Force Field Parameters for the Photosystem II Reaction Center

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Our recent experimental results [1] led to the hypothesis that at a room temperature the reduced pigment pheophytin *a* (PHO) induces conformational changes of the photosystem II reaction center (PSII RC) pigment-protein complex. The conformational changes affect excitonic interaction of the RC chlorophylls, which was observed in absorption and CD spectra. In order to better interpret our experiments, theoretical approach such as molecular dynamics simulation is useful tool through the use of dynamic conformational analysis of PSII RC. At present the complete force field (FF) parameters applied in MD are not available for the photosynthetic pigments of PSII RC, namely partial atomic charges and force constants of chlorophyll *a*, plastoquinone and both neutral and reduced form of PHO. From that reason we have developed new FF parameters calculated by quantum chemical method on the pigments with known experimental 3D structure. New FF parameters were successfully applied in preliminary MD simulations on the pigment-protein complex PSII RC (experimental structure pdbID 1S5L). This work is supported by MSMT (MSM6007665808, GACR206/02/D177) and by AVCR (AVOZ60870520).

[1] Vacha F., Durchan M., Siffel P., *Biochim Biophys Acta,* 2002, **147** 1554.

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