**Dear Prof.** **Ivan Juranic,**

Please find in the attachment the word file of our manuscript entitled

**"**Determination of pKa for caffeic acid in mixed solvent using

net analyte signal and ab initio theory**"**

which is submitted for consideration for publication in Journal of the Serbian Chemical Society. In the present paper the behavior of acidity constants of caffeic acid in binary mixture ethanol/water was studied by applying net analyte signal on UV-Vis spectrophotometric data and ab initio quantum mechanical method. Our findings are:

1. The results obtained by NAS indicated that the proposed method is an effective method for calculation of acid dissociation constants of caffeic acid solution with high spectral overlap.
2. The obtained results for investigation of pKa1 and pKa2 of caffeic acid in a mixture of water and ethanol revealed that the reduction of solvent polarity leads to an increase of pKa1 and pKa2.
3. In strong alkaline solution, the oxidation of the acid is inevitable; therefore the accuracy of the pka3 value is poor.
4. The calculated Gibbs energy by ab initio shows that para-hydroxy group is more acidic than meta-hydroxy group.
5. The obtained pKa values by ab initio quantum mechanical method are in good agreement with NAS.
6. The red shifts of different species of caffeic acid obtained using the ab initio quantum mechanical method are in good agreement with the results of UV–Vis spectroscopy.

The manuscript has not been previously published, is not currently submitted for reviewing to any other journal, and will not be submitted elsewhere before a decision is made by this journal. Hope you find it interesting. I am looking forward to hearing your positive reply. Thank you very much for your cooperation in this regard.

Yours sincerely,

Ali Benvidi,

Prof. of Analytical Chemistry,

Department of Chemistry,

Yazd University, Yazd, Iran,

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