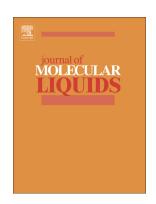
Accepted Manuscript

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PII: S0167-7322(17)32084-6

DOI: doi:10.1016/j.molliq.2017.10.049

Reference: MOLLIQ 8011

To appear in: Journal of Molecular Liquids

Received date: 13 May 2017

Revised date: 17 September 2017 Accepted date: 10 October 2017

Please cite this article as: Lixia Yuan, Min Liu, Bin Sun, Jie Liu, Xilian Wei, Zhengping Wang, Bingquan Wang, Jun Han, Calorimetric and spectroscopic studies on the competitive behavior between (–)-epigallocatechin-3-gallate and 5-fluorouracil with human serum albumin. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2017.10.049

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ACCEPTED MANUSCRIPT

Calorimetric and spectroscopic studies on the competitive behavior between (–)-epigallocatechin-3-gallate and

5-fluorouracil with human serum albumin

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Abstract: The combination of several drugs is often necessary, especially during long-term therapy. Drug-protein interaction has attracted a great deal of research interest because only the free drug fraction exerts pharmacological and/or toxicological effects. Herein, the binding interactions of serum transport protein, human serum albumin (HSA), with individual or combined anticancer drugs, (-)-epigallocatechin-3-gallate (EGCG) and 5-fluorouracil (FU), were investigated using isothermal titration calorimetry (ITC), circular dichroism (CD), and dynamic light scattering (DLS). DLS measurements showed that EGCG has a larger effect on the hydrodynamic diameter of HSA than FU. The adding order of EGCG and FU has an important influence on the size of the EGCG + FU + HSA complex. Fitting of the ITC data suggested that there are two sets of sites for the individual and combined binding of EGCG and FU to HSA. The obtained thermodynamic parameters revealed that electrostatic, hydrogen bonding, and van der Waals interactions may contribute to the stronger affinity of EGCG while hydrophobic interactions, van der Waals forces,

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