6
-163.39 (0.35) C22 - C2 - O1 - C6
72.12 (0.45) C21 - C2 - O1 - C6
157.40 (0.36) O4 - C4 - O3 - C2
-24.33 (0.48) C5 - C4 - O3 - C2
51.15 (0.41) O1 - C2 - O3 - C4
165.54 (0.34) C22 - C2 - O3 - C4
-69.50 (0.41) C21 - C2 - O3 - C4

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.860	2.095	121.15	2.645	O4
N2-H2	0.860	1.991	132.93	2.652	O6
N2-H2	0.860	2.518	131.07	3.150	O6 [-x+2, -y, -z+2]

Table S9. Bond lengths [Å] and angles [°] for compound **16**
Code number 1794r31.

C(2)-O(1)	1.428(3)
C(2)-O(3)	1.439(3)
C(2)-C(21)	1.506(4)
C(2)-C(22)	1.507(4)
C(4)-O(4)	1.218(3)
C(4)-O(3)	1.358(3)
C(4)-C(5)	1.439(3)
C(5)-C(7)	1.421(3)
C(5)-C(6)	1.441(3)

C(6)-O(6)	1.211(3)
C(6)-O(1)	1.363(3)
C(7)-N(2)	1.347(3)
C(7)-N(1)	1.349(3)
C(8)-N(2)	1.449(4)
C(9)-N(2)	1.461(4)
C(10)-C(15)	1.384(4)
C(10)-C(11)	1.399(3)
C(10)-N(1)	1.437(3)
C(11)-C(12)	1.396(4)
C(11)-C(16)	1.537(4)
C(12)-C(13)	1.382(5)
C(13)-C(14)	1.363(5)
C(14)-C(15)	1.377(4)
C(16)-C(17)	1.530(4)
C(16)-C(19)	1.535(4)
C(16)-C(18)	1.541(4)

O(1)-C(2)-O(3)	108.2(2)
O(1)-C(2)-C(21)	111.9(2)
O(3)-C(2)-C(21)	111.0(2)
O(1)-C(2)-C(22)	105.9(2)
O(3)-C(2)-C(22)	106.2(2)
C(21)-C(2)-C(22)	113.1(3)
O(4)-C(4)-O(3)	116.2(2)
O(4)-C(4)-C(5)	127.0(2)
O(3)-C(4)-C(5)	116.7(2)
C(7)-C(5)-C(4)	120.1(2)
C(7)-C(5)-C(6)	121.5(2)
C(4)-C(5)-C(6)	117.2(2)
O(6)-C(6)-O(1)	116.9(2)
O(6)-C(6)-C(5)	126.9(3)
O(1)-C(6)-C(5)	116.1(2)
N(2)-C(7)-N(1)	118.6(2)
N(2)-C(7)-C(5)	122.3(2)
N(1)-C(7)-C(5)	119.2(2)
C(15)-C(10)-C(11)	121.3(2)
C(15)-C(10)-N(1)	117.7(2)

C(11)-C(10)-N(1)	121.1(2)
C(12)-C(11)-C(10)	115.5(3)
C(12)-C(11)-C(16)	120.5(2)
C(10)-C(11)-C(16)	124.0(2)
C(13)-C(12)-C(11)	123.3(3)
C(14)-C(13)-C(12)	119.5(3)
C(13)-C(14)-C(15)	119.5(3)
C(14)-C(15)-C(10)	120.9(3)
C(17)-C(16)-C(19)	106.6(2)
C(17)-C(16)-C(11)	110.7(2)
C(19)-C(16)-C(11)	111.7(2)
C(17)-C(16)-C(18)	110.1(2)
C(19)-C(16)-C(18)	106.0(2)
C(11)-C(16)-C(18)	111.4(2)
C(7)-N(1)-C(10)	125.1(2)
C(7)-N(2)-C(8)	123.2(2)
C(7)-N(2)-C(9)	122.8(2)
C(8)-N(2)-C(9)	114.0(2)
C(6)-O(1)-C(2)	118.12(19)
C(4)-O(3)-C(2)	117.21(19)

Torsion angles [°] for **16** (1794r31).

O(4)-C(4)-C(5)-C(7)	14.9(4)
O(3)-C(4)-C(5)-C(7)	-169.7(2)
O(4)-C(4)-C(5)-C(6)	-152.9(3)
O(3)-C(4)-C(5)-C(6)	22.5(3)
C(7)-C(5)-C(6)-O(6)	-15.7(4)
C(4)-C(5)-C(6)-O(6)	151.9(3)
C(7)-C(5)-C(6)-O(1)	168.4(2)
C(4)-C(5)-C(6)-O(1)	-24.0(3)
C(4)-C(5)-C(7)-N(2)	164.2(2)
C(6)-C(5)-C(7)-N(2)	-28.5(4)
C(4)-C(5)-C(7)-N(1)	-16.5(4)
C(6)-C(5)-C(7)-N(1)	150.7(2)
C(15)-C(10)-C(11)-C(12)	1.5(4)
N(1)-C(10)-C(11)-C(12)	-179.3(2)
C(15)-C(10)-C(11)-C(16)	-178.9(3)
N(1)-C(10)-C(11)-C(16)	0.2(4)

C(10)-C(11)-C(12)-C(13)	0.7(4)
C(16)-C(11)-C(12)-C(13)	-178.9(3)
C(11)-C(12)-C(13)-C(14)	-1.5(5)
C(12)-C(13)-C(14)-C(15)	0.1(5)
C(13)-C(14)-C(15)-C(10)	2.0(5)
C(11)-C(10)-C(15)-C(14)	-2.9(4)
N(1)-C(10)-C(15)-C(14)	177.9(3)
C(12)-C(11)-C(16)-C(17)	119.5(3)
C(10)-C(11)-C(16)-C(17)	-60.0(3)
C(12)-C(11)-C(16)-C(19)	0.8(4)
C(10)-C(11)-C(16)-C(19)	-178.7(2)
C(12)-C(11)-C(16)-C(18)	-117.6(3)
C(10)-C(11)-C(16)-C(18)	62.9(3)
N(2)-C(7)-N(1)-C(10)	-37.6(4)
C(5)-C(7)-N(1)-C(10)	143.1(2)
C(15)-C(10)-N(1)-C(7)	-32.7(4)
C(11)-C(10)-N(1)-C(7)	148.1(3)
N(1)-C(7)-N(2)-C(8)	154.0(3)
C(5)-C(7)-N(2)-C(8)	-26.8(4)
N(1)-C(7)-N(2)-C(9)	-24.4(4)
C(5)-C(7)-N(2)-C(9)	154.9(3)
O(6)-C(6)-O(1)-C(2)	169.8(2)
C(5)-C(6)-O(1)-C(2)	-13.9(3)
O(3)-C(2)-O(1)-C(6)	50.3(3)
C(21)-C(2)-O(1)-C(6)	-72.4(3)
C(22)-C(2)-O(1)-C(6)	163.9(2)
O(4)-C(4)-O(3)-C(2)	-167.5(2)
C(5)-C(4)-O(3)-C(2)	16.6(3)
O(1)-C(2)-O(3)-C(4)	-51.7(3)
C(21)-C(2)-O(3)-C(4)	71.5(3)
C(22)-C(2)-O(3)-C(4)	-165.1(3)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.853	1.923	142.84	2.654	O4

Table S10. Bond lengths [A] and angles [deg] for compound **17xH_2O**
Code number1072dm6.

C(2)-O(3)	1.431(6)
C(2)-O(1)	1.430(6)
C(2)-C(21)	1.472(10)
C(2)-C(22)	1.513(12)
C(4)-O(4)	1.218(5)
C(4)-O(3)	1.348(6)
C(4)-C(5)	1.430(6)
C(5)-C(6)	1.406(6)
C(5)-C(7)	1.457(6)
C(6)-O(6)	1.223(5)
C(6)-O(1)	1.362(6)
C(7)-N(2)	1.313(6)
C(7)-N(1)	1.340(6)
C(8)-C(13)	1.367(7)
C(8)-C(9)	1.383(6)
C(8)-N(1)	1.412(6)
C(9)-C(10)	1.375(8)
C(10)-C(11)	1.365(8)
C(11)-C(12)	1.370(9)
C(12)-C(13)	1.367(8)
C(14)-N(2)	1.466(6)
C(15)-N(2)	1.467(7)
O(3)-C(2)-O(1)	109.5(4)
O(3)-C(2)-C(21)	107.0(6)
O(1)-C(2)-C(21)	107.1(6)
O(3)-C(2)-C(22)	108.4(6)
O(1)-C(2)-C(22)	111.5(5)
C(21)-C(2)-C(22)	113.1(7)
O(4)-C(4)-O(3)	116.7(4)
O(4)-C(4)-C(5)	127.4(4)
O(3)-C(4)-C(5)	115.9(4)
C(6)-C(5)-C(4)	120.5(4)
C(6)-C(5)-C(7)	119.4(4)
C(4)-C(5)-C(7)	119.5(4)
O(6)-C(6)-O(1)	116.0(4)
O(6)-C(6)-C(5)	126.4(4)
O(1)-C(6)-C(5)	117.6(4)
N(2)-C(7)-N(1)	118.8(4)
N(2)-C(7)-C(5)	120.7(4)
N(1)-C(7)-C(5)	120.5(4)
C(13)-C(8)-C(9)	120.2(4)
C(13)-C(8)-N(1)	120.8(4)

C(9)-C(8)-N(1)	119.0(4)
C(10)-C(9)-C(8)	119.1(5)
C(11)-C(10)-C(9)	120.5(5)
C(10)-C(11)-C(12)	120.0(5)
C(13)-C(12)-C(11)	120.0(5)
C(12)-C(13)-C(8)	120.1(5)
C(7)-N(1)-C(8)	124.4(4)
C(7)-N(2)-C(14)	121.0(4)
C(7)-N(2)-C(15)	123.5(4)
C(14)-N(2)-C(15)	115.3(4)
C(6)-O(1)-C(2)	117.9(4)
C(4)-O(3)-C(2)	117.6(4)

Torsion angles [deg] for **17xH_2O** (1072dm6).

O(4)-C(4)-C(5)-C(6)	174.6(5)
O(3)-C(4)-C(5)-C(6)	-4.8(6)
O(4)-C(4)-C(5)-C(7)	2.9(7)
O(3)-C(4)-C(5)-C(7)	-176.5(4)
C(4)-C(5)-C(6)-O(6)	-168.4(5)
C(7)-C(5)-C(6)-O(6)	3.3(7)
C(4)-C(5)-C(6)-O(1)	10.7(6)
C(7)-C(5)-C(6)-O(1)	-177.6(4)
C(6)-C(5)-C(7)-N(2)	58.7(6)
C(4)-C(5)-C(7)-N(2)	-129.6(4)
C(6)-C(5)-C(7)-N(1)	-121.3(5)
C(4)-C(5)-C(7)-N(1)	50.5(5)
C(13)-C(8)-C(9)-C(10)	-1.6(7)
N(1)-C(8)-C(9)-C(10)	-179.6(5)
C(8)-C(9)-C(10)-C(11)	0.4(8)
C(9)-C(10)-C(11)-C(12)	1.8(8)
C(10)-C(11)-C(12)-C(13)	-2.9(8)
C(11)-C(12)-C(13)-C(8)	1.7(7)
C(9)-C(8)-C(13)-C(12)	0.5(6)
N(1)-C(8)-C(13)-C(12)	178.5(4)
N(2)-C(7)-N(1)-C(8)	-166.9(4)
C(5)-C(7)-N(1)-C(8)	13.1(6)
C(13)-C(8)-N(1)-C(7)	53.0(6)
C(9)-C(8)-N(1)-C(7)	-129.0(5)
N(1)-C(7)-N(2)-C(14)	5.8(6)
C(5)-C(7)-N(2)-C(14)	-174.1(4)
N(1)-C(7)-N(2)-C(15)	-169.2(4)
C(5)-C(7)-N(2)-C(15)	10.9(6)
O(6)-C(6)-O(1)-C(2)	-164.6(5)
C(5)-C(6)-O(1)-C(2)	16.2(7)
O(3)-C(2)-O(1)-C(6)	-45.7(7)
C(21)-C(2)-O(1)-C(6)	-161.4(6)
C(22)-C(2)-O(1)-C(6)	74.3(6)
O(4)-C(4)-O(3)-C(2)	152.8(5)
C(5)-C(4)-O(3)-C(2)	-27.8(7)

O(1)-C(2)-O(3)-C(4)	52.2(7)
C(21)-C(2)-O(3)-C(4)	168.0(6)
C(22)-C(2)-O(3)-C(4)	-69.7(6)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.790	2.127	151.33	2.845	O20 [x+1/2, -y, z-1/2]
O20-H21	0.879	2.090	151.87	2.895	O4
O20-H22	0.991	1.906	164.63	2.874	O6 [x-1/2, -y+1, z+1/2]

Table S11. Bond lengths [A] and angles [deg] for compound **18xTHF**
Code number 975dm1.

N(1)-C(7)	1.333(5)
N(1)-C(8)	1.432(5)
N(2)-C(7)	1.319(5)
N(2)-C(17)	1.457(5)
N(2)-C(18)	1.465(5)
C(2)-O(1)	1.424(6)
C(2)-O(3)	1.431(5)
C(2)-C(21)	1.516(7)
C(2)-C(22)	1.516(6)
C(4)-O(4)	1.216(5)
C(4)-O(3)	1.375(5)
C(4)-C(5)	1.420(5)
C(5)-C(6)	1.416(5)
C(5)-C(7)	1.461(5)
C(6)-O(6)	1.215(5)
C(6)-O(1)	1.376(5)
C(8)-C(9)	1.394(6)
C(8)-C(13)	1.395(6)
C(9)-C(10)	1.390(7)
C(9)-C(14)	1.529(7)
C(10)-C(11)	1.387(7)
C(11)-C(12)	1.373(7)
C(11)-C(15)	1.514(7)
C(12)-C(13)	1.391(7)
C(13)-C(16)	1.497(6)
O(2A)-C(1A)	1.360(18)
O(2A)-C(4A)	1.380(18)
C(1A)-C(2A)	1.430(17)
C(2A)-C(3A)	1.372(18)

C(3A)-C(4A)	1.315(17)
O(2B)-C(1B)	1.40(2)
O(2B)-C(4B)	1.438(19)
C(1B)-C(2B)	1.43(2)
C(1B)-C(4B)	1.87(4)
C(2B)-C(3B)	1.41(2)
C(3B)-C(4B)	1.44(2)

C(7)-N(1)-C(8)	125.6(3)
C(7)-N(2)-C(17)	121.5(3)
C(7)-N(2)-C(18)	122.5(3)
C(17)-N(2)-C(18)	115.8(3)
O(1)-C(2)-O(3)	109.6(3)
O(1)-C(2)-C(21)	111.2(4)
O(3)-C(2)-C(21)	109.9(4)
O(1)-C(2)-C(22)	106.3(4)
O(3)-C(2)-C(22)	106.1(4)
C(21)-C(2)-C(22)	113.5(4)
O(4)-C(4)-O(3)	116.7(3)
O(4)-C(4)-C(5)	127.2(4)
O(3)-C(4)-C(5)	116.0(4)
C(6)-C(5)-C(4)	121.0(4)
C(6)-C(5)-C(7)	118.2(3)
C(4)-C(5)-C(7)	120.5(3)
O(6)-C(6)-O(1)	116.1(4)
O(6)-C(6)-C(5)	127.0(4)
O(1)-C(6)-C(5)	116.7(4)
N(2)-C(7)-N(1)	118.6(3)
N(2)-C(7)-C(5)	121.7(3)
N(1)-C(7)-C(5)	119.7(4)
C(9)-C(8)-C(13)	121.5(4)
C(9)-C(8)-N(1)	118.9(4)
C(13)-C(8)-N(1)	119.4(4)
C(10)-C(9)-C(8)	117.9(4)
C(10)-C(9)-C(14)	120.5(4)
C(8)-C(9)-C(14)	121.6(4)
C(11)-C(10)-C(9)	122.2(4)
C(12)-C(11)-C(10)	117.9(4)
C(12)-C(11)-C(15)	121.7(6)
C(10)-C(11)-C(15)	120.4(5)
C(11)-C(12)-C(13)	122.7(5)
C(12)-C(13)-C(8)	117.7(4)
C(12)-C(13)-C(16)	120.0(4)
C(8)-C(13)-C(16)	122.3(4)
C(6)-O(1)-C(2)	117.9(3)
C(4)-O(3)-C(2)	118.0(3)
C(1A)-O(2A)-C(4A)	115(2)
O(2A)-C(1A)-C(2A)	98.7(18)
C(3A)-C(2A)-C(1A)	106.1(17)
C(4A)-C(3A)-C(2A)	113(2)

C(3A)-C(4A)-O(2A)	101(2)
C(1B)-O(2B)-C(4B)	82(2)
O(2B)-C(1B)-C(2B)	101.6(16)
O(2B)-C(1B)-C(4B)	49.7(13)
C(2B)-C(1B)-C(4B)	80.6(13)
C(3B)-C(2B)-C(1B)	99.8(15)
C(2B)-C(3B)-C(4B)	98.4(15)
O(2B)-C(4B)-C(3B)	101.0(17)
O(2B)-C(4B)-C(1B)	47.9(12)
C(3B)-C(4B)-C(1B)	81.2(12)

Torsion angles [deg] for **18xTHF** (975dm1).

O(4)-C(4)-C(5)-C(6)	-169.5(4)
O(3)-C(4)-C(5)-C(6)	9.0(6)
O(4)-C(4)-C(5)-C(7)	3.9(7)
O(3)-C(4)-C(5)-C(7)	-177.6(3)
C(4)-C(5)-C(6)-O(6)	164.3(5)
C(7)-C(5)-C(6)-O(6)	-9.2(7)
C(4)-C(5)-C(6)-O(1)	-10.0(6)
C(7)-C(5)-C(6)-O(1)	176.5(4)
C(17)-N(2)-C(7)-N(1)	-10.9(5)
C(18)-N(2)-C(7)-N(1)	165.2(3)
C(17)-N(2)-C(7)-C(5)	170.5(4)
C(18)-N(2)-C(7)-C(5)	-13.4(5)
C(8)-N(1)-C(7)-N(2)	165.3(3)
C(8)-N(1)-C(7)-C(5)	-16.1(5)
C(6)-C(5)-C(7)-N(2)	117.5(4)
C(4)-C(5)-C(7)-N(2)	-56.1(5)
C(6)-C(5)-C(7)-N(1)	-61.0(5)
C(4)-C(5)-C(7)-N(1)	125.4(4)
C(7)-N(1)-C(8)-C(9)	117.4(4)
C(7)-N(1)-C(8)-C(13)	-67.4(5)
C(13)-C(8)-C(9)-C(10)	2.4(6)
N(1)-C(8)-C(9)-C(10)	177.5(4)
C(13)-C(8)-C(9)-C(14)	-176.1(4)
N(1)-C(8)-C(9)-C(14)	-0.9(6)
C(8)-C(9)-C(10)-C(11)	0.9(7)
C(14)-C(9)-C(10)-C(11)	179.4(5)
C(9)-C(10)-C(11)-C(12)	-3.2(7)
C(9)-C(10)-C(11)-C(15)	177.2(5)
C(10)-C(11)-C(12)-C(13)	2.4(7)
C(15)-C(11)-C(12)-C(13)	-178.0(5)
C(11)-C(12)-C(13)-C(8)	0.7(7)
C(11)-C(12)-C(13)-C(16)	-178.7(4)
C(9)-C(8)-C(13)-C(12)	-3.2(6)
N(1)-C(8)-C(13)-C(12)	-178.3(4)
C(9)-C(8)-C(13)-C(16)	176.2(4)

N(1)-C(8)-C(13)-C(16)	1.1(6)
O(6)-C(6)-O(1)-C(2)	164.8(4)
C(5)-C(6)-O(1)-C(2)	-20.2(6)
O(3)-C(2)-O(1)-C(6)	48.3(5)
C(21)-C(2)-O(1)-C(6)	-73.4(5)
C(22)-C(2)-O(1)-C(6)	162.7(4)
O(4)-C(4)-O(3)-C(2)	-159.3(4)
C(5)-C(4)-O(3)-C(2)	22.0(5)
O(1)-C(2)-O(3)-C(4)	-49.5(5)
C(21)-C(2)-O(3)-C(4)	73.0(5)
C(22)-C(2)-O(3)-C(4)	-163.9(4)
C(4A)-O(2A)-C(1A)-C(2A)	27(3)
O(2A)-C(1A)-C(2A)-C(3A)	-21(2)
C(1A)-C(2A)-C(3A)-C(4A)	10(3)
C(2A)-C(3A)-C(4A)-O(2A)	6(3)
C(1A)-O(2A)-C(4A)-C(3A)	-22(4)
C(4B)-O(2B)-C(1B)-C(2B)	-67(3)
O(2B)-C(1B)-C(2B)-C(3B)	45(4)
C(4B)-C(1B)-C(2B)-C(3B)	0(3)
C(1B)-C(2B)-C(3B)-C(4B)	1(4)
C(1B)-O(2B)-C(4B)-C(3B)	67(3)
C(2B)-C(3B)-C(4B)-O(2B)	-44(4)
C(2B)-C(3B)-C(4B)-C(1B)	0(3)
C(2B)-C(1B)-C(4B)-O(2B)	114(3)
O(2B)-C(1B)-C(4B)-C(3B)	-114(3)
C(2B)-C(1B)-C(4B)-C(3B)	0(3)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.836	2.079	151.42	2.842	O4 [-x+1/2, y+1/2, -z+1/2]

Table S12. Bond lengths [Å] and angles [°] for compound **19xH_2O**

Code numbercw2169.

C(2)-O(1)#1	1.427(3)
C(2)-O(1)	1.427(3)
C(2)-C(21)	1.497(6)
C(2)-C(22)	1.504(5)
C(5)-C(6)	1.397(3)
C(5)-C(6)#1	1.397(3)
C(5)-C(7)	1.484(5)

C(6)-O(6)	1.230(3)
C(6)-O(1)	1.368(3)
C(7)-N(2)	1.310(4)
C(7)-N(1)	1.319(4)
C(8)-N(1)	1.492(5)
C(8)-C(9)	1.516(4)
C(8)-C(9)#1	1.516(4)
C(8)-C(10)	1.518(6)
C(11)-C(12)#1	1.436(7)
C(11)-C(12)	1.436(7)
C(11)-N(2)	1.490(4)
C(11)-C(13)#1	1.522(8)
C(11)-C(13)	1.522(8)
C(11)-C(14)#1	1.537(9)
C(11)-C(14)	1.537(9)
C(12)-C(14)#1	1.295(13)
C(12)-C(13)#1	1.507(16)
C(13)-C(13)#1	1.36(2)
C(13)-C(12)#1	1.507(16)
C(14)-C(12)#1	1.295(13)
C(14)-C(14)#1	1.542(18)

O(1)#1-C(2)-O(1)	111.0(3)
O(1)#1-C(2)-C(21)	110.22(18)
O(1)-C(2)-C(21)	110.22(18)
O(1)#1-C(2)-C(22)	107.08(18)
O(1)-C(2)-C(22)	107.08(18)
C(21)-C(2)-C(22)	111.1(3)
C(6)-C(5)-C(6)#1	122.4(3)
C(6)-C(5)-C(7)	118.07(14)
C(6)#1-C(5)-C(7)	118.07(14)
O(6)-C(6)-O(1)	116.54(19)
O(6)-C(6)-C(5)	126.8(2)
O(1)-C(6)-C(5)	116.61(19)

N(2)-C(7)-N(1)	115.1(3)
N(2)-C(7)-C(5)	122.0(3)
N(1)-C(7)-C(5)	122.9(3)
N(1)-C(8)-C(9)	111.33(19)
N(1)-C(8)-C(9)#1	111.3(2)
C(9)-C(8)-C(9)#1	109.3(3)
N(1)-C(8)-C(10)	104.4(3)
C(9)-C(8)-C(10)	110.2(2)
C(9)#1-C(8)-C(10)	110.2(2)
C(12)#1-C(11)-C(12)	145.1(7)
C(12)#1-C(11)-N(2)	107.4(3)
C(12)-C(11)-N(2)	107.4(3)
C(12)#1-C(11)-C(13)#1	111.9(7)
C(12)-C(11)-C(13)#1	61.2(7)
N(2)-C(11)-C(13)#1	105.4(4)
C(12)#1-C(11)-C(13)	61.2(7)
C(12)-C(11)-C(13)	111.9(7)
N(2)-C(11)-C(13)	105.4(4)
C(13)#1-C(11)-C(13)	53.2(10)
C(12)#1-C(11)-C(14)#1	109.5(7)
C(12)-C(11)-C(14)#1	51.5(5)
N(2)-C(11)-C(14)#1	114.1(3)
C(13)#1-C(11)-C(14)#1	108.5(6)
C(13)-C(11)-C(14)#1	140.1(5)
C(12)#1-C(11)-C(14)	51.5(5)
C(12)-C(11)-C(14)	109.5(7)
N(2)-C(11)-C(14)	114.1(3)
C(13)#1-C(11)-C(14)	140.1(5)
C(13)-C(11)-C(14)	108.5(6)
C(14)#1-C(11)-C(14)	60.2(8)
C(14)#1-C(12)-C(11)	68.3(5)
C(14)#1-C(12)-C(13)#1	124.6(7)
C(11)-C(12)-C(13)#1	62.2(5)
C(13)#1-C(13)-C(12)#1	117.2(5)

C(13)#1-C(13)-C(11)	63.4(5)
C(12)#1-C(13)-C(11)	56.6(4)
C(12)#1-C(14)-C(11)	60.2(5)
C(12)#1-C(14)-C(14)#1	117.5(5)
C(11)-C(14)-C(14)#1	59.9(4)
C(7)-N(1)-C(8)	132.0(3)
C(7)-N(2)-C(11)	135.1(3)
C(6)-O(1)-C(2)	118.13(18)

Selected torsion angles

-170.29 (0.18) C6_$1 - C5 - C6 - O6
-4.44 (0.40) C7 - C5 - C6 - O6
6.86 (0.43) C6_$1 - C5 - C6 - O1
172.71 (0.23) C7 - C5 - C6 - O1
-83.23 (0.22) C6 - C5 - C7 - N2
83.23 (0.22) C6_$1 - C5 - C7 - N2
96.77 (0.22) C6 - C5 - C7 - N1
-96.77 (0.22) C6_$1 - C5 - C7 - N1
66.80 (1.76) C12_$1 - C11 - C12 - C14_$1
-107.31 (0.50) N2 - C11 - C12 - C14_$1
154.31 (0.70) C13_$1 - C11 - C12 - C14_$1
137.49 (0.69) C13 - C11 - C12 - C14_$1
17.06 (0.49) C14 - C11 - C12 - C14_$1
-87.51 (1.75) C12_$1 - C11 - C12 - C13_$1
98.38 (0.51) N2 - C11 - C12 - C13_$1
-16.82 (0.52) C13 - C11 - C12 - C13_$1
-154.31 (0.70) C14_$1 - C11 - C12 - C13_$1
-137.25 (0.61) C14 - C11 - C12 - C13_$1
160.42 (0.40) C12_$1 - C11 - C13 - C13_$1
18.46 (0.44) C12 - C11 - C13 - C13_$1
-97.93 (0.31) N2 - C11 - C13 - C13_$1
74.02 (0.98) C14_$1 - C11 - C13 - C13_$1
139.46 (0.45) C14 - C11 - C13 - C13_$1
-141.97 (0.83) C12 - C11 - C13 - C12_$1

101.64 (0.46) N2 - C11 - C13 - C12_$1
-160.42 (0.41) C13_$1 - C11 - C13 - C12_$1
-86.40 (1.18) C14_$1 - C11 - C13 - C12_$1
-20.96 (0.58) C14 - C11 - C13 - C12_$1
146.08 (0.81) C12 - C11 - C14 - C12_$1
-93.56 (0.49) N2 - C11 - C14 - C12_$1
77.95 (1.25) C13_$1 - C11 - C14 - C12_$1
23.62 (0.64) C13 - C11 - C14 - C12_$1
161.42 (0.43) C14_$1 - C11 - C14 - C12_$1
-161.42 (0.43) C12_$1 - C11 - C14 - C14_$1
-15.34 (0.39) C12 - C11 - C14 - C14_$1
105.02 (0.33) N2 - C11 - C14 - C14_$1
-83.48 (1.07) C13_$1 - C11 - C14 - C14_$1
-137.80 (0.47) C13 - C11 - C14 - C14_$1
180.00 (0.00) N2 - C7 - N1 - C8
0.00 (0.00) C5 - C7 - N1 - C8
-61.13 (0.22) C9 - C8 - N1 - C7
61.13 (0.22) C9_$1 - C8 - N1 - C7
180.00 (0.00) C10 - C8 - N1 - C7
180.00 (0.00) N1 - C7 - N2 - C11
0.00 (0.00) C5 - C7 - N2 - C11
-88.24 (0.57) C12_$1 - C11 - N2 - C7
88.24 (0.57) C12 - C11 - N2 - C7
152.31 (0.55) C13_$1 - C11 - N2 - C7
-152.31 (0.55) C13 - C11 - N2 - C7
33.33 (0.47) C14_$1 - C11 - N2 - C7
-33.33 (0.47) C14 - C11 - N2 - C7
-162.24 (0.23) O6 - C6 - O1 - C2
20.31 (0.31) C5 - C6 - O1 - C2
-44.98 (0.32) O1_$1 - C2 - O1 - C6
77.44 (0.29) C21 - C2 - O1 - C6
-161.54 (0.26) C22 - C2 - O1 - C6

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1	0.860	2.062	164.84	2.901	O2 [x, y, z+1]
N2-H2	0.860	2.204	159.47	3.024	O2 [x, y, z+1]
O2-H11	0.949	1.895	156.51	2.791	O6 [-x+3/2, -y+3/2, z-1/2]

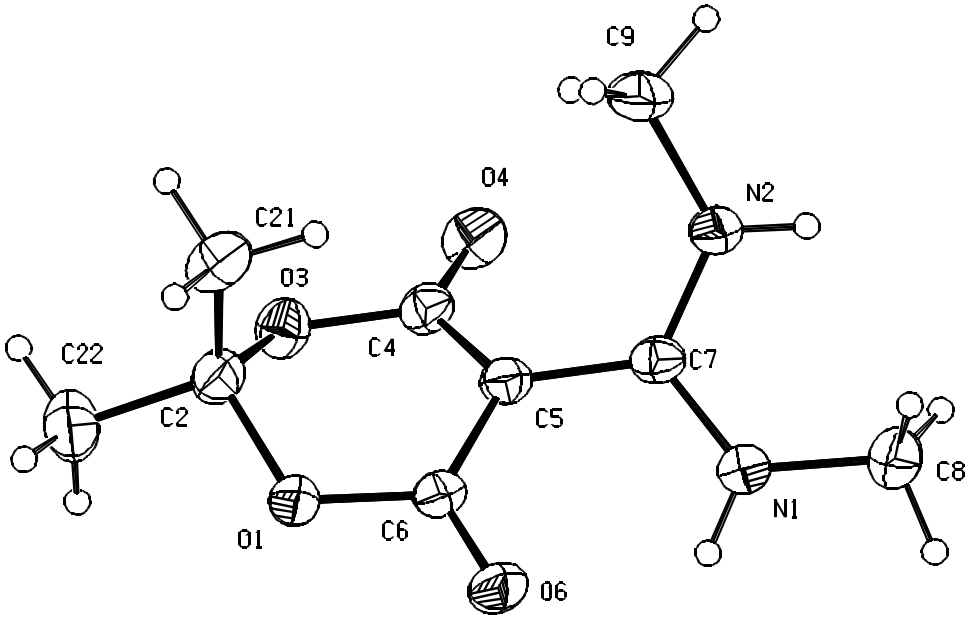

Figure S1. View of compound **10**

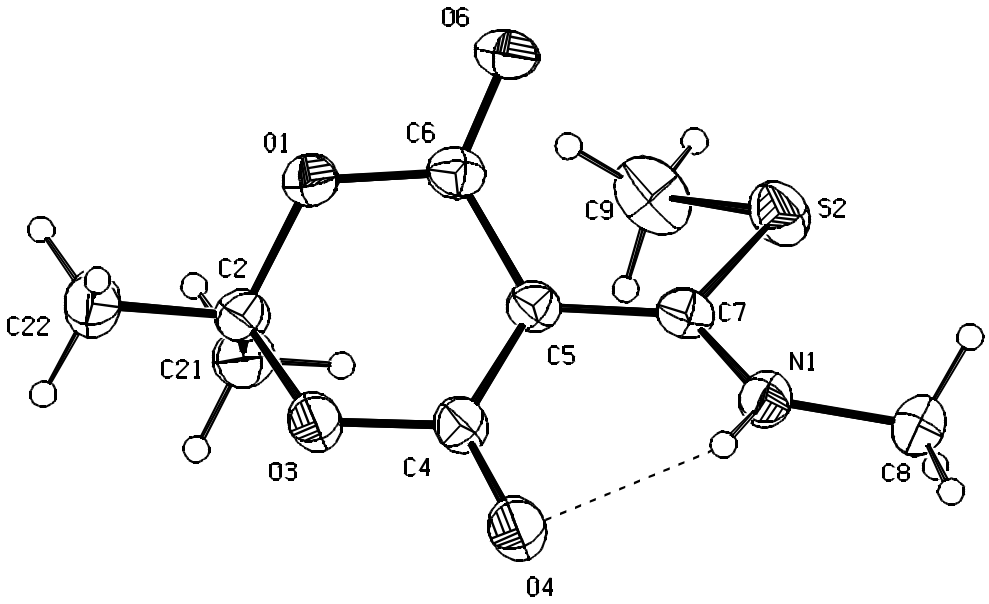

Figure S2. View of compound **11**

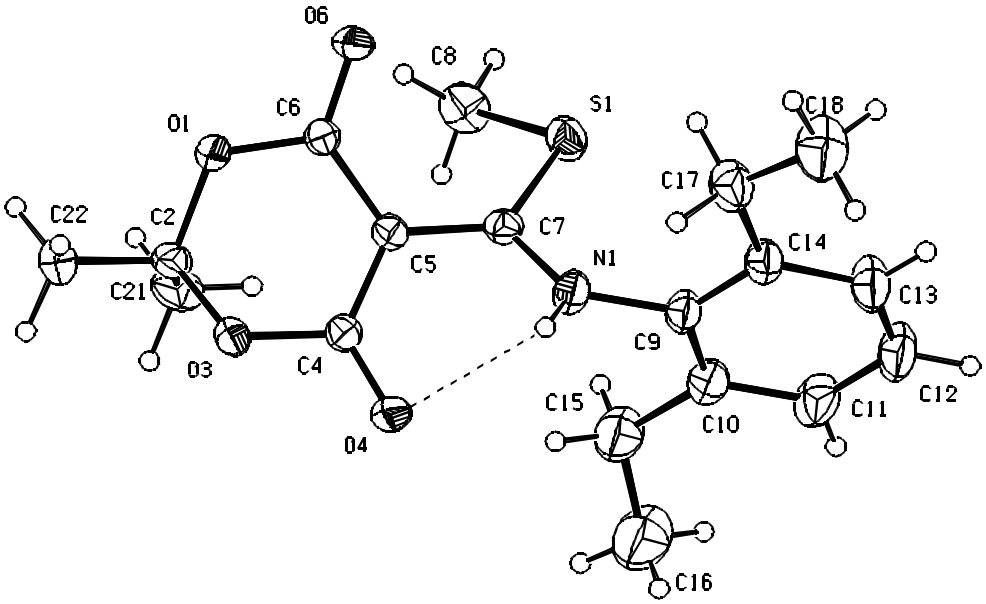

Figure S3. View of compound **13**

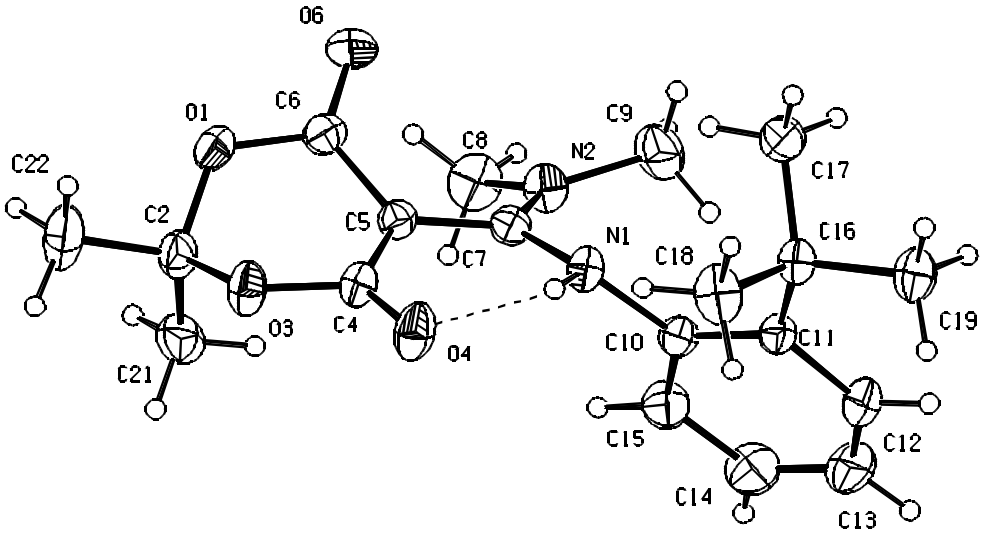

Figure S4. View of compound **16**

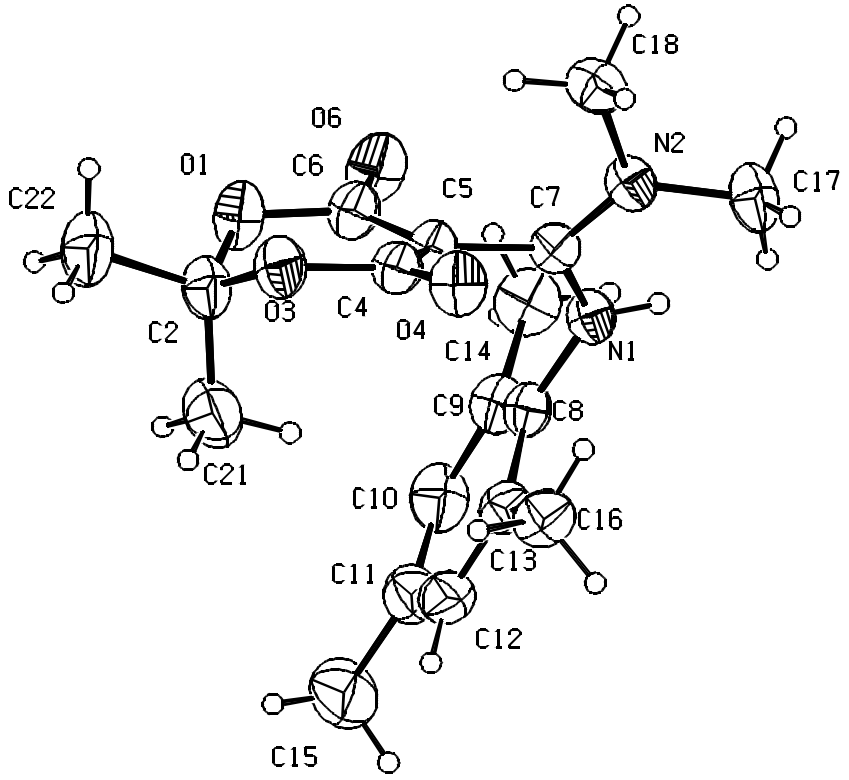

Figure S5. View of compound **18**

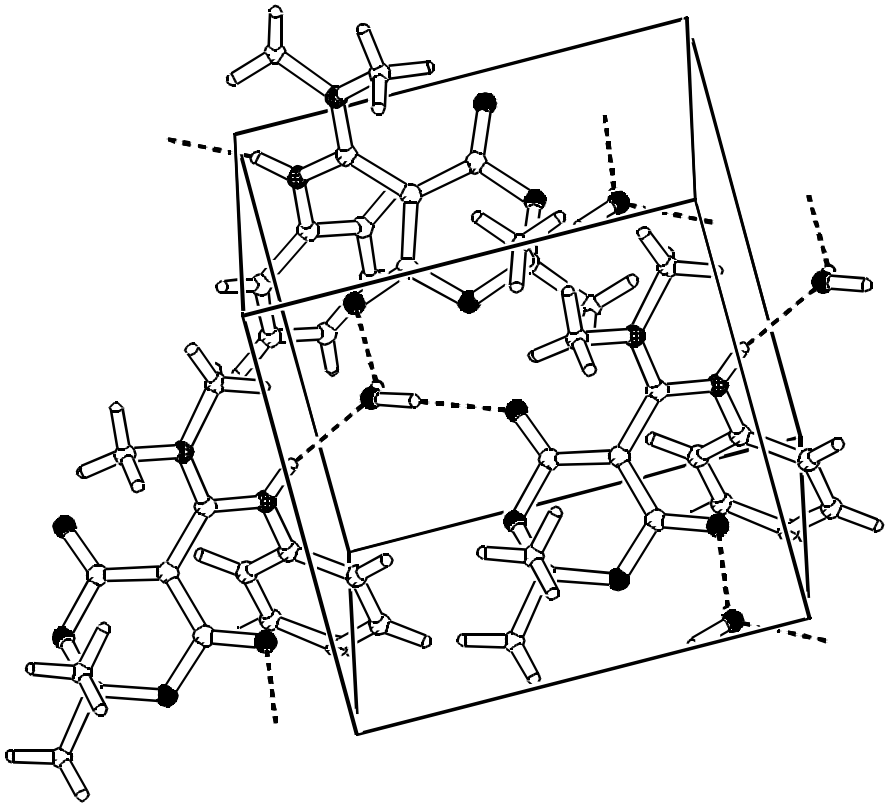

Figure S6. Packing diagram for **(17).H_2O** showing H-bonding

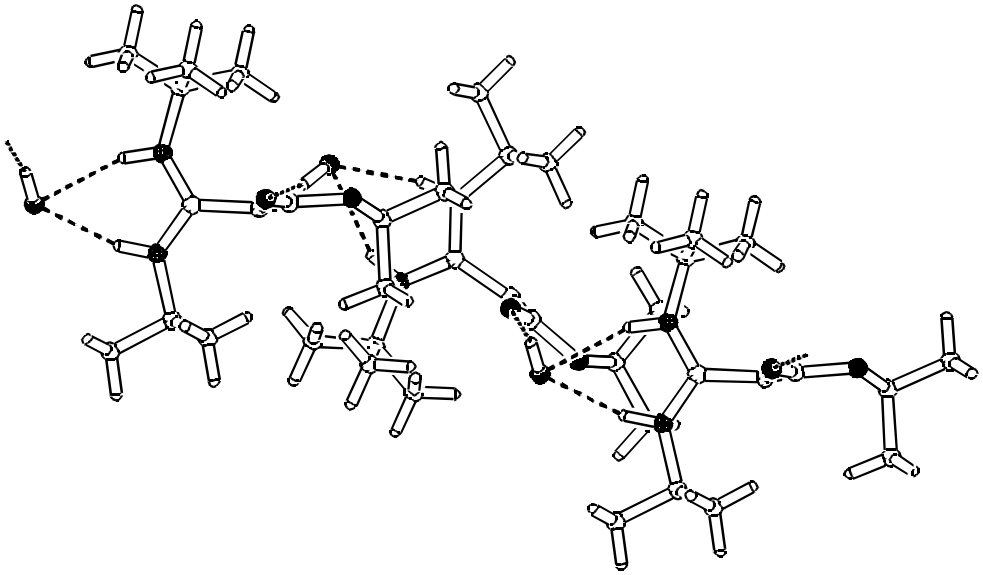

Figure S7. Packing diagram for **(19).H_2O** showing H-bonding