SUPPLEMENTARY MATERIAL

CHIRAL ACTION AT A DISTANCE: REMOTE SUBSTITUENT EFFECTS ON THE OPTICAL ACTIVITY OF CALYCULINS A AND B

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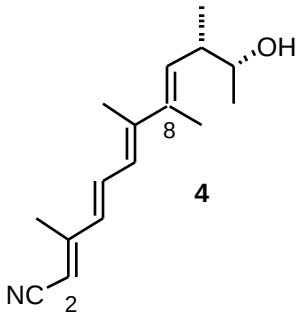
Minimized dihedral angles for calyculin fragment 4:



4

Dihedral Angle	X-Ray Structure[1]	MM2*	**HF 6-31G****
C1-C2-C3-C4	2.2	0.2	0.0
C2-C3-C4-C5	176.8	181.1	180.1
C3-C4-C5-C6	175.4	178.6	179.9
C4-C5-C6-C7	178.8	167.8	180.7
C5-C6-C7-C8	177.0	178.9	178.7
C6-C7-C8-C9	186.5	213.2	190.2

Dihedral Angle	**DFT (B3LYP, 631G*)**	MP2(6-31G)	**MP2(6-31G*)**
C1-C2-C3-C4	0.1	0.1	0.1
C2-C3-C4-C5	180.4	180.2	180.2
C3-C4-C5-C6	180.1	179.8	179.8
C4-C5-C6-C7	180.1	180.0	180.6
C5-C6-C7-C8	179.5	178.2	178.1
C6-C7-C8-C9	184.9	198.6	194.2

[1] Kato, Y.; Fusetani, N.; Matsunaga, S.; Hashimoto, K.; Fujita, S.; Furuya, T. *J. Am. Chem. Soc.* **1986**, *108*, 2780.