COMPARISON OF 6-311G(D) AND 3-21G (DFT/HF) METHODS OF 3-METHYL-4-[3-(3-METHOXYBENZOX)BENZYLDENAMINO]-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONE

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3-Methyl-4-aminio-4,5-dihydro-1H-1,2,4-triazol-5-one reacted with 3-[3-(methoxybenzoxyl)-benzaldehyde to afford:

3-methyl-4-[3-(3-methoxybenzoxyl)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one (Medetalibeyoğlu, 2015). The compound was optimized and using B3LYP/6-311G(d) HF/6-311G(d) and B3LYP/3-21G HF/3-21G basis sets (Frinch et al., 2009; Wolinski, Hilton & Pulay, 1990). 1H-NMR and 13C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 (Wolinski, 1990). Theoretically calculated IR data of the compound were calculated in gas phase by using 6-311G(d) and 3-21G basis sets of B3LYP and HF methods and are multiplied with appropriate adjustment factors and the data obtained according to B3LYP and HF methods are formed using theoretical infrared spectrum. The identification of calculated IR data was used in visual program (Marnitz, 2004). Experimentally (Medetalibeyoğlu, 2015) and theoretically UV-vis values in ethanol were calculated and compared. Additionally, this compound were found bound angles, bond length, dipole moments, the HOMO-LUMO energy and total energy of the molecule with muliken changes from both methods. The obtained data with both methods were compared.

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Keywords: B3LYP, HF, GIAO, 1.2,4-triazol-5-one

COMPARISON OF OPINIONS OF STUDENTS AND UNIVERSITY TEACHERS FROM MEDICAL UNIVERSITY OF WARSAW ON E-ASSESSMENT – A PRELIMINARY REPORT

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Until now, test exams at Warsaw Medical University were mostly carried out in the paper-and-pen test form. Beginning in the academic year 2014-2015, it is possible to get a credit and pass a test exam on the ASK Systems e-exam platform. The study aimed to compare opinion of students and university teachers from Medical University of Warsaw on e-assessment. Study group were 181 people - 148 students: study group consisted of 79 students, who took part in e-assessment on ASK Systems E-exam platform, (Group 1 - 59 students), and students, who did not take part in e-assessment (Group 2 - 89 students) and 33 university teachers (Group 3). Group 1 - 59 women, mean age: 24.56. 25 of students has already took part in an e-exam apart from university. Group 2 - 55 women, 25 men, mean age: 22.53. 80 of students has already took part in an e-exam apart from university. Group 3 - mean age: 46.57, 14 of women, 15 teachers took part in e-assessment. Participation in the study was voluntary. An anonymous questionnaire survey. E-questionnaire consisted of 56 statements in 5 thematic domains. 5 step Likert scale. Links to the questionnaire were placed on an external server, which ensured anonymity. Reliability assessment of the questionnaire: Cronbach's Alpha coefficient. Analysis of significance of differences between Groups 1, 2, and 3 by parametric Kruskal-Wallis test, α=0.05. Among the study groups, statistically significant differences of opinions and attitudes towards exams concerned the following: phrasing questions that would be impossible to phrase in the case of a traditional pen-and-paper test.

Keywords: E-assessment, Quality of assessment, Modern technologies, Health sciences students, University teachers, Attitudes

COMPUTER-ASSISTED ACADEMIC LITERACY DEVELOPMENT: GETTING STARTED

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Given the challenges South African universities face when it comes to the levels of academic literacy of both prospective and enrolled students, additional aids for improving individual skills cannot go amiss. Although some academic literacy skills are part of the Home Language and First Additional Language curricula - as cited by other studies that are currently underway - these skills are, it would seem, underrepresented in assessments and examinations in high school. The proposed project aims to investigate the possibilities of creating a computer adaptive learning system that specifically focuses on the improvement of spelling and academic vocabulary acquisition, but could potentially be used to develop a

Keywords: Computer-assisted learning, Academic literacy, South African universities, Reading proficiency, Writing proficiency

COMPLEX NETWORK OF SOCIAL NETWORK TAGS

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Complex network studies, as an interdisciplinary framework, span a large variety of subjects including social media. Having the “universality” property, majority of the complex networks display common structures as a result of the underlying self-organizing principles. In social networks, several mechanisms generate miscellaneous structures like friendship networks, mention networks, tag networks etc. Focusing on tag networks (namely, hashtag in twitter), we constructed a tag network having hashtags as nodes, where the co-occurrences of these tags in a single entry define the links connecting them. We observed that the universal properties of the networks like small-world property, clustering and scale-free degree distribution is also observed in the network of social network tags. We also presented the visualization of this network provided by the software Gephi.