

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

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**Abstract.** The aim of the work was to identify the main components of orchid extracts and to study their interaction with silica. Composition of sixteen orchid extracts was investigated by means of high performance liquid chromatography and laser desorption/ionization mass spectrometry; as it was shown in this study, flavonoids and phenolic acids were the main bioactive compounds available in the extracts. The interaction between various phenols and silica silanol groups was studied by quantum chemical method. Results show that the strength of interaction of phenols with silica increased in the following order: ferullic, feruloylquinic and fertaric acids < kaempferol, apingenin << chlorogenic and caffeic acids, rhamnetin, quercetin, luteolin, epicatechin gallate. The common feature of compounds characterized by the strongest interaction with silanol groups is the presence of a phenol ring with two neighbouring hydroxyl groups. The hydrogen bonds formed between these groups and silanol groups are much shorter (about 0.17 nm) than those formed by other hydroxyl groups of phenols (up to 0.28 nm).

**Keywords:** orchid extract, phenolic compound, fumed silica, quantum chemical calculation.

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