

SPECTROSCOPIC STUDIES (GEOMETRY OPTIMIZATION, E → Z ISOMERIZATION, UV/VIS, EXCITED STATES, FT-IR, HOMO-LUMO, FMO, MEP, NBO) OF NEW AZOMETHINE DYES FOR BIOLOGICAL APPLICATIONS

A. Pazniak¹, S. Shahab^{1,2,3}, M. Sheikhi⁴, E. Dikumar²

¹*Belarusian State University, ISEI BSU,*

Minsk, Republic of Belarus

apoznk@mail.ru

²*Institute of Physical Organic Chemistry of National Academy of Sciences of Belarus,*

Minsk, Republic of Belarus

siyamakshahab@mail.ru

dikumar@ifoch.bas-net.by

³*Institute of Chemistry of New Materials of National Academy of Sciences of Belarus,*

Minsk, Republic of Belarus

⁴*Young Researchers and Elite Club, Gorgan Branch, Islamic Azad University,*

Gorgan, Iran

m.sheikhi2@gmail.com

Three new azomethine compounds have been predicted and synthesized. Their equilibrium geometric parameters, IR, NMR, UV/Vis and electronic absorption spectra have been presented and discussed.

Keywords: antioxidant activity, azomethine, electronic spectrum, geometry optimization.

In the present work the geometries and adsorption properties of the three new molecules were investigated by Density Functional Theory (DFT) in the solvent for the first time.

In the present work, first time the molecular structures of three newly synthesized azomethine dyes:

(1Z)-N-benzylidene-4-((E)-1-(oxim)ethyl)benzenamine,

4-((1Z)-4-((E)-1-(oxim)ethyl)phenylimino)methylphenol,

(Z)-1-(4-((Z)-4-methoxybenzylidene)amino)phenyl)ethanone oxime have been investigated using Density Functional Theory (DFT/B3LYP/6-31+G*) in dimethylformamide (DMF). The electronic spectra of azomethine dyes in a DMF solvent was carried out by TD-DFT method. After quantum-chemical calculations three new azomethine dyes for optoelectronic applications were synthesized. FT-IR spectra of the title compounds are recorded and discussed. The computed absorption spectral data of the azomethine dyes are in good agreement with the experimental data, thus allowing an assignment of the UV spectra. The molecular HOMO-LUMO, excitation energies and oscillator strengths for E and Z isomers of the dyes have also been calculated and presented. Optical Properties of the PVA-films containing new substances have been also investigated[1].

BIBLIOGRAPHY

1. *Shahab, S.* Interaction between new synthesized derivative of (E,E)-azomethines and BN(6,6-7) nanotube for medical applications: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis, excited state), FMO, MEP and HOMO-LUMO investigations/S. Shahab, at all. // J. of Molec. Struct. – 2017. – Vol. 1, № 1146. – P. 881–888.

A METHOD FOR IMRT TREATMENTS OF PROSTATE CANCER IMPROVEMENT

M. Piatkevich, E. Titovich, N. Makarava, D. Kazlouski, A. Kaprusynka, V. Hertsyk

N. N. Alexandrov National Cancer Centre of Belarus,

Minsk, Republic of Belarus

MaxPetkevichN@gmail.com

The aim of the research work is to analyze modern methods in planning and elaboration of a new method for obtaining a volume-modulated dose distribution for irradiating prostate cancer by IMRT method.

Keywords: Radiation therapy, prostate cancer, IMRT, VMAT, medical linear accelerator, planning.

Data from the World Health Organization shows a steady increase in morbidity and mortality from prostate cancer, which makes this problem significant. With the implementation of modern medical accelerators in the treatment of prostate cancer, radiotherapy became the dominant technique for these treatments. Its main principle is to bring a high radiation dose strictly to the tumor, minimizing the dose to surrounding normal tissues and organs. Despite the existence of modern methods of irradiation in external beam radiation therapy, the possibility of their universal use in all oncology institutions is limited by the need for expensive equipment and its constant updating, which involve considerable financial costs. This fact makes it impossible to use modern methods of radiotherapy in clinics, where insufficient attention is paid to financing. The aim of the study is to search for an alternative to the VMAT method, in perspective of the lack of this technique in many oncological dispensaries of post-Soviet countries due to inadequate funding, lack of technical equipment and expensive licenses.

For the prostate cancer treatments, VMAT and IMRT (equidistantly spaced 9 irradiation fields) are used in most clinical cases. The main advantage of the VMAT method is a short time of irradiation of the patient (3-5 min.), which increases the potential number of patients treated in comparison with other methods of irradiation. When patients are irradiated using IMRT, the most effective coverage of the target with the prescribed dose is achieved, while the irradiation of adjacent tissues and organs is minimal.

In connection with the described difficulties, it is proposed to obtain a volume-modulated dose distribution by improving the established planning algorithm by the IMRT method. Creating a volume modulated dose distribution by the IMRT method allows not using more modern expensive equipment (specialized medical linear accelerators) to introduce the VMAT method, but at the same time, results in decreasing of the patient irradiation time compared to the standard approach to IMRT.

The patient irradiation course according to the developed method IMRTnew consists of several irradiation plans, which are calculated with a shift in the angle of rotation of the accelerator gantry by a certain number of degrees. Each calculated plan is assigned to a certain day of treatment from the total number of days of the entire course of exposure.

The use of 7 irradiation fields in each individual plan reduced the patient exposure time by more than 20% compared to the standard IMRT plan. The results obtained from the developed IMRTnew method are equivalent or better than using the VMAT method.

ANTIOXIDANT PROPERTIES OF JUICES CONTAINING CHERRY, RASPBERRY AND STRAWBERRY

P. Podorovskaya, E. Tarun, D. Selina

Belarusian State University, BSU ISEI,

Minsk, Republic of Belarus

padarouskap@gmail.com

The comparative study of the antioxidant activity of the packaged juices of cherry, raspberries and strawberry. The dependence of the fluorescence intensity of fluorescein from the logarithm of the concentration of juice, of which graphically determined indicators IC_{50} .

Keywords: antioxidant activity, juices of cherry, raspberries, strawberry, fluorescein.

Excess concentration of free radicals in the body is the central risk factor for cardiovascular, oncological diseases and other pathologies. Flavonoids have strong antioxidant properties and can be used to prevent various diseases. Many berries include flavonoids such as quercetin and rutin, as well as anthocyanins and other phenolic glycosides that act as free radical inhibitors [1-3].

A comparative study of the antioxidant activity of 4 packaged juices of various brands containing cherries: «Rich» (Russia) (1), «Sochny» (Belarus) (2), «Fruto-nanya» (Russia) (3), «My family» (Belarus) (4) (table 1); 5 packaged juices containing raspberries: «My family» (Belarus) (1), «Dobry» (Belarus) (2), «Fruto-nanya» (Russia) (3) and (4), «Soki Pridonya» (5) (Table 2) and 4 packaged juices containing strawberries: «Odesski» (Ukraine) (1), «My Family» (Belarus) (2), «Fruto-nanya» (Russia) (3) and (4) (Table 3). Also, a comparison of these juices with juices from fresh berries is made. The method of determining the antioxidant activity with respect to activated forms of oxygen is based on measuring the fluorescence intensity of the oxidizable compound and its decrease under the influence of active oxygen species. In this work, fluorescein is used to detect free radicals, which has a high extinction coefficient and close to 1 quantum yield of fluorescence. Generation of free radicals was carried out using the Fenton system, in which hydroxyl radicals are formed during the reaction of the iron complex with EDTA and hydrogen peroxide.