私は、下記研究課題に係る研究費について、以下のとおり研究成果を報告します。また当該研究費の執行について、規程等を遵守し、適正に使用いたしました。

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2. 研究課題名
   IR-MALDIにおけるマトリックス分子の赤外光吸収強度の理論的研究

3. 交付額
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To investigate the correlation between the wavelength dependence of ionization threshold fluence of target molecule in matrix-assisted laser desorption/ionization by infrared laser (IR-MALDI) and the IR absorption spectrum of matrix molecule, we have analyzed the IR absorption spectra of four matrix molecules by using density functional theory and correlated ab initio molecular orbital method. The calculated IR absorption spectra of the isolated molecules showed more qualitative correlation with the wavelength dependence of ionization threshold fluence than those of the solid state structures. We can consider that a portion of matrix molecules lost the ordered crystal structure and that the transition to the diluted or isolated state occurred at the early process of IR laser irradiation.

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