

Table 1 Conformational descriptors of the central and peripheral five-membered rings (torsion angles, degrees)

(Intra-ring) torsions are numbered as follows, oxygen atoms *italicized*

Central rings	Peripheral rings

The two values in each entry are for molecules $m = 1, 2$

Rings A						
Ring mn	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>	
m1	-23.7(6), -32.5(7)	30.1(6), 36.1(3)	-23.8(7), -23.6(7)	7.4(7), 1.5(7)	10.0(6), 18.2(6)	
m2	-35.9(6), -29.7(6)	36.4(7), 32.8(6)	-21.0(7), -21.3(7)	-2.7(7), 1.2(7)	22.7(6), 16.9(6)	
m3	-35.1(5), -37.1(6)	37.4(6), 36.7(7)	-23.3(6), -19.7(7)	-0.2(6), -4.7(6)	20.7(6), 24.2(6)	
m4	-35.8(6), -37.8(5)	36.7(7), 39.6(6)	-19.6(7), -24.0(7)	-5.5(7), -1.2(7)	25.3(6), 23.1(6)	
m5	-39.7(6), -37.2(7)	39.1(6), 27.5(7)	-21.8(7), -5.9(7)	-4.4(7), -18.5(7)	25.7(6), 32.8(6)	
Rings B						
	<i>f</i>	<i>g</i>	<i>h</i>	<i>i</i>	<i>j</i>	
m1	8.7(8), 1.8(5)	11.0(7), 16.7(5)	-27.7(6), -29.6(6)	33.0(6), 30.0(8)	-25.4(7),	-
						19.9(6)
m2	-4.7(5), 4.9(7)	23.8(6), 16.8(7)	-34.6(6), -33.0(7)	31.7(6), 36.4(7)	-16.1(6),	-
						25.2(7)
m3	0.8(7), -6.0(5)	20.9(7), 25.1(5)	-35.5(7), -35.5(5)	36.1(7), 31.4(6)	-22.4(7),	-
						15.6(6)
m4	-7.6(5), 0.0(7)	25.4(5), 21.8(7)	-34.3(6), -36.2(7)	29.5(6), 36.4(7)	-13.4(6),	-
						22.2(7)
m5	-3.3(7), -21.6(5)	22.9(7), 28.4(5)	-34.3(7), -24.7(6)	32.2(8), 9.9(6)	-17.6(8), 7.2(6)	
Rings C						
	<i>k</i>	<i>l</i>	<i>m</i>	<i>n</i>	<i>o</i>	
m1	9.7(6), -17.4(10)*	12.8(6), -3.0(13)*	-31.5(6), 24.8(13)*	36.7(6), -33.9(10)*	-28.5(6),	
						32.0(8)*
m2	-36.6(8)*, -19.2(8)	27.7(10)*, -3.2(9)	-6.9(11)*, 26.4(10)	-15.6(9)*, -36.3(9)	32.6(7), 34.3(8)	

m3	-18.3(6), -35.8(7)	-3.6(6), 19.8(7)	26.3(7), 5.9(8)	-36.5(7), -26.8(7)	33.4(67), 37.9(7)
m4	-30.3(8), -20.6(6)	21.1(8), -2.1(7)	-1.8(8), 25.9(7)	-16.8(8), -38.0(7)	28.6(7), 35.5(6)
m5	-21.2(6), -32.7(7)	-1.0(6), 13.4(8)	24.9(9), 13.5(8)	-37.1(7), -32.2(7)	35.6(6), 39.2(7)

- -3.1(11), 24.8(15), -33.5(15), 30.8(13), -16.0(10) (ring 21); -8.5(9), -16.9(9), 37.9(9), -43.9(8), (-) (ring 22) are the counterpart values for the disordered components.