Dear Professor Nikolić,

Please find enclosed manuscript entitled

**Redox properties of alkyl-substituted 4-aryl-2,4-dioxobutanoic acids**

meant to be published as **Original scientific paper**.

This work is a part of our ‘long-time’ study of aryldiketo acids (ADKs) and their derivatives. ADKs represent a group of small organic molecules that comprise 2,4-dioxobutanoic acid scaffold. Along with well-known HIV-1 integrase (IN) inhibition, they exert widespread biological activities. The aim of this work to evaluate effects of aryl substitutions on properties of dioxobutanoic moiety that is involved in key interactions with metal ions within active sites of target enzymes. The effect of pH on electronic properties of nine congeners was examined using cyclic voltammetry and differential pulse polarography. Compounds were chosen as a simple set of congeners, bearing Me-groups on phenyl ring which should not be involved in electrochemical reactions, leaving diketo moiety as sole electrophore. Substitution pattern was systematically varied, yielding a set having different torsion between phenyl ring and aryl keto group (Ar-C(O)). Protonation state of ADKs at different pH values was determined from experimentally obtained p*K*as. The results showed that the equal number of protons and electrons is involved in the oxidation and reduction reactions at the surface of electrode. Quantitative linear correlations between reduction potentials and energies of frontier orbitals, calculated for neutral, monoanionic and corresponding radical anionic species, and steric parameter were found.

To the best of our knowledge there are no similar reports for ADKs.

Along with the manuscript we are sending the supplementary data.

We hope that results presented within this work and the way of presentation will be suitable for the publication in Journal of the Serbian Chemical Society.

**Hereby we confirm that the manuscript submitted to the Journal for review is original, has been written by the stated authors and has not been published elsewhere; is currently not being considered for publication by any other journal and will not be submitted for such a review while under review by the Journal; the manuscript contains no libelous or other unlawful statements and does not contain any materials that violate any personal or proprietary rights of any other person or entity.**

On behalf of authors, respectfully

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