Electronic supplementary information *for*

Intramolecular interaction of synthetic chlorophyll heterodyads with different π-skeletons

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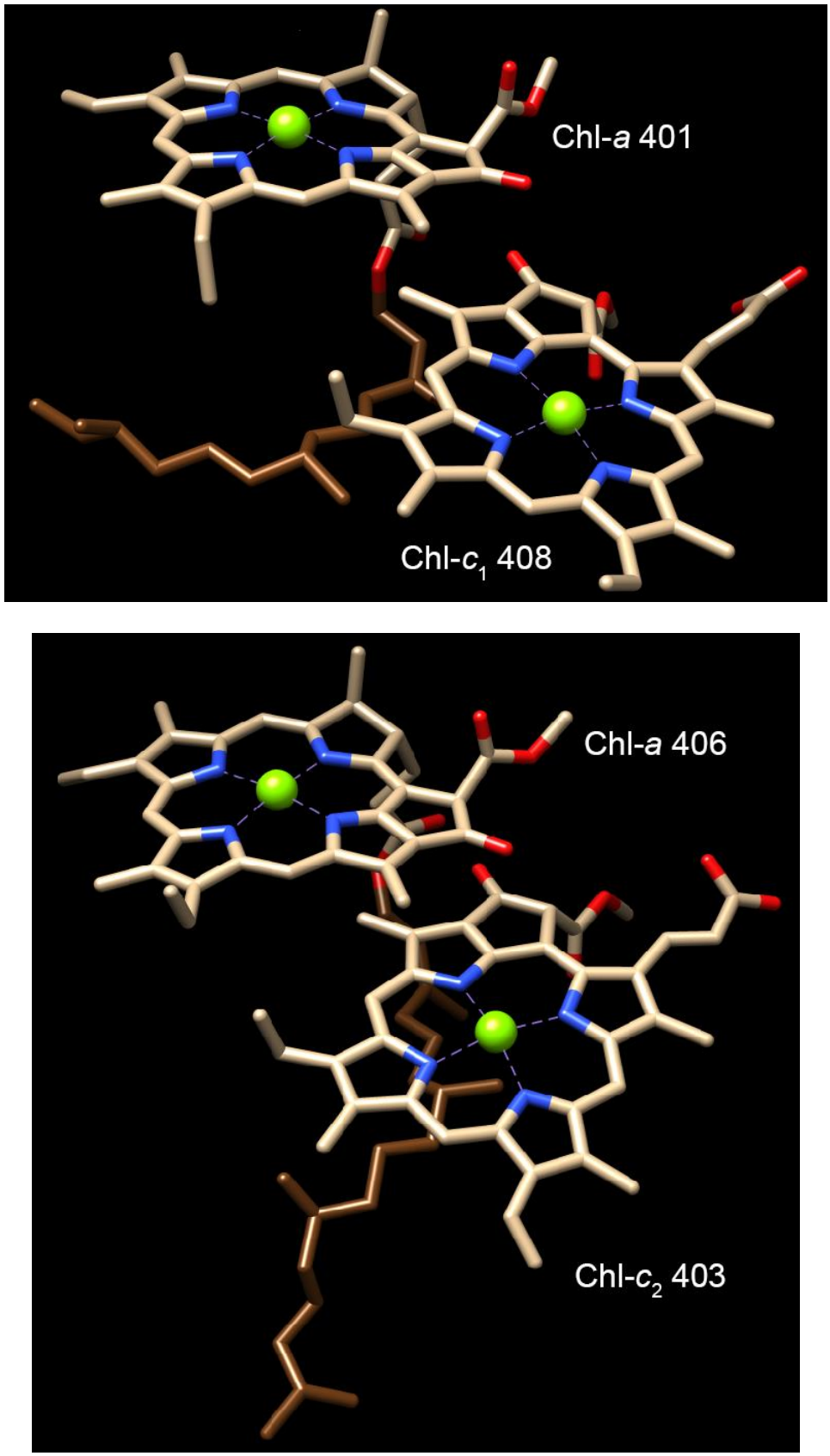


Fig. S1 Interaction of Chl-*a* 401 with Chl-c_1 408 (upper) and Chl-*a* 406 with Chl-c_2 403 (upper) in FCP based on PDB #6A2W.

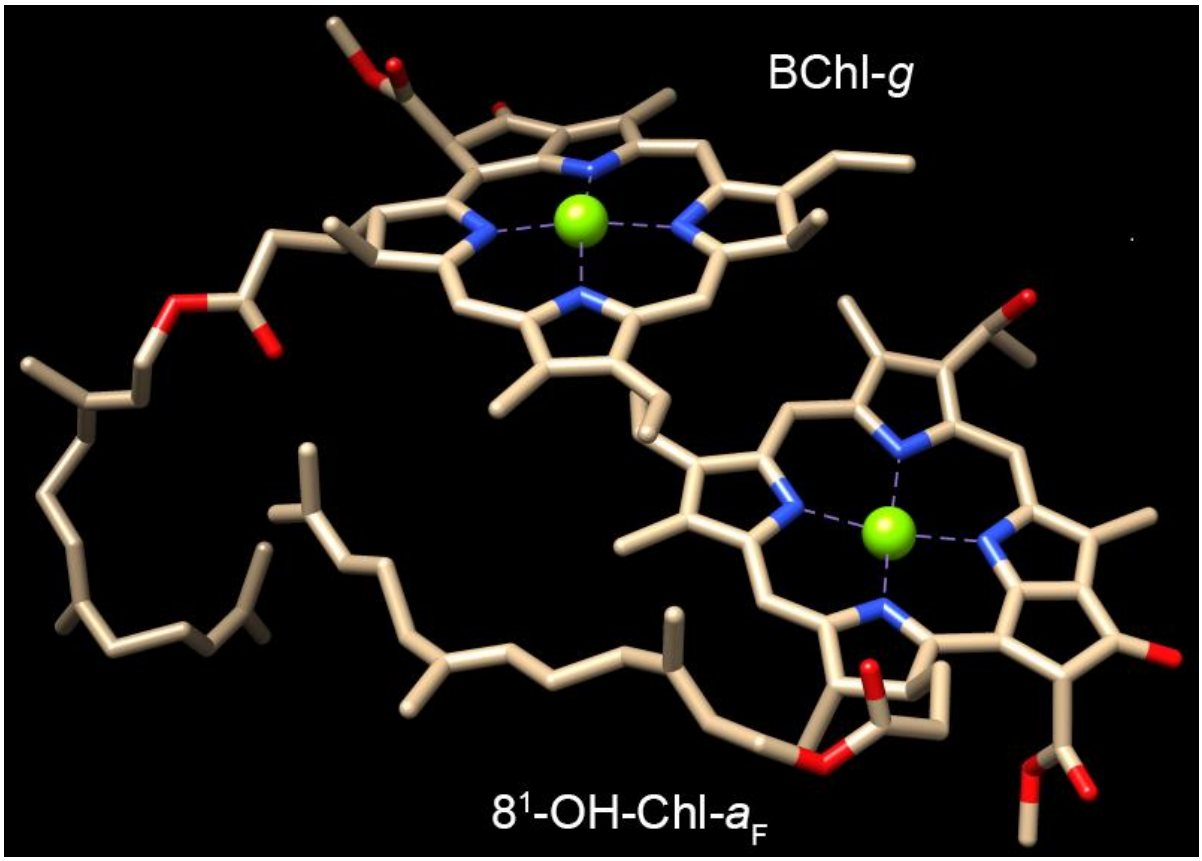


Fig. S2 Interaction of BChl-*g* with 8^1-OH-Chl-a_F in heliobacterial RC based on PDB #5V8K.

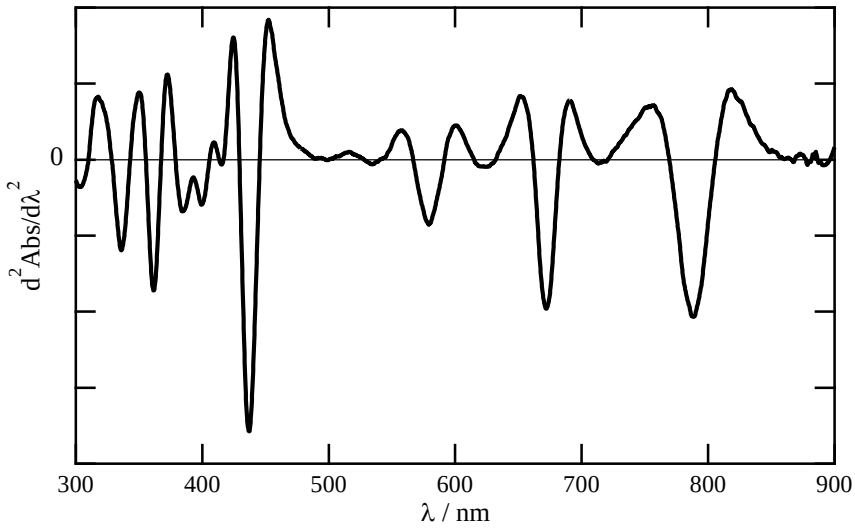


Fig. S3 Second derivative in electronic absorption spectrum of **ZnB–ZnC** (5 μM) in 1%(v/v) methanol and benzene.

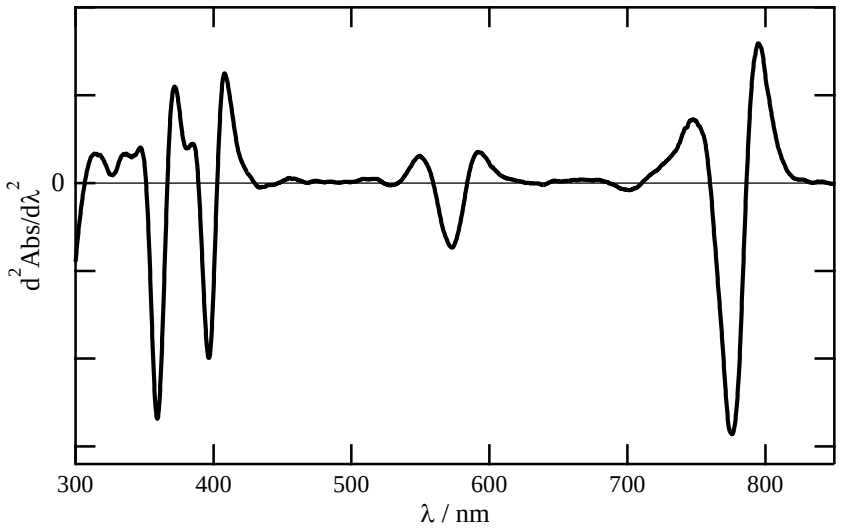


Fig. S4 Second derivative in electronic absorption spectrum of **ZnB** (5 μM) in 1%(v/v) methanol and benzene.

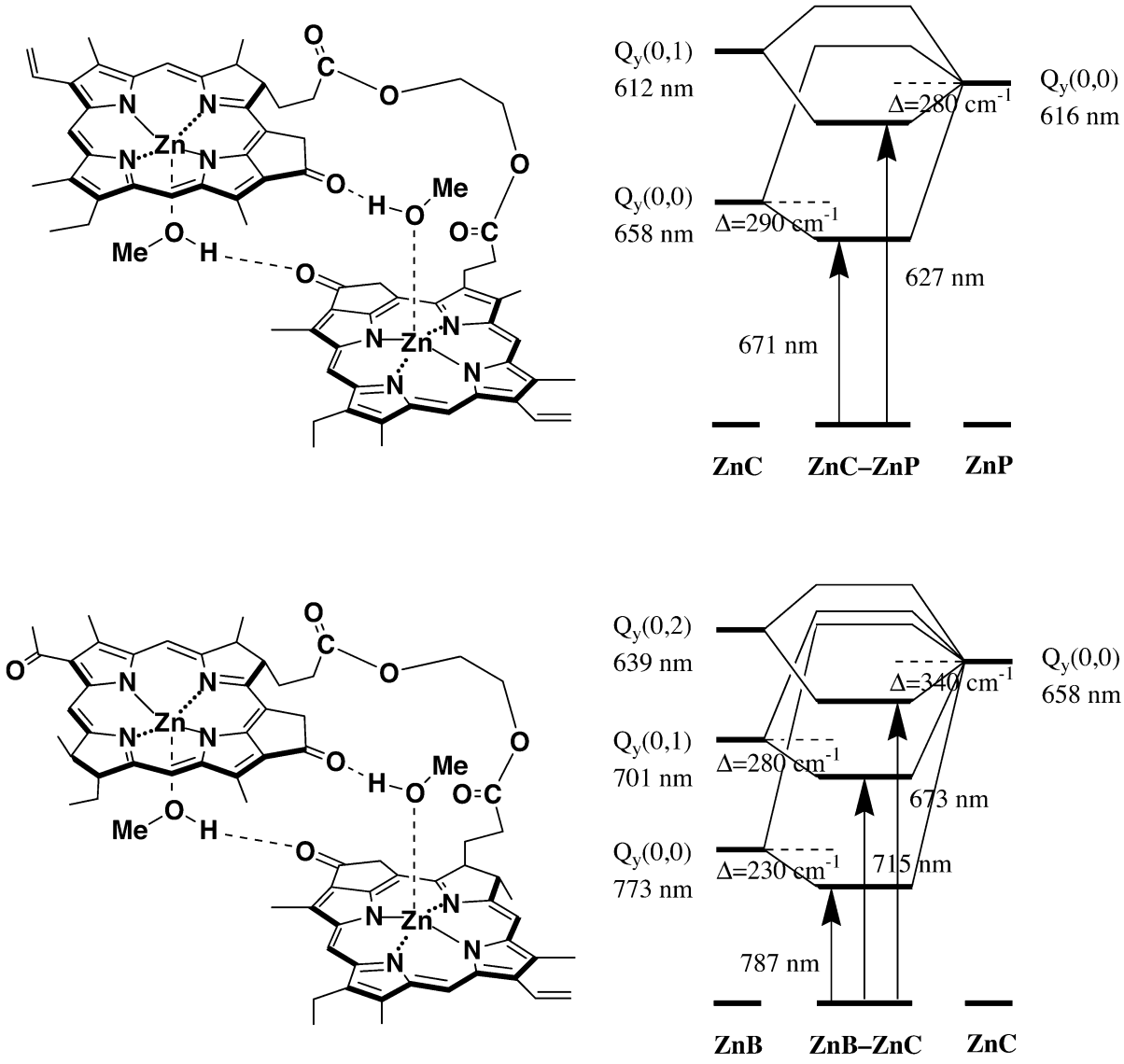
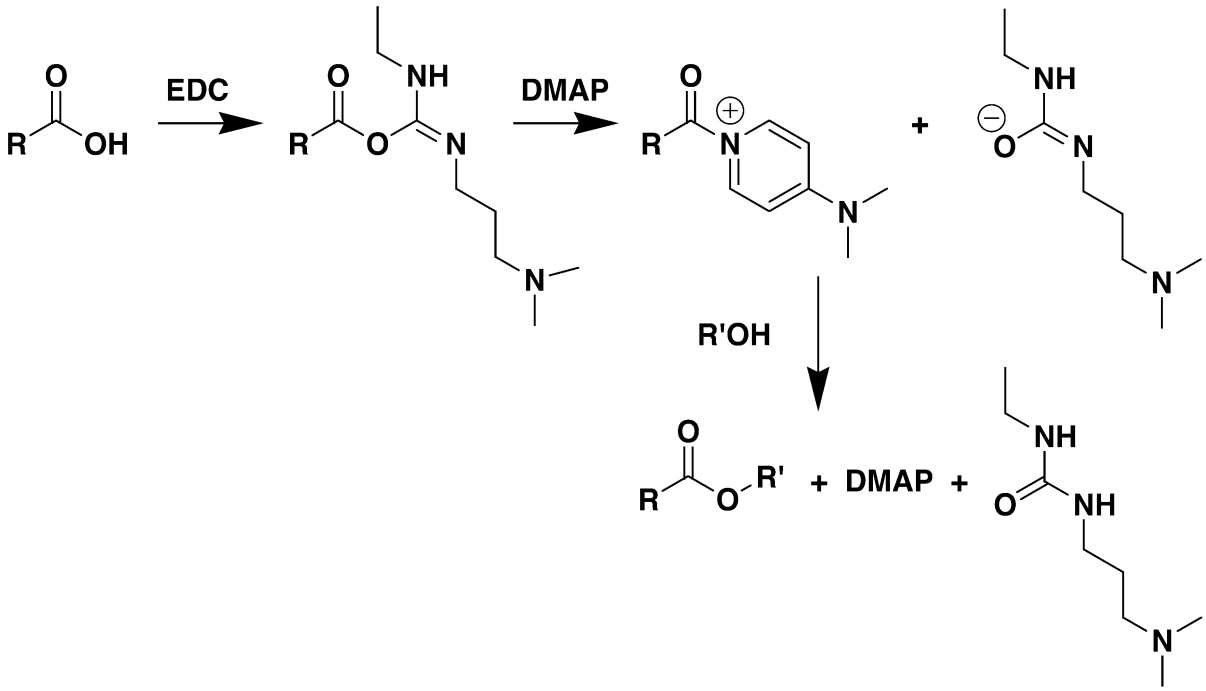


Fig. S5 Proposed conformers of methanol-locked heterodyads (left) and the estimated energy levels of their excitonically coupled Q_y bands (right): **ZnC–ZnP**·2MeOH (upper) and **ZnB–ZnC**·2MeOH (lower).



Scheme S1 Steglich esterification of carboxylic acid (RCOOH) with alcohol (R'OH) using EDC and DMAP [step (vii) in Fig. 5].