水中における (-)- エピガロカテキン -3-*O*- ガレートを用いた高次機能の開発

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Development of High-Order Functions Using (–)-Epigallocatechin-3-*O*-Gallate in Water

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ABSTRACT The high-order functions of molecular capture and chiral recognition of tea gallated catechins (–)-epigallocatechin-3-*O*-gallate (EGCg) in water were investigated. A solution of equimolar amounts of a variety of heterocyclic compounds and EGCg in water afforded adhesive precipitates containing the heterocyclic compounds and EGCg at a molar ratio of 1:1, based on the integrated value of NMR proton signals. The molecular capture abilities of a variety of heterocyclic compounds using EGCg from the aqueous solutions were evaluated with the ratios of the heterocyclic compounds included in the precipitates of EGCg complex to the total heterocyclic compounds used. In the ^{1}H NMR spectrum of a solution containing cyclo(L-Pro-Gly), cyclo(D-Pro-Gly), and EGCg in a D_2O solution, a difference in the chemical shift of the ^{1}H NMR signal for some protons of the Pro residue was observed. Judging from the crystal structures of the 2:2 EGCg complexes of cyclo(L-Pro-Gly), cyclo(D-Pro-Gly), the difference in the chemical shift derived mainly from a magnetic anisotropic shielding effect by the ring current from the B ring of EGCg. In the ^{1}H NMR spectrum of a solution containing the pharmaceuticals racemic (*R, S*)-propranolol, (*R, S*)-diprophylline, (*R, S*)-proxyphylline and EGCg in D_2O, splitting of the ^{1}H NMR signals of the pharmaceuticals was observed. It was suggested that the pharmaceuticals formed diastereomers of EGCg complexes, as a result chirality of the pharmaceuticals was recognized by EGCg in the D_2O solution.

抄録　茶ガレート型カテキンの (-)- エピガロカテキン -3-*O*- ガレート（EGCg）を用いて、分子補足や不斉認識などの高次機能の開発を行った。水中で EGCg は等モル量の様々なヘテロ環化合物と、1:1 ヘテロ環化合物・EGCg 錯体をつくり沈殿する。そこで、EGCg を用いたヘテロ環化合物の分子補足能を求めた。分子補足能は、用いたヘテロ環化合物に対する沈殿中に含まれているヘテロ環化合物の比率により評価した。EGCg は cyclo（L-Pro-Gly）および cyclo（D-Pro-Gly）とも 2:2 錯体をつくることが X 線結晶構造解析よりわかった。その際、^{1}H NMR スペクトルにおいて、いくつかのプロリン残基のプロトンシグナルが分離することより、EGCg が cyclo（Pro-Gly）の不斉を認識することがわかった。さらに、EGCg は水中で、医薬品であるラセミ体の（*R*、*S*）- プロプラノロール、（*R*、*S*）- ジプロフィリン、（*R*、*S*）- プロキシフィリンの不斉も識別することもわかった。