

Списък на научните трудове на гл. ас. д-р Валя Николова

Катедра Фармацевтична и приложна органична химия,

Факултет по химия и фармация,

СУ „Св. Климент Охридски”

Публикации:

1. **V. Dimitrova**, S. Ilieva, B. Galabov, “Electrostatic potential at atomic sites as a reactivity descriptor for the hydrogen bonding complexes of monosubstituted acetylenes and ammonia”, *Journal of Physical Chemistry A*, 106, (2002), 11801-11805.

IF* = 2.871 (2002); брой цитати: 50

2. **V. Dimitrova**, S. Ilieva, B. Galabov, “Electrostatic potential at nuclei as a reactivity index in hydrogen bond formation. Complexes of ammonia with C-H, N-H and O-H proton donor molecules”, *Journal of Molecular Structure (Theochem)*, 637, (2003), 73-80.

IF = 0.97 (2003); брой цитати: 18

3. B. Galabov, P. Bobadova-Parvanova, S. Ilieva, **V. Dimitrova**, „The electrostatic potential at atomic sites as a reactivity index in the hydrogen bond formation“, *Journal of Molecular Structure (Theochem)*, 630, (2003), 101-112.

IF = 0.97 (2003); брой цитати: 39

4. **V. Dimitrova**, S. Ilieva, B. Galabov, „A quantitative characterization of the reactivity of substituted phenols for the proton transfer reaction“, *Bulgarian Chemical Communications*, 37(4), (2005), 356-360.

IF = 0.349 (2005); брой цитати: 0

5. B. Galabov, **V. Nikolova**, J. Wilke, H. F. Schaefer, W. Allen, „Origin of the S_N^2 benzylic effect“, *Journal of American Chemical Society*, 130, (2008), 9887-9896.

IF = 8.091 (2008); брой цитати: 59

6. D. Cheshmedzhieva, **V. Dimitrova**, B. Hadjieva, S. Ilieva, „Rationalizing IR intensities in terms of electronic parameters“, *Journal of Molecular Structure*, 1009, (2012), 69-73.

IF = 1.404 (2012); брой цитати: 2

7. **V. Nikolova**, D. Cheshmedzhieva, S. Ilieva, B. Galabov, „The nature of intramolecular interactions determining the σ^α constants for aromatic systems“, *Journal of Molecular Structure*, 1023, (2012), 31-36.

IF = 1.404 (2012); брой цитати: 1

*Импакт фактор (IF)

8. B. Galabov, **V. Nikolova**, S. Ilieva, „Does the molecular electrostatic potential reflect the effects of substituents in aromatic systems?“, *Chemistry a European Journal*, (2013), 5194-5155.

IF = 5.696 (2013); брой цитати: 17

9. **V. Nikolova**, S. Ilieva, B. Galabov, H. F. Schaefer, „Experimental measurement and theory of substituent effects in π -hydrogen bonding: complexes of substituted phenols with benzene“, *Journal of Organic Chemistry*, 79, (2014), 6823-6831.

IF = 2.59 (2014); брой цитати: 13

10. **V. Nikolova**, B. Galabov, „Effects of structural variations on the hydrogen bond pairing between adenine derivatives and thymine“, *Macedonian Journal of Chemistry and Chemical Engineering*, 34(1), (2015), 159-167.

IF = 0.40 (2015); брой цитати: 1

11. **V. Nikolova**, S. Angelova, N. Markova, T. Dudev, „Gallium as a therapeutic agent: a thermodynamic evaluation of the competition between Ga^{3+} and Fe^{3+} ions in metalloproteins“, *Journal of Physical Chemistry B*, 9 (120), (2016), 2241-2248.

IF = 3.177 (2016); брой цитати: 6

12. T. Dudev, **V. Nikolova**, „Determinants of Fe^{2+} over M^{2+} ($\text{M}=\text{Mg, Mn, Zn}$) Selectivity in non-heme proteins“, *Inorganic Chemistry*, 55 (24), (2016), 12644-12650.

IF = 4.7 (2016); брой цитати: 1

13. **V. Nikolova**, D. Cheshmedzhieva, S. Ilieva, B. Galabov, „Hydrogen bonding reactivities of atomic sites in the nucleobases“, *Bulgarian Chemical Communications*, 49, Special Issue D, (2017), 8-18.

IF = 0.238 (2017); брой цитати: 0

14. **V. Nikolova**, B. Galabov, „Theoretical vs. experimental IR frequency shifts upon π -hydrogen bonding: complexes of substituted phenols with hexamethylbenzene“, *Contributions, Section of Natural, Mathematical and Biotechnical Sciences, MASA*, 38(1), (2017), 33-41.

IF = няма; брой цитати: 0

15. **V. Nikolova**, S. Angelova, T. Dudev, „IIA/IIB group metal cations hosted by β -cyclodextrin: a DFT study“, *Bulgarian Chemical Communications*, 49, (2017), 189-194.

IF = 0.238 (2017); брой цитати: 0

16. S. Angelova, **V. Nikolova**, N. Molla, T. Dudev, „Factors governing the host-guest interactions between IIA/IIB group metal cations and α -cyclodextrin: a DFT/CMD study“, *Inorganic Chemistry*, 56, (2017), 1981-1987.

IF = 4.7 (2017); брой цитати: 1

17. S. Angelova, **V. Nikolova**, T. Dudev, „Determinants of the host-guest interactions between α -, β - and γ -cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study“, *Phys. Chem. Chem. Phys.*, 19, (2017), 15129-15136.

IF = 4.123 (2017); брой цитати: 0

18. S. Angelova, **V. Nikolova**, S. Pereva, T. Spassov, T. Dudev, „ α -cyclodextrin: how effectively can its hydrophobic cavity be hydrated?“, *Journal of Physical Chemistry B*, 121, (2017), 9260-9267.

IF = 3.146 (2017); брой цитати: 2

19. B. Galabov, **V. Nikolova**, D. Cheshmrdzhieva, B. Hadjieva, H. F. Schaefer III, „Hyperconjugative effects in π -hydrogen bonding: theory and experiment“, *Journal of Computational Chemistry*, 39 (10),(2018), 527-534.

IF = 3.221 (2017); брой цитати: 0

20. S. Angelova, **V. Nikolova**, T. Dudev, „Divalent metal ions to lactose: a DFT computational study“, *Bulgarian Chemical Communications*, 50, (2018), 126-130.

IF = 0.238 (2017); брой цитати: 0

Други:

1. **Валя Николова**, „Атомният електростатичен потенциал като индекс на реактивоспособност при процеси на водородно свързване и химични реакции“, Автореферат на дисертация за присъждане на образователната и научна степен "доктор" по 4.2. Химически науки (Теоретична химия), 2008г.
2. **Валя Николова**, „Теоретични изследвания върху процеси на комплексообразуване: атомен електростатичен потенциал като индекс на реактивоспособност при водородно свързване; взаимодействия на циклодекстрини с метални йони“, Хабилитационен труд, 2018г.