

Table S3 ADCH charges of Chl *a* and β -Car.

	Chl <i>a</i>		β -Car	
	Atom number	Charge	Atom number	Charge
The 10 most nucleophilic sites	33(N)	-1.38892	27(C)	-0.299
	17(N)	-1.32207	8(C)	-0.27114
	25(N)	-1.04662	13(C)	-0.26381
	6(N)	-0.84214	39(C)	-0.2638
	40(O)	-0.36304	14(C)	-0.261
	15(O)	-0.33233	40(C)	-0.26098
	54(C)	-0.26199	38(C)	-0.25166
	32(C)	-0.2606	12(C)	-0.25161
	59(C)	-0.2571	37(C)	-0.24612
	38(C)	-0.24565	36(C)	-0.24593
The 10 most electrophilic sites	37(C)	0.045864	—	—
	34(C)	0.048415	—	—
	26(C)	0.063676	—	—
	7(C)	0.087852	—	—
	18(C)	0.089661	—	—
	10(C)	0.095933	—	—
	21(C)	0.103877	34(C)	0.012958
	14(C)	0.174205	1(C)	0.013084
	39(C)	0.182005	9(C)	0.029998
1(Mg)	4.055369	26(C)	0.035806	