

Supporting Information

Towards the Rational Design of Novel Drugs based on Solubility, Partitioning/Distribution, Biomimetic Permeability and Biological Activity exemplified by 1,2,4-Thiadiazole Derivatives

Tatyana V. Volkova^a, Irina V. Terekhova^a, Oleg I. Silyukov^a, Alexey N. Proshin^b, Annette Bauer-Brandl^c, German L. Perlovich^{a,*}

^aInstitute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russia

^bInstitute of Physiologically Active Compounds, Russian Academy of Sciences, 142432 Chernogolovka, Russia

^cDepartment of Physics, Chemistry and Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark

*Tel: +7 4932 533784; Fax: +7 4932 336237;

E-mail: glp@isc-ras.ru.

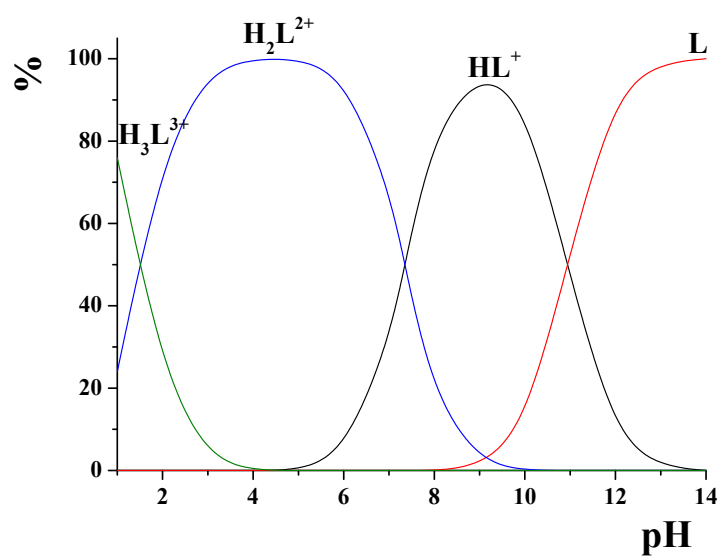
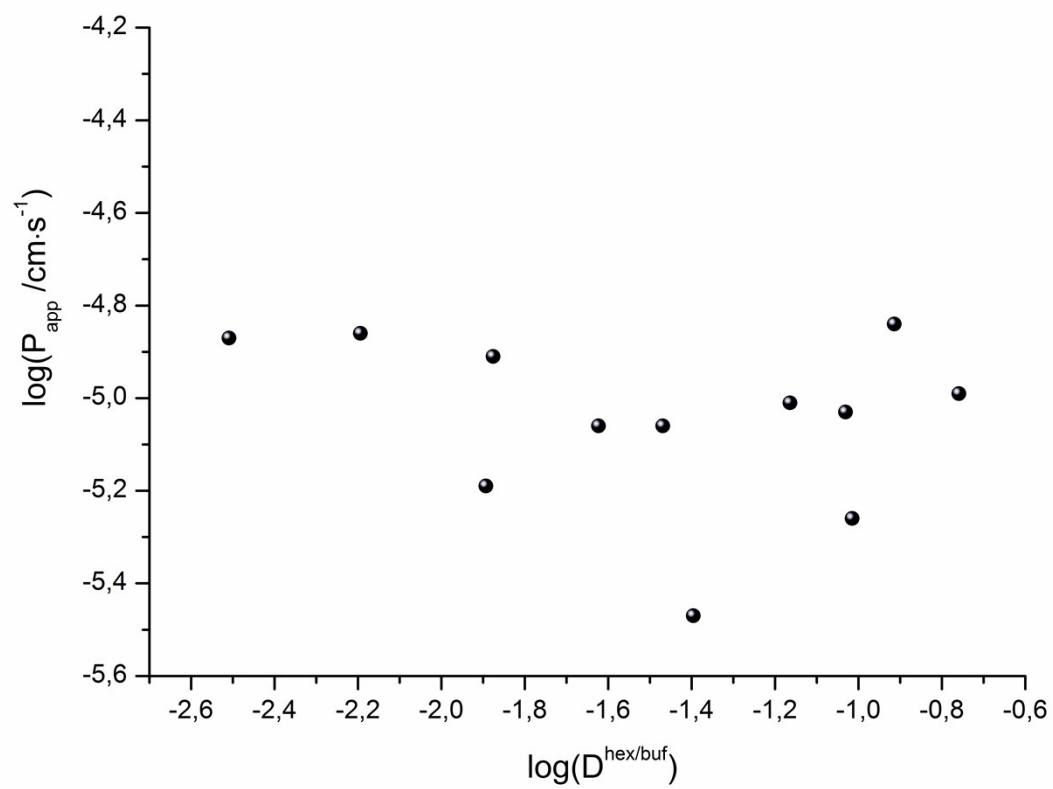
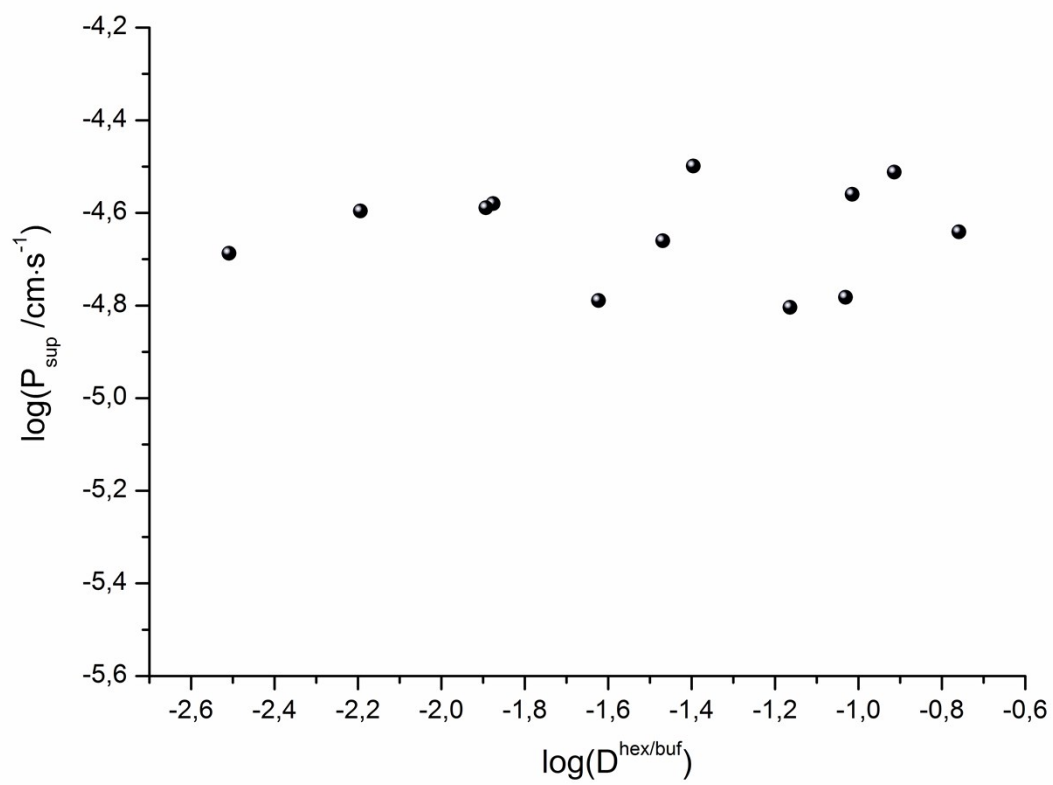


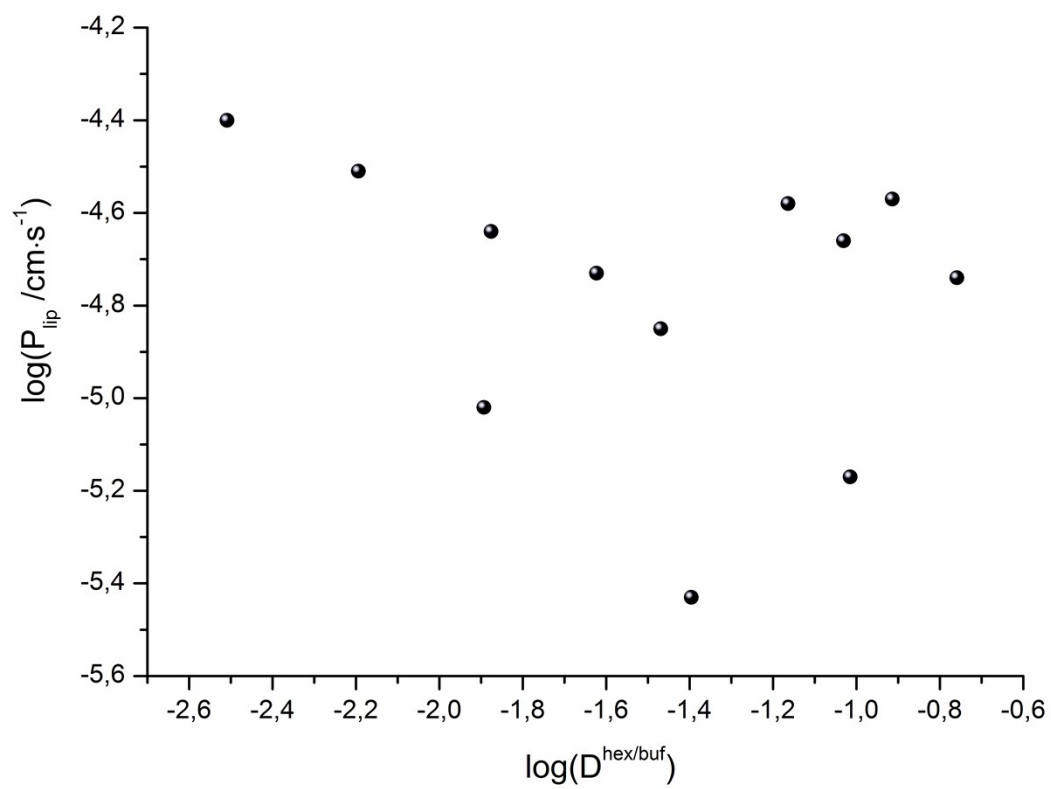
Fig. 1SI. Dependence of content of the ionized forms of the molecules on the pH of buffer solution of compound **2**.



a



b



c

Fig. 2SI. Relationships $\log P_{app}$, $\log P_{sup}$, $\log P_{lip}$ with $\log D^{hex/buf}$

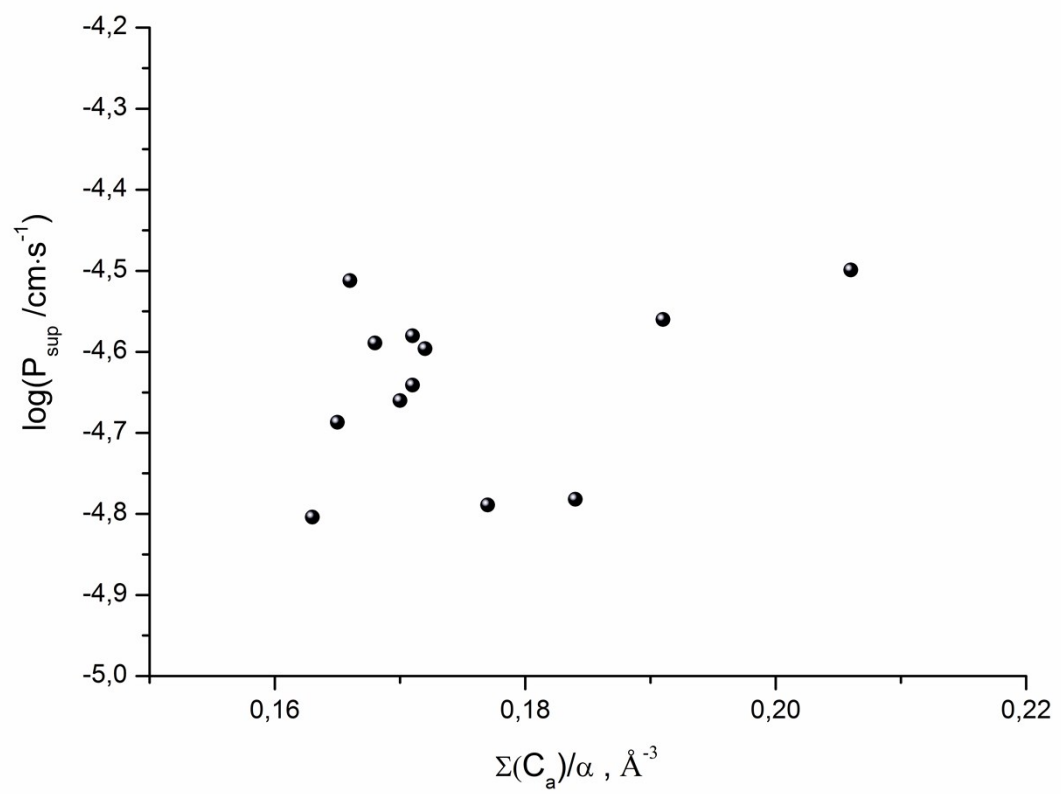


Fig. 3SI. Relationship $\log P_{\text{sup}}$ with $\Sigma(C_a)/\alpha$