Supporting Information for

Stereochemical Determination of the Unique Acrylate Moiety at the 17-Position in Chlorophylls-*c* from a Diatom *Chaetoseros calcitrans* and Its Effect upon Electronic Absorption Properties

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Table S1. The red-shift values $\Delta\lambda$s[a] of absorption maxima induced by esterification at the 17^2-COOH as well as $8^1,8^2$- and $17^1,17^2$-dehydrogenations of natural Chls-*c* and their analogs.

	Δλ / nm		
	Soret	Qx	Qy
Esterification			
Chl-c_1 → Chl-c_1-phy	2.4	0.6	0.4
Chl-c_2 → Chl-c_2-phy	2.0	0.8	0.6
$8^1,8^2$-Dehydrogenation			
Chl-c_1 → Chl-c_2	3.8	3.0	1.4
Chl-c_1-phy → Chl-c_2-phy	3.6	3.2	1.6
PChl-*a* → 8-vinyl-PChl-*a*	5.6	3.0	2.0
$17^1,17^2$-Dehydrogenation			
Chl-c_1-phy → PChl-*a*	15.0	7.2	5.6
Chl-c_2-phy → 8-vinyl-PChl-*a*	13.0	7.4	5.2

[a]All $\Delta\lambda$s were calculated using λ_{max} from Table 2.

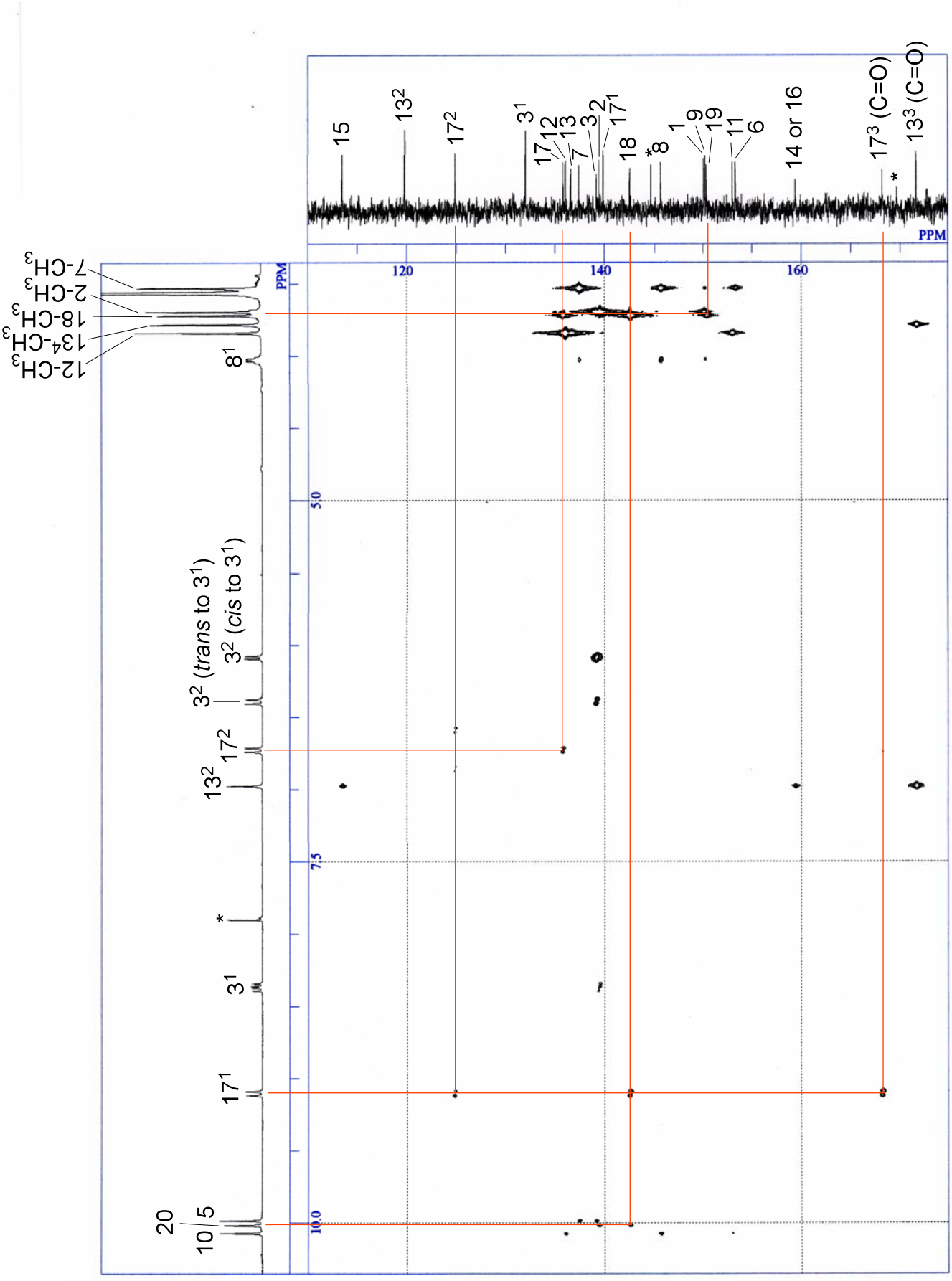

Figure S1. Partial HMBC spectrum ($^{n}J_{CH}$ = 10Hz) of Chl-c_1 in THF-d_8 at room temperature. The key correlations to assign the 17^1-H and 17^2-H in the acrylate are indicated by the red lines. Impurities are indicated by asterisks.

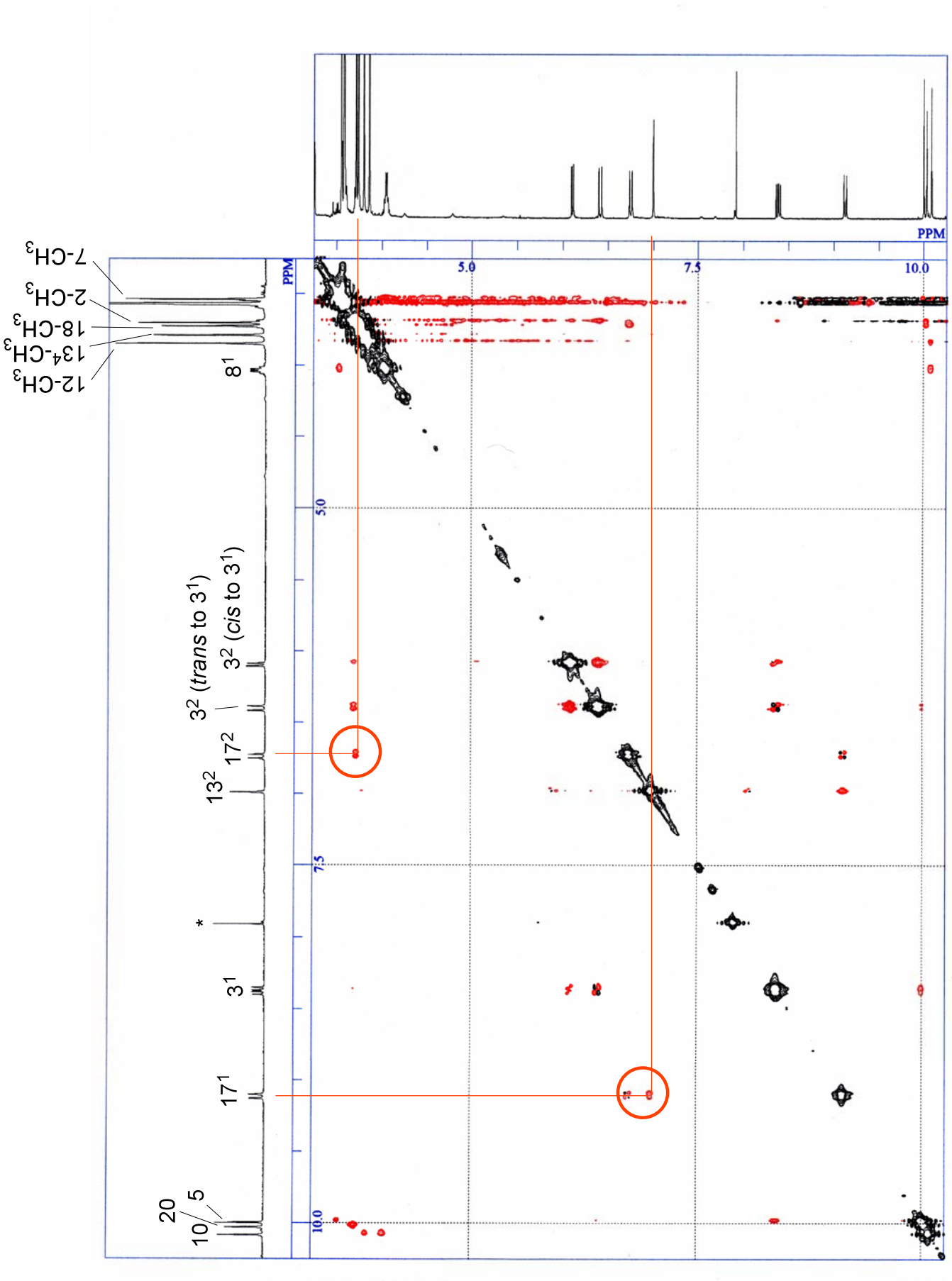

Figure S2. Partial NOESY spectrum (τ_m = 600 msec) of Chl-c_1 in THF-d_8 at room temperature. The two NOE correlations identifying the conformation of the 17-acrylate, 17^1-H/13^2-H and 17^2-H/18-CH_3 are indicated by the red circles. An impurity is indicated by an asterisk.

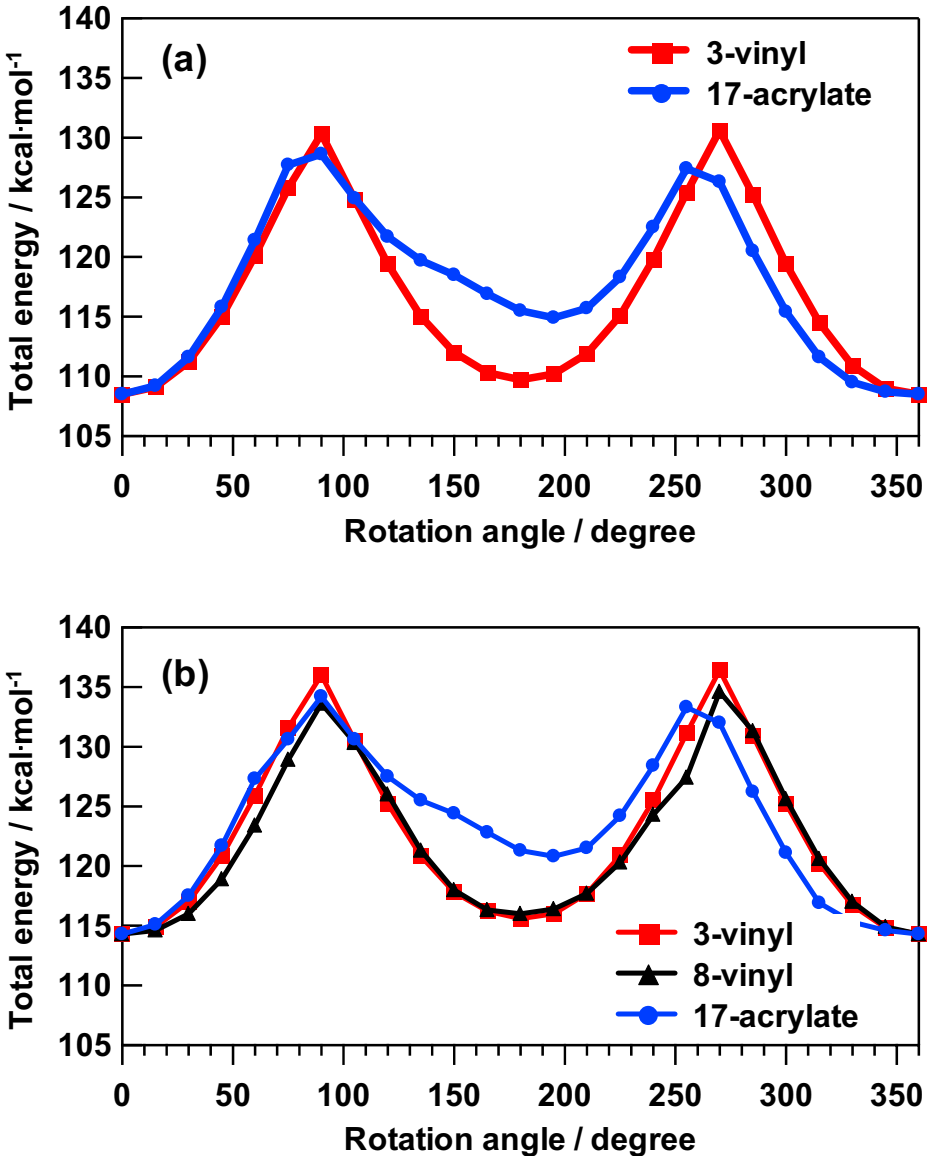

Figure S3. Total calculated energies of Chl-c_1 (a) and Chl-c_2 (b) as a function of the clockwise rotation around the C17–C17^1 bond for the acrylate, the C3–C3^1 for the 3-vinyl and the C8–C8^1 for the 8-vinyl subsitituents.

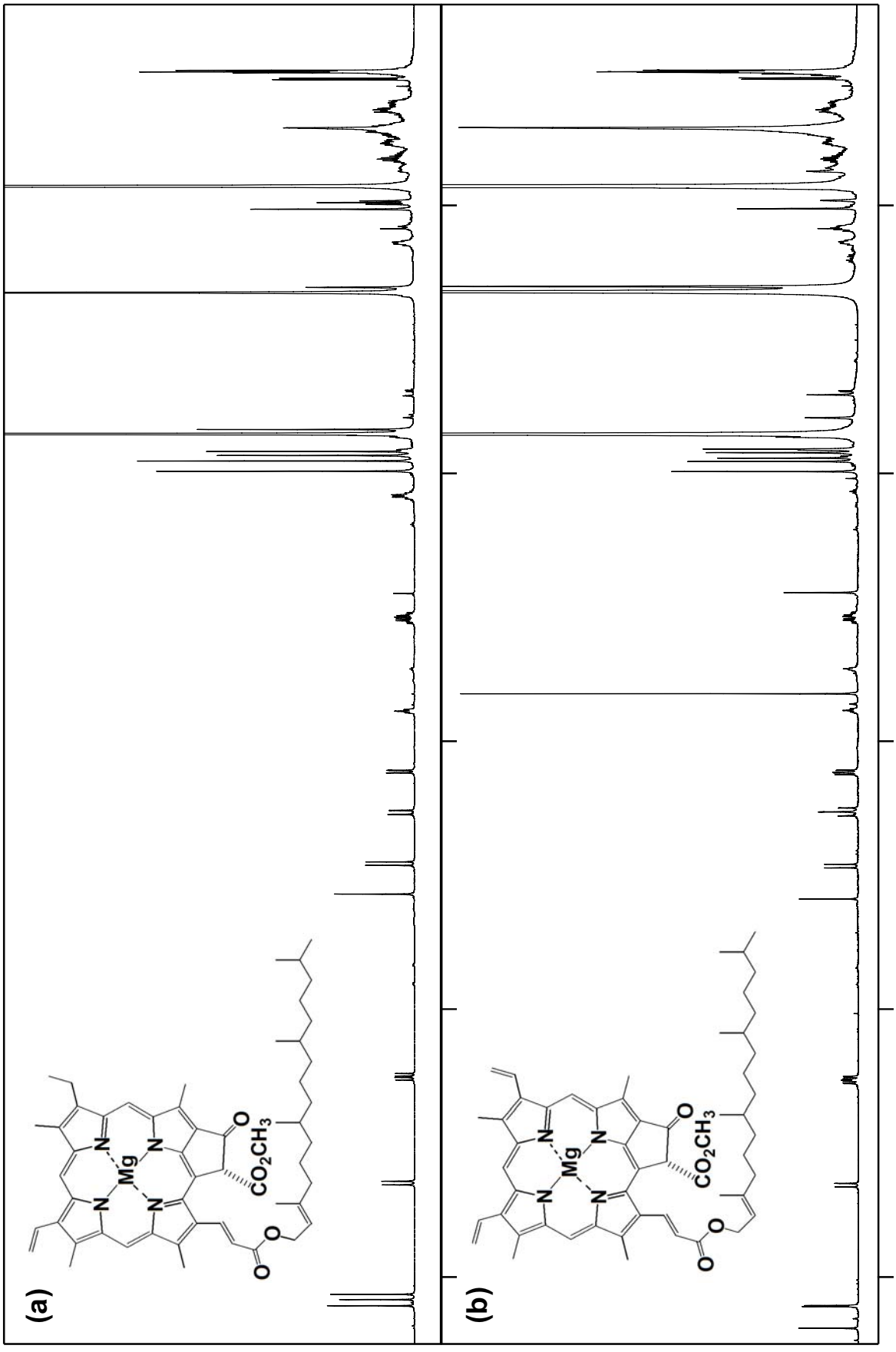

Figure S4. ^{1}H-NMR spectra of the synthetic Chl-c_1-phy (a) and Chl-c_2-phy (b) in THF-d_8 at room temperature.

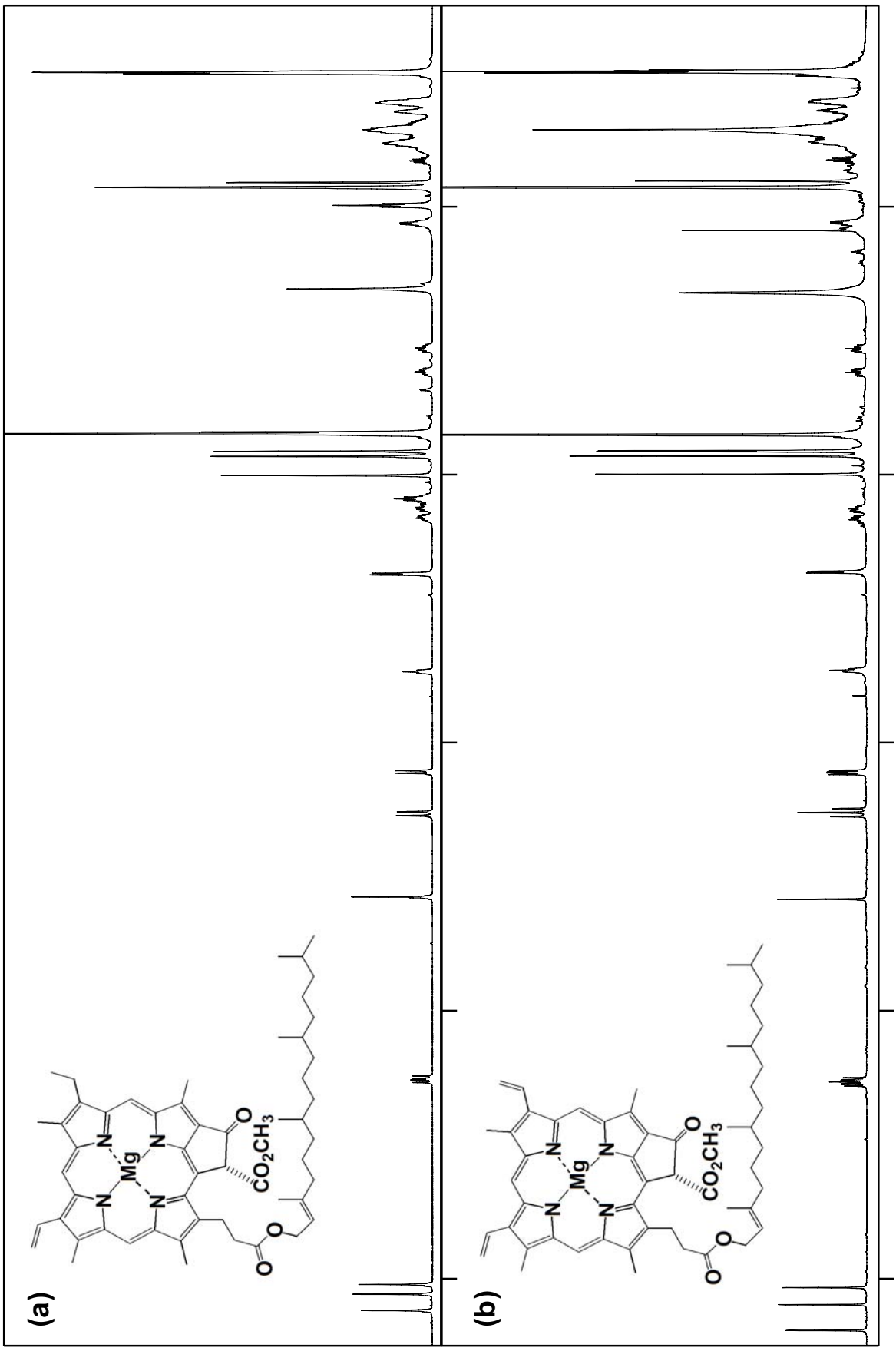

Figure S5. ^{1}H-NMR spectra of the synthetic PChl-*a* (a) and 8-vinyl-PChl-*a* (b) in THF-d_8 at room temperature.