# Poster session Programme Advisory Committee for Condensed Matter Physics (25 January, 2024)

Poster abstract	Remarks
1. Morris Water Maze and Open Field: development of web service prototypes for	
automating videodata analysis for behavioral tests	
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<ul> <li>Within a JINR MLIT-LRB project, the BIOHLIT information system, assigned to automate data analysis for investigating the influence of ionizing radiation, is being developed.</li> <li>One of the components of implemented investigations is related to the study of different rodent cognitive dimensions and behavior features using specialized test systems, such as the Morris Water Maze and the Open Field, which are located at the Laboratory of Radiation Biology. To automate videodata analysis, a web service prototype for the Morris Water Maze behavioral test was developed. It is designed to generate datasets needed for the classification of motion trajectories of rodents (search strategy). The developed web service enables to monitor the correctness of generated trajectories and form a dataset in different representations. Based on computer vision methods, a tracking algorithm for rodents was proposed in the Morris Water Maze test system.</li> <li>Using a convolution neural network, preliminary results related to the trajectory classification were obtained. The results demonstrate the necessity of both the extension of the training sample and the representation of trajectories with characteristic marks. A web service prototype for the Open Field behavioral test was developed. It allows one to solve the rodent tracking problem, to build a heat map, to count the sectors covered and present common analysis for users.</li> <li>All investigations are performed with the help of the ML/DL/HPC ecosystem of the HybriLIT heterogeneous computing platform.</li> </ul>	
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### 2. Photoactivated NETosis

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In response to a variety of physiological and pharmacological stimuli, neutrophils release decondensed chromatin, also known as neutrophil extracellular traps (NETs). In recent years, studies have been performed on photoactivated NET formation, mainly by ultraviolet (UV) radiation. In following studies, it has been demonstrated, for the first time, that NET formation is activated not only by UV but also by three spectra of visible light: blue, green, and orange, in a dose-dependent manner [1]. Moreover, a hypothesis about the primary photoacceptors of photoactivated NETosis was put forward and proven, since understanding the molecular mechanisms of various forms of NETosis for regulating the unwanted formation of NETosis is very important [2].

NETosis was induced by irradiation with wavelength-switchable LED sources. Raman spectroscopy was used for searching and identifying special biomarkers of photoactivated NETosis and fluorescence microscopy was applied for visualization and quantification of NET release, respectively. Furthermore, using inhibitory analysis, we established that photoactivated NETosis proceeds through NADPH oxidase and PAD4 signaling pathways. The citrulline's low-frequency vibrational modes and the distinctive raman frequencies of different reactive oxygen species (ROS) were recorded for the first occasion by Raman spectroscopy. The development of new drugs designed to suppress NETosis, especially when induced by exposure to intense UV and visible light, can help to mitigate light-induced photoaging and other damaging effects of electromagnetic radiation.

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# 3. Origin of high pressure phase transition in the Ln<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> (Ln = La, Nd, Pr) Carply- Galy phases.

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#### Abstract

The investigation of the layered perovskite-like compound  $Ln_2Ti_2O_7$  (Ln = La, Nd, Pr) involved a comprehensive examination of its structural and vibrational characteristics employing X-ray diffraction and Raman spectroscopy under pressures reaching 30 GPa. The findings suggest the occurrence of a gradual structural phase transition from the initial ferroelectric monoclinic P2<sub>1</sub> phase to the paraelectric monoclinic P2<sub>1</sub>/m phase at approximately  $P_{Nd_2Ti_2O_7}$ =19.0 Gpa,  $P_{La_2Ti_2O_7} = 16.7$  Gpa and  $P_{Pr_2Ti_2O_7} = 13.8$  GPa. This pressure-induced transition manifested anomalies in unit cell compression and alterations in the pressure-dependent behavior of vibrational modes [1]. The monoclinic crystal structure of  $P2_1$  symmetry, as predicted by group theory, presented 132 Raman-active modes. A discernible increase in observed mode wavenumbers was noted at pressures below the phase transition pressure, with anomalies in the pressure behavior of specific vibrational modes near the transition pressure being linked to changes in pressure coefficients [2]. Noteworthy alterations were observed in certain vibrational modes, such as the disappearance of some and the appearance of new modes post-transition, signifying a distortion in the  $TiO_6$  octahedra [3]. These anomalies, occurring in proximity to specific pressures, indicate the continuous nature of the phase transition. Furthermore, anomalies in the pressure behavior of lattice parameters were observed at approximately around 14.0 GPa -19.0 GPa, signifying a structural phase transformation. The anisotropic nature of lattice compression was evident, with the c-axis in the monoclinic phases displaying the highest compressibility. The average compressibility of the "c" parameter was approximately three times greater than that of the "a" and "b" parameters. Even post-structural phase transition, a pronounced compression anisotropy persisted. Additionally, a marked increase in the monoclinic angle " $\beta$ " in the vicinity of the transition pressure was documented.

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# 4. Coarse-grained simulation of phospholipid membrane self-assembly in the presence of amyloid beta peptides

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At present, there is a hypothesis about the key role of amyloid beta peptide in the onset of Alzheimer's disease. It is considered that its interaction with cell membranes causes a disruption of their permeability and integrity, which may trigger further neurodegenerative processes [1]. The experimental study showed that the peptide took part in the morphological changes of the phospholipid membrane during its transition through the main lipid phase transition temperature [2]. However, this research did not allow us to look into the processes and resulting structures at the atomic level. The latter results are better achieved in the theoretical studies we have carried out recently.

In order to describe the assembly process of phospholipid membranes in the presence of amyloid beta peptides, the interaction of  $A\beta(25-35)$  with zwitterionic DPPC phospholipids has been simulated using the coarse-grained molecular dynamics method in the GROMACS 2019.3 software package. We have found that the system assembles into bicelle-like structures with peptides on the rim at the temperature below the phase transition of the lipid, while it assembles into a system of small vesicles with peptides embedded in the lipid bilayer at the temperature above the phase transition temperature. The results obtained are in good agreement with those obtained experimentally and complement the picture of what is happening in phospholipid membranes loaded with amyloid beta peptides [3].

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#### 5. Convolutional neural network for reconstruction of neutron tomography data.

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Convolutional neural network (CNN) is a powerful tool for working with various images. There is a significant potential for using CNN in neutron tomography tasks [1-3]. The use of CNN makes it possible to improve the accuracy of reconstruction of 3D models, as they are able to identify even complex features and image structures. On the other hand, neutron tomography generates large amounts of data, and CNNs are well suited to efficiently process such data. CNN's parallel processing capabilities allow for faster analysis of large datasets, thereby improving overall performance. In this way, they can reduce data processing time, which is especially important for scientific applications of neutron tomography.

This paper presents the results of the development of a convolutional neural network for the reconstruction of three-dimensional data from an incomplete set of radiographic projections. The effectiveness of this approach is demonstrated in comparison with conventional reconstruction algorithms. The minimum required number of projections for tomographic reconstruction using CNN is also determined.

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6. Numerical study of the influence of model parameters on the effect of magnetic moment reversal in systems of  $\varphi_0$  Josephson junctions with pulsed and inductive current sources

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A study of the periodic structure of magnetic moment reversal domains in the systems of the  $\varphi_0$ -junction superconductor-ferromagnet-superconductor depending on the values of model parameters was carried out. Variants of a  $\varphi_0$ -junction system with pulsed and inductive current sources, described by the Cauchy problem for a system of nonlinear ordinary differential equations, were considered. This problem is solved numerically in a wide range of varying model parameters. To speed up mass calculations, parallel versions of computer code were developed, and their efficiency was confirmed by test calculations. The calculations were performed on the HybriLIT computing resources of the JINR Multifunctional Information and Computing Complex.

# 7. DNA DSB formation kinetics in mature neurons of primary rat hippocampal cell culture after exposure to ionizing radiation with different physical characteristics <u>Hramco T.S.<sup>1,2</sup></u>, Krupnova M.E.<sup>1</sup>, Pahomova N.V.<sup>1</sup>, Shamina D.D.<sup>1</sup>, Yasinskaya A.V.<sup>1,2</sup>,

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The modern challenges of space radiobiology and radiation therapy raise the problem of ionizing radiation's negative impact on the brain, which is known for variable radiosensitivity of its structures. The hippocampus is considered one of the most radiosensitive brain structures due to the adult neurogenesis processes and long-term memory disruption. The negative effects of radiation highly depend on the radiation source and the physical characteristics of exposure, which explains a wide range of DNA damage types induced in neurons.

To examine the effects of various sources of ionizing radiation on mammalian neuron cells, the method of primary rat hippocampal cell culture was used. This method is widely implemented *in vitro* to study molecular and cellular processes in the brain. In our work, we investigated the influence of protons, nitrogen ions, and  $\gamma$ -rays on DNA double-strand break (DSB) formation – one of the most severe types of DNA damage. The DNA DSB number and complexity were evaluated based on radiation-induced DNA repair protein foci (RIF) formation: phosphorylated histone H2AX ( $\gamma$ H2AX) and repair protein 53BP1.

The primary rat hippocampal cell culture was prepared from newborn rats (P0-P1, *Sprague Dawley*). Initially isolated rat hippocampal formation was trypsinized, and a single cell suspension was plated onto Petri dishes precoated with poly-L-lysine. To remove non-neuronal cells from the culture, part of the samples was exposed to a 3  $\mu$ M Ara-C solution for 24h at day *in vitro* (DIV) 4. Afterwards, all the samples were cultivated under the recommended conditions until the moment of irradiation.

Samples of primary rat hippocampal cell culture were irradiated with <sup>60</sup>Co  $\gamma$ -rays (3 Gy, 1.25 MeV, 0.3 keV/µm), protons (3 Gy, 150 MeV), or <sup>15</sup>N ions (1.25 Gy, 14 MeV/nucleon, 175 keV/µm) at DIV16, 18, and 10, correspondingly. 1, 4, and 24 h post-irradiation cells were fixed in 4% PFA solution. Then, DNA DSBs were visualized by indirect immunocytochemical staining with combinations of the primary and secondary antibodies conjugated with FITC and Texas Red fluorescent dyes. For  $\gamma$ -irradiation, the colocalization of  $\gamma$ H2AX and 53BP1 protein markers was used to identify the DNA DSBs without specific cell-type markers. For proton or nitrogen irradiation, the  $\gamma$ H2AX protein marker only was used to identify the DNA DSBs with a cell-type marker of mature neurons, MAP2. The fluorescent images were received with AxioImager.M2 equipped with ApoTome.2.

Several conclusions can be drawn from the obtained results. The number of RIF is significantly higher after proton irradiation than after  $\gamma$ -irradiation, which may be due to the specifics of proton energy transfer. The RIF formation peak shifts with increasing LET to later post-irradiation time. The number of RIF is 2.4 times higher 1h after nitrogen irradiation compared to  $\gamma$ -irradiation; 24h after nitrogen irradiation, the RIF number remained constant in contrast to proton irradiation: 21  $\gamma$ H2AX foci for <sup>15</sup>N-ions, and 13  $\gamma$ H2AX foci for protons. Foci cluster complexity grows as LET increases, which is clearly indicated by the dominance of foci clusters with a higher number of individual foci.

# 8. Chromosomal abnormalities in blood lymphocytes of *Macaca mulatta* monkeys after irradiation of monkeys' heads with <sup>12</sup>C ions

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The attention of many researchers is directed to the assessment of risks and dangers associated with the effects of cosmic radiation on crew members during long space missions outside Earth's magnetosphere [1, 2]. Along with the study of cognitive functions [3], it seems important to evaluate the radiobiological markers of cytogenetic damage caused by various types of ionizing radiation, the exposure to which will be encountered during flight.

The paper presents data on chromosomal abnormalities in blood lymphocytes of *Macaca Mulatta* monkeys after total exposure to <sup>137</sup>Cs  $\gamma$ -rays under hypokinesia and partial irradiation of the animals' heads with accelerated <sup>12</sup>C ions at a dose of 1 Gy with an interval of 8 days. The studies were carried out 24 hours and 19, 39, 92, 446 and 550 days after carbon ion irradiation.

Cytogenetic analysis of chromosomal abnormalities was performed in the control and irradiated monkeys. The level of aberrations in the control did not exceed 1.8 %. The highest yield of cells with chromosomal abnormalities was recorded 24 hours after irradiation with <sup>12</sup>C ions and was at least 13%, which is seven times higher than in the control. By 550 days, a decrease in the level of aberrations was observed in blood lymphocytes of irradiated monkeys; nevertheless, it still exceeded the control values by 2.5–3 times. A similar trend was observed for dicentrics and centric rings, which are markers of radiation exposure: their level gradually decreased. By the end of the study period, their number still significantly exceeded the control data, and they accounted for more than 20% of the total number of aberrations. The main type of aberrations was fragments (up to 50%). The observed decrease in the total number of chromosomal aberrations, including markers of radiation exposure, is probably related to the elimination of cells with unstable chromosomal aberrations from circulating blood over time.

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#### 9. Induction of DNA double-stranded breaks in tumor cells in the presence of DNA repair modifiers under the action of protons

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In recent years, beams of accelerated protons have been increasingly used in radiation therapy for oncological diseases. An important reason for the exceptional interest of specialists in the use of this type of radiation in radiation oncology is the differences in the distribution of absorbed doses in the irradiated tumor under the influence of protons and photon radiation. It is well known, that the maximum energy during the passage of particles through tissue matter is transferred at the end of their path (in the Bragg peak) and the dose distribution is characterized by high conformity with respect to the irradiated target: maximum damage to the tumor area and less damage to adjacent healthy tissue.

Among the wide range of different DNA lesions induced by ionizing radiation, the most severe violations leading to cell death are simultaneous violations of the integrity of both DNA strands, namely double-strand breaks (DSBs). Double-strand breaks are formed either as a result of the direct rupture of two complementary sections, the so-called direct DSBs, which are caused by energy transfer to the local DNA segment and result in the violation of its integrity, or are formed from other lesions as "repair costs" during the action of repair enzymes. This type of damage is classified as enzymatic DSBs.

Since the yield of enzymatic DNA DSBs during irradiation depends on a number of biological factors, the frequency of their formation can be influenced by modifying DNA repair processes. To study the features of induction and repair of DNA damage under the action of different quality ionizing radiation and the contribution of enzymatic DNA DSBs, we used DNA repair inhibitors – arabinoside cytosine (AraC), hydroxyurea (HU) and ligase IV inhibitor – SCR7.

Using the DNA comet assay, it was shown that the number of DNA DSBs after combined action of modifiers (AraC/SCR7 and AraC/HU) and ionizing radiation significantly exceeds the number of DNA DSBs formed only under the action of ionizing radiation without the use of modifiers. The kinetics of DNA DSB repair in tumor cell cultures under the influence of various DNA repair inhibitors is complex and is characterized by an increase in the yield of DNA damage up to 6 hours of post-irradiation incubation, after which the amount of damage begins to decrease. However, even 24 hours after exposure to ionizing radiation, the number of DNA DSBs under the action of inhibitors exceeds the control level of damage.

Damage repair caused by radiation is a set of simultaneously occurring but multidirectional processes: firstly, the formation of enzymatic DSBs from single-strand breaks and damaged bases occurs due to the work of base excision repair and repair of AP sites, and secondly, repair along the path of non-homologous end joining of both direct DNA DSBs and formed enzymatic DSBs. The implementation of these biological effects in distant post-radiation period will be largely determined by the residual pool of cluster damage.

#### 10. High pressure effect on crystal structure of vdW magnet Fe<sub>3</sub>GeTe<sub>2</sub>

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Recently, a long-range magnetic ordering has been discovered in 2D van der Waals structures, which can be maintained at sufficiently high temperatures within the monolayer [1]. In addition, van der Waals two-dimensional magnets attract close attention in connection with the search and research of exotic phenomena, including those that occur under extreme conditions (high pressure and low temperatures). Metallic Fe<sub>3</sub>GeTe<sub>2</sub> is one of the most interesting representatives of this family of compounds due to having a higher critical temperature ( $T_C \sim 220$ K) [2]. Its great potential has also been highlighted by recent experiments showing that  $T_C$  can be increased even up to room temperature [3]. On the other hand, its electronic and magnetic properties are far from being clearly understood. The very basic picture for the magnetic moment is still under debate, as is the effect of high pressure on crystalline and magnetic properties.

High pressure investigation is a direct method of controlled change in magnetic interactions due to variations in interatomic distances and angles. Investigations at high pressures provides a unique opportunity to study the relationship between changes in structural parameters and magnetic properties, which is necessary to understand the nature and mechanisms of physical phenomena observed in the van der Waals materials.

This work is devoted to the investigation of the crystal structure and vibrational properties of Fe<sub>3</sub>GeTe<sub>2</sub> in wide pressure range using the combination of X-ray diffraction and Raman spectroscopy (FLNP, JINR, Dubna, Russia). It was found that the initial hexagonal crystal structure of Fe<sub>3</sub>GeTe<sub>2</sub> is preserved in the studied pressure range up to 19 GPa. The baric dependences of the parameters and volume of the unit cell, bond lengths and angles for Fe<sub>3</sub>GeTe<sub>2</sub> are obtained. An sostructural phase transition manifests at high pressure of  $P \sim 7$  GPa. The observed isostructural ransition is accompanied by anomalies in the baric dependences of the parameters and volume of he unit cell, interatomic distances and angles. The observed anomalies in the baric behavior of nteratomic distances oriented along the *c* axis indicate the competing nature of intraplane and nterplane interactions. A significant decrease in the interatomic distances Fe-Fe and an increase in he angles Fe1-Te(Ge)-Fe1,2 also indicates an increase in the antiferromagnetic state and a corresponding suppression of the ferromagnetic state. The anomalous behavior of the frequencies and half-widths of the Fe<sub>3</sub>GeTe<sub>2</sub> vibrational modes in the vicinity of the isostructural transition associated with the anomalous behavior of the interatomic distance and angles was also found.

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# 11. Features in the formation of lipid bilayers from soy phospholipids and DMPC on a silicon substrate

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The use of special biodegradable systems for the transfer of biologically active substances has become widespread [1]. Such systems have a number of advantages: increasing the bioavailability of drugs, the possibility of targeted delivery of drug compounds and reducing the number of side effects compared to the same drugs, but in their usual form [2].

Studies on the interaction of such systems with the cell membrane or lipid bilayer have currently been carried out in insufficient quantities [3]. To better understand the mechanism of penetration, it is necessary to start with the creation of a model membrane and study the process of interaction of nanodrugs with the model membrane.

The aim of the experiment was to investigate the differences in the formation of lipid bilayers from soybean phospholipids with different purities (S80 and S100) and dimyristoylphosphatidylcholine (DMPC). The experiment was carried out using the time-of-flight neutron reflectometry method at the Joint Institute for Nuclear Research on the neutron reflectometer "GRAINS". The peculiarity of this installation is that it has a horizontal sample plane, and it is also possible to use a washable cell. A silicon crystal was chosen as a substrate, on which an oxide layer was grown in the laboratory. Solutions were prepared in heavy water with a phospholipid concentration of 0.1%

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### 12. Development of Python-based tools for modeling the dynamics of systems based on Josephson junctions

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Active research into possible applications of systems based on Josephson junctions, superconducting electronics and spintronics [1, 2] necessitates the development of effective tools for the mathematical modeling of such systems. As part of a joint project between MLIT and BLTP, an ecosystem based on the Jupyter environment is being developed using Python libraries and publishing materials in the form of a Jupyter Book. A distinctive feature of this representation is the ability to accompany the computational code with a description of the problem being solved with formulas and graphs. It should be noted that a number of tasks require numerous resource-intensive calculations, which leads to the need for the significant speedup of computational schemes implemented in Python and the development of parallel algorithms.

Developed algorithms for calculating the current-voltage characteristic of a Josephson junction under the influence of external radiation and computing the dependence of the width of the Shapiro step on the amplitude of external radiation, as well as implemented approaches for speeding up computational circuits using specialized Python libraries, will be presented. The developed materials are publicly available on the ML/DL/HPC ecosystem of the HybriLIT platform (MLIT JINR) [3] in the form of Jupyter Book [4, 5].

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# 13. The neurobiological effects of exposure to accelerated charged particles

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The study of effects of accelerated charged particles on behavior and morphological changes in the central nervous system (CNS) is an important task in space and medical radiobiology. Assessment of this neurobiological effects will help make hadron therapy more safety and decrease the risks of interplanetary space flights. The report will present a comparative analysis of behavioral reactions and morphological changes in early and late periods in the brain of adult rats after exposure to gamma radiation, protons of various energies and carbon ions.

JINR accelerators and sources were used to irradiate animals SD rats. During the research, the behavior of animals was analyzed at the Open Field Test, T-maze, and stand for recording visual reactions. To analyze morphological changes in brain tissue, staining with cresylviolet, Congo red, and the TUNEL method was used. A quantitative assessment of neurons with various types of morphological changes in the cortex, cerebellum, and hippocampus of 1 Gy irradiated animals was carried out.

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# 14. Effect of DNA synthesis inhibitor AraC on DNA double-strand breaks formation in normal and tumor cells under proton irradiation

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Treatment of malignant neoplasms is an extremely complex and multistage process, requiring the involvement of various methods of action on tumor cells, involving both different irradiation techniques and radiosensitizing agents. Cytosine arabinoside (AraC) is one of radiosensitizing compounds. AraC is an inhibitor of DNA polymerases and is incorporated into replicating DNA strands, resulting in inhibition of strand initiation and extension. It can also be used in combination with irradiation, enhancing the effect of the latter due to the formation of additional enzymatic DNA double-strand breaks from single-stranded substrate. Which we showed in the course of experiments on different types of cells: normal and tumor cells.

The cultures of normal human skin fibroblasts (NHDF 22873, Lonza, CC2509) and tumor cells (human glioblastoma, U87) were used for the experiments. 1 h before irradiation, fibroblasts and U87 cells were treated with 20 mM of AraC-solution dissolved in cultural media. The irradiation of samples was carried out by protons at the phasotron facility (DNLP JINR) and <sup>15</sup>N-ions at the U400-M facility (FLNR JINR) at a dose of 1.25 Gy.

DNA double-strand breaks were visualized by immunocytochemical staining using primary antibodies specific to DNA double-strand breaks proteins - phosphorylated histone H2AX ( $\gamma$ H2AX) and repair protein 53BP1. The survival of glioblastoma cells (U87) was assessed by counting the macrocolonies formed by the cells after 10 days of postirradiation cultivation. The samples were stained with cresyl violet dye.

It was found that the number of foci per cell decreases with time after proton irradiation under normal conditions in both cell cultures. However, the presence of the AraC inhibitor induces increase of a persistent foci number until the 24 h: 6-fold higher growth in the fibroblasts and 3-fold higher in the glioblastoma cells compared to the number of foci in cells that were not exposed to the inhibitor.

## 15. mFISH analysis of chromosome aberrations induced *in vitro* in human lymphocytes by γ-rays <sup>60</sup>Co and 130 kVp X-rays

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We exploited classical metaphase method of chromosome aberrations analysis and advanced multicolor FISH method to investigate the biological efficiency of 130 kVp X-rays (CellRad, Precision, USA) of different quality (added filtration) and their suitability as a reference radiation in radiobiological research. For this study, human lymphocytes were irradiated in vitro with 130 kVp X-rays + 0.5 mm Al built-in added filtration (mean energy 48.8 keV, effective energy 25.4 keV) or 0.1 mm Cu custom-made added filtration (mean energy 57.7 keV, effective energy 38.5 keV) at doses 1-4 Gy, harvested 48 h after irradiation and aberrations in metaphases of the first post-irradiated cell cycle were assessed. The cytogenetic effects of X-ray radiation were compared with the results obtained at the  $\gamma$ -<sup>60</sup>Co unit (ROKUS-M, JINR) and with the results obtained earlier by one of the authors at the 250 kVp X-ray unit (Seifert, GSI, Germany) [1,2]. Classical metaphase analysis revealed no clear differences in biological efficiency of 130 kVp X-rays with both added filtration compared to 250 kVp X-rays. The modern powerful method of molecular cytogenetics multicolor FISH (mFISH) based on the entire genome painting allows visualizing more chromosome rearrangements with higher precision than routine method. As a result, chromosome aberration analysis by means of mFISH revealed no statistically significant difference in biological efficiency of 130 kVp + 0.1 mm Cu and 250 kVp X-rays (p = 0.137) and statistically significant higher efficiency of 130 kVp X-rays + Al 0.5 mm as compared to 130 kVp X-rays + Cu 0.1 mm (p = 0.019, RBE = 1.11  $\pm$  0.17). y-rays <sup>60</sup>Co induced the lowest aberration frequency among radiation species under study. Noteworthy, the aberration spectra induced by all radiation types used were shown to be similar (~20 % simple breaks, 60% simple exchanges and 20% complex aberrations). Altogether our data show that 130 kVp + 0.1 mm Cu X-rays may be used as a reference radiation in radiobiological research.

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### 16. Structural features of the fragment of cast iron cauldrons of Medieval Golden Horde: neutron tomography data

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The spatial arrangement of the internal pores inside several fragments of ancient cast iron cauldrons related to the medieval Golden Horde period was studied using the neutron tomography method. In our work, we tried to identify the structural features of fragments from cast iron cauldrons of the medieval Golden Horde [1], as a representative of the products from the ancient iron casting process. We have selected two groups of iron-cast fragments from the Selitrennoye settlement is a leftover old Saray-Batu city in the lower parts of the Volga River and the Bolgar settlement in the central Volga region. Both settlements were capitals of the Golden Horde during the 13–15th centuries AD, but the difference in geographic location and historical area appoints them as manufactory centers with modified technological approaches for casting and processing cast iron within the borders of one ancient state in a similar historical period. The experiment was carried out at the DRAGON facility at the National Research Center "Kurchatov Institute" at the IR-8 reactor [2].

We obtained differences in the structural features of the internal structure of fragments of cast iron cauldrons [3], but these results are preliminary due to insufficient statistics.

The high neutron penetration into a cast iron material provides sufficient data for detailed analysis of the three-dimensional imaging data. The size, elongation, and orientation distributions of the observed internal pores were obtained. The imaging and quantitative analytical data are considered structural markers for the location of cast iron foundries, as well as a feature of the medieval casting process.

Also, the study of algorithms for describing porosity or granularity is an important area for studying the properties and characteristics of materials in general, relating not only to cultural heritage items, but also for materials science studies of various metal alloys, concretes, ores, etc.

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## 17. Characterization of Activated Carbon from Rice Husk for Enhanced Energy Storage Devices

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Rechargeable chemical current sources occupy an important place in the development of renewable energy sources and electric vehicles. As part of the development of energy-intensive and efficient rechargeable energy storage devices, an urgent task is to improve the lithium-ion batteries that are used today.

The production of activated carbon (AC) from lignocellulosic biomass through chemical activation is gaining global attention due to its scalability, economic viability, and environmental advantages. Chemical activation offers several benefits, including energy efficiency, reduced carbonization time, and lower temperature requirements. In this study, potassium hydroxide (KOH) was employed for chemical activation, resulting in activated carbon with a high specific surface area of ~3050 m<sup>2</sup>/g. The structural analysis revealed the presence of over 15% of few-layered graphene in the activated carbon matrix. X-ray diffraction (XRD) technique was employed to investigate the activated carbon derived from rice husk (RH). The potential applications of activated carbon obtained from rice husks through chemical activation were explored, including its use for heavy metal removal, elimination of organic pollutants, and as an active material in hybrid energy storage devices. Furthermore, a scaling methodology for the production of activated carbon was proposed, facilitating its industrial implementation.

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