

## CHROMATOGRAPHIC ANALYSIS OF ORCHID EXTRACTS AND QUANTUM CHEMICAL CALCULATIONS OF INDIVIDUAL COMPONENTS INTERACTION WITH SILICA

Olga Kazakova <sup>a\*</sup>, Roman Ivannikov <sup>b</sup>, Iryna Laguta <sup>a</sup>, Oksana Stavinskaya <sup>a</sup>, Viktor Anishchenko <sup>c</sup>, Olga Severinovska <sup>a</sup>, Ludmila Buyun <sup>b</sup>

<sup>a</sup>Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,  
17, General Naumov str., Kiev 03164, Ukraine

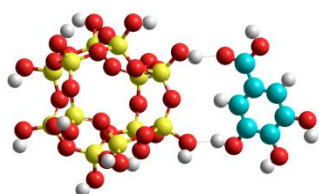
<sup>b</sup>M.M. Gryshko National Botanic Garden of National Academy of Sciences of Ukraine,  
1, Timiryazevska str., Kiev 01014, Ukraine

<sup>c</sup>L.M. Litvinenko Institute of Physical-Organic Chemistry and Coal Chemistry of National Academy of  
Sciences of Ukraine, 50, Kharkivs'ke hwy., Kiev 02160, Ukraine

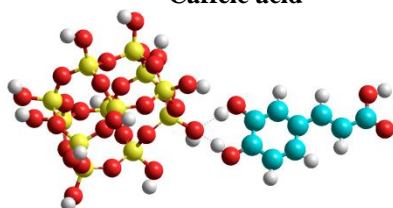
\*e-mail: kazakova\_olga@ukr.net

Received: 22 April 2020/ Revised final: 23 May 2020/ Accepted: 27 May 2020

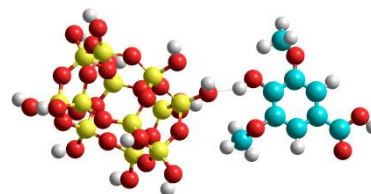
**Gallic acid**



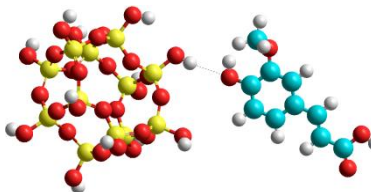
**Caffeic acid**



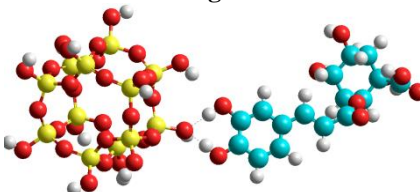
**Sinapic acid**



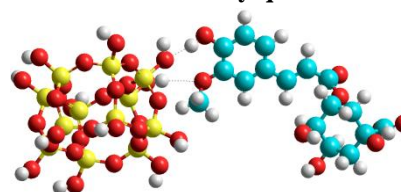
**Ferulic acid**



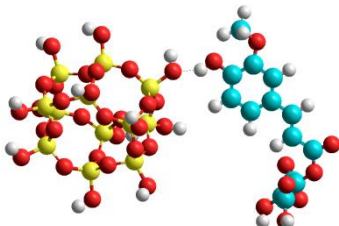
**Chlorogenic acid**



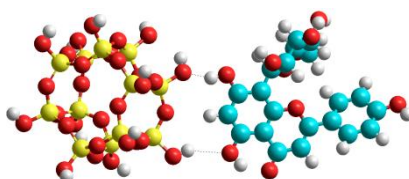
**Feruloylquinic acid**



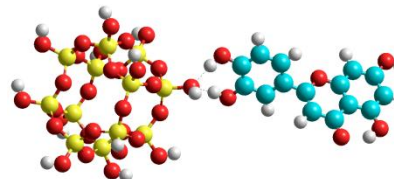
**Fertaric acid**



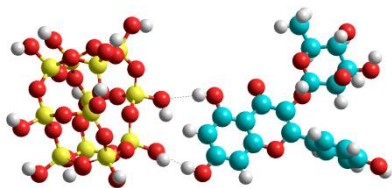
**Apigenin-8-C-glucoside**



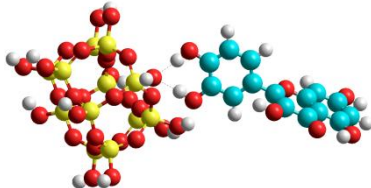
**Luteolin**



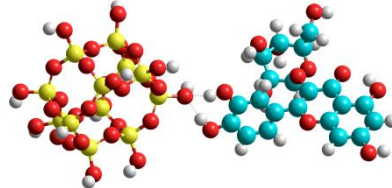
**Kaempferol 3-*O*-rhamnoside**



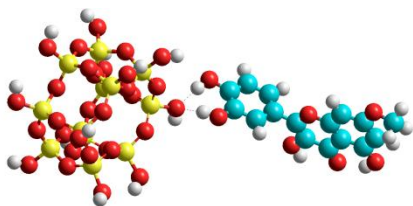
**Quercetin**



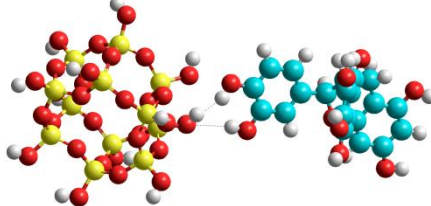
**Quercetin-3-*O*-glucoside**



**Rhamnetin**



**Epigallocatechin gallate**



**Figure S1. Optimized structure of the adsorption complexes of phenolic compounds on silica surface (atoms: H – light-grey, C – light-blue, O – red; Si – yellow; PM6 geometry, Gaussian 09) taking into account the solvation effects (SMD, Gaussian 09).**