

論文 / 著書情報
Article / Book Information

題目(和文)	
Title(English)	Gas phase spectroscopic study of bio and bio-relevant molecules: Role of inter- and intramolecular interactions on conformations
著者(和文)	SohnWoonyong
Author(English)	Woonyong Sohn
出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第9736号, 授与年月日:2015年3月26日, 学位の種別:課程博士, 審査員:藤井 正明,原 正彦,山元 公寿,野村 淳子,酒井 誠
Citation(English)	Degree:., Conferring organization: Tokyo Institute of Technology, Report number:甲第9736号, Conferred date:2015/3/26, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

Abstract

UV and IR spectra of homophenylalanine (HPhe), Ac-HPhe-Gly-Gly-NH₂, adrenaline, mono-hydrated adrenaline and a complex of catechol and Ser-Ile-Val-Ser-Phe-NH₂ and acetaminophen were measured by laser desorption supersonic jet technique. Conformers of the target molecules were found by UV-UV hole-burning spectroscopy and assigned by IR dip spectra together with quantum chemical calculations.

We studied HPhe and demonstrated combination of simulated UV and IR spectra is powerful to assign the conformation. We investigated Ac-HPhe-Gly-Gly-NH₂ and found β -turn- β -turn structure, the most stable conformer of Ac-Phe-Gly-Gly-NH₂, was not observed. We investigated adrenaline and its mono-hydrated cluster and demonstrated the most stable conformation is changed by hydration of a single water molecule. It is rationalized by enhancement of NH- π interaction. We succeeded to measure REMPI and IR spectra of the complex of catechol and Ser-Ile-Val-Ser-Phe-NH₂, which is a model of the adrenaline-accepted receptor. This provides the possibility to understand molecular recognition in neuro system at molecular level. We investigated acetaminophen and found four species. It was demonstrated that acetaminophen has two conformers and each conformer gives two independent transitions starting from the most stable 0a₁ and the hot 1e internal rotational levels.

Keywords: laser desorption, supersonic jet, gas phase, UV-UV hole burning spectroscopy, IR dip spectroscopy, conformer, homophenylalanine, adrenaline, acetaminophen