

**Table S2** Main geometric parameters of Chl *a* and  $\beta$ -Car.

	Chl <i>a</i>		$\beta$ -Car	
Interatomic distance	R(2,7)	1.3768	R(5,6)	1.3565
	R(2,37)	1.4121	R(6,7)	1.4702
	R(3,10)	1.3913	R(7,8)	1.3545
	R(3,18)	1.409	R(8,9)	1.4512
	R(6,7)	1.3742	R(9,10)	1.3684
	R(6,7)	1.3742	R(10,11)	1.4334
	R(7,8)	1.5152	R(11,16)	1.3647
	R(8,9)	1.5476	R(16,17)	1.4412
	R(9,10)	1.5258	R(17,18)	1.3734
			R(18,19)	1.4277
		R(19,20)	1.3688	
Dihedral angle	D(37,2,7,6)	3.3702	D(7,8,9,15)	1.0031
	D(2,7,8,9)	-165.507	D(15,9,10,11)	-0.0248
	D(7,6,10,3)	-179.69	D(11,16,17,35)	0.0737
	D(18,3,10,6)	2.0755	D(35,17,18,19)	-0.1153
	D(18,3,10,9)	-173.856		
	D(21,17,18,3)	178.3279		