Spectral properties of reaction center of photosystem II (RC PS II) and some chosen pigment molecules were studied by methods of quantum chemistry. Absorption spectra of six monomer unit of RC PS II were computed with semiempirical method and on the DFT level. Spectra of monomers obtained by the semiepirical ZINDO method are red shifted and spectra obtained by TDDFT are blue shifted from measured spectrum of chlorophyll a. The shift is a result of applied method. Next, electron transitions of chosen part of chlorophyll-pheophytin complex of RC PS II were obtained by semiempirical method. A goal was to describe differences, which follows from enlarging size of the reaction complex. A difference in the spectra correlates with various groups of pigments, which belong to active and inactive branches. Red shift of spectral lines was found only for the central dimer in comparison with electron transitions of chlorophyll a. Spectra of selected pigment molecules (chlorophylls, bacteriochlorophylls, carotenoids, phycobilins) were calculated on the DFT level and a good agreement with experimental data was achieved. An expected spectral-lines dependence on molecular structures was obtained. The relationship of some substituents, the length of unsaturated chains of chromofor and some modification of structure was searched.