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CONTENTS

PHYSICS

**Aimaganbetova Z.K., Kulshymbayev Y.A., Zhanturina N.N., Beketova G.K.**  
First-principles calculation of the electronic properties of the Double Halide Perovskite  $\text{Cs}_2\text{Ag}_{0.2}\text{Na}_{0.4}\text{In}_{0.6}\text{Ti}_{0.4}\text{Cl}_6$  based on the quantum ESPRESSO software.....14

**Amangeldinova S., Zhuniskhan S., Kalzhigitov N., Kurmangaliyeva V.**  
Study of the cluster structure of  $^5\text{He}$  and  $^5\text{Li}$  mirror nuclei in two-cluster approximation.....35

**Chokin K., Otunchi Ye., Kozhahmetova A., Kasenova A., Shongalova A.**  
Development and testing of a laboratory pyrometallurgical installation for recycling lithium-ion batteries.....46

**Issayeva A., Beisebayeva A., Madybekova G., Shynazbekova Sh., Issa A.**  
Comparative analysis of physico-chemical characteristics of drinking, spring and natural water in the South Kazakhstan.....65

**Kim V.Yu., Aimuratov Y.K.**  
Search for transient cosmic events by scanning the sky with wide-field telescopes.....78

**Koshtybayev T.B., Tatenov A.M., Aliyeva M.E., Tugelbaeva G.T., Zhanaliyeva G.Zh.**  
Study of the electromagnetic field based on thermodynamics principles.....89

**Mukamedenkyzy V., Akberdiyev B.**  
Numerical investigation of the effect of inclination angle on the stability of mechanical equilibrium in Ar–N<sub>2</sub> binary gas mixtures.....105

**Myasnikova L.N., Uzakbaeva S.S., Shanina Z.K., Bekeshev A.Z.**  
Kinetic properties of high-density polyethylene filled with chromium spinel powder.....119

**Nurbayev B.M., Dmitriyeva E.A., Kemelbekova A.E.**  
The role of low-dimensional layered structures in enhancing the stability of tin-based perovskite materials.....136

**Sattinova Z., Ermakhanova F., Assilbekov B., Taimuratova L.**  
Influence of various cooling conditions and heat transfer coefficients on solidification during the formation of beryllium ceramic products.....149

**Shestakova L.I., Serebryanskiy A.V., Spassyuk R.R., Omarov Ch.T.**  
Search for gas of comet-meteor origin in the inner Solar System: caii ion emission.....165

**Ualikhanova U., Tursynkazy F., Syzdykova A.M., Altayeva G.S., Altaibayeva A.B.**  
Studying the amplitude of  $f(T)$  gravitational waves using Bessel functions.....179

<b>Zhexenbayeva G.A., Nasirova D.M., Aimanova G.K., Shomshekova S.A.</b> Photometric study of the symbiotic object V725 Tau.....	194
<b>Zhusupova N.K., Zhadyranova A.A.</b> Bounce cosmology in $f(T, \mathcal{T})$ gravity based on energy condition analysis.....	205
<b>Ziyatbekova G., Abdimanapova P., Sagyntay O., Nurym A., Ilinov R.</b> Using artificial intelligence to predict diseases based on medical data.....	225

## CHEMISTRY

<b>Almassov N.Zh., Zhumagaliyeva A.N., Duisenbekov S.E., Zhakiyev N.K.</b> Design and optimization of hybrid renewable energy systems for hydrogen production in Kazakhstan.....	236
<b>Amangeldi B., Zhanikulov N., Taimasov B., Aitureev M.M., Dauletiyarov M.</b> Calculation of the Raw material composition for obtaining white Portland cement clinker.....	251
<b>Baeshov A., Tashenov E.A., Atykhanova S.B., Koshkarbayeva Sh.T.</b> Preparation of cadmium sulfide by electrochemical method using a composite sulfur–graphite electrode.....	267
<b>Baisalova G.Zh., Azhikhanova Zh., Taltenov A.A., Kuzhatova P.</b> Determination of the total phenolic content in perennial herbaceous plants of the flora of Kazakhstan.....	277
<b>Darmenbayeva A.S., Rajasekharan R., Zhussipnazarova G.M., Mukazhanova Zh.B., Begenova B.E.</b> Composites based on chitosan and cellulose: synthesis, properties, and application prospects.....	287
<b>Erkasov R.Sh., Zhamkenova A.S., Sergazina S.M., Nurmukhanbetova N.N., Kassenova N.B.</b> Halide-dependent modulation of hydrogen bonding in Mn(II) complexes with protonated acetamide: a QAIM, NCI, and energy decomposition study.....	304
<b>Kalimoldina L.M., Shaikhova Zh.E., Kaliyeva B.K., Bubish Sh., Askarova Sh.K.</b> The effect of silver nanoparticles on the germination of bean, lemon, tangerine and avocado seeds.....	320
<b>Kurtebayeva A.A., Alvarez-Torrellas S., Gomes H.T., Orynbayev S.A., Kalmakhanova M.S.</b> Activated-carbon-enhanced polymeric membranes for efficient elimination of emerging contaminants.....	334

<b>Massenova A.T., Zhumakanova A.S., Torlopov I.I., Rakhmetova K.S., Abilmagzhanov A.Z.</b> Optimization of the hierarchical zeolite ZSM-5 synthesis process by steam-assisted alkaline modification.....	350
<b>Mutushev A.Zh., Nuraly A.M., Sanat A.S., Shaukharova M.A., Yessimsiitova Z.B.</b> The effect of light-converting films on the accumulation of bioactive compounds and the quality of fruits.....	366
<b>Nefedov A.N., Taikenova A.T.</b> Current state of organic corrosion inhibitor application in oil refining.....	379
<b>Omarov B.T., Altybayev Zh.M., Serikbayeva B.S.</b> Production of biohumus by vermicomposting of organic wastes and study of its agroecological effectiveness.....	399
<b>Rakhman D.M., Kappasuly A., Makhayeva D.N., Kazybayeva D.S., Irmukhametova G.S.</b> Development and investigation of mucoadhesive hydrogels based on gellan–cysteine complexes.....	414
<b>Sabyrzhanova A.E., Bolatkyzy N., Berganaeva G.E., Dyusebaeva M.A.</b> Study of amino acids and fatty acids in the aerial part of <i>Plantago major</i> .....	428
<b>Satayeva S., Akhmetova F., Urazova A., Aituganova S., Yerniyazova K.</b> The influence of PEPA concentration on the physical, mechanical, and operational properties of ED-20 epoxy adhesives.....	439
<b>Zamanbek A.Zh., Koshkarbayeva Sh.T., Satayev M.S.</b> Methods of Obtaining Silver Nanoparticles and Antibacterial Properties.....	450
<b>Zhortarova A.A., Salkeyeva L.K., Minayeva Ye.V., Ibrayev M.K., Fazylov S.D.</b> New possibilities for the synthesis and phosphorylation of phosphonoacetic acid ester.....	462

## МАЗМҰНЫ

### ФИЗИКА

<b>Аймағанбетова З.К., Құлшымбаев Е.А., Жантурина Н.Н., Бекетова Г.К.</b> Quantum Espresso бағдарламасы негізінде Cs <sub>2</sub> Ag <sub>0.2</sub> Na <sub>0.4</sub> In <sub>0.6</sub> Ti <sub>0.4</sub> Cl <sub>6</sub> кос галогенді перовскиттің электрондық қасиеттерін бірінші принциптік есептеу.....	14
<b>Амангелдинова С., Жүнісхан С., Калжигитов Н., Курманғалиева В.</b> Екі кластерлік жуықтауда 5He және 5Li айналық ядроларының кластерлік құрылымын зерттеу.....	35
<b>Чокин К., Отунчи Е., Кожаметова А., Касенова А., Шонғалова А.</b> Литий-ионды аккумуляторларды қайта өндеуге арналған зертханалық пирометаллургиялық қондырғыны әзірлеу және сынау.....	46
<b>Исаева А.Б., Бейсебаева А.С., Мадыбекова Г.М., Шиназбекова Ш.С., Иса А.Б.</b> Сравнительный анализ физико-химических характеристик питьевой, родниковой и природной воды юга Казахстана.....	65
<b>Ким В.Ю., Аймуратов Е.К.</b> Кең бұрышты телескоптармен аспанды сканерлеу арқылы өтпелі ғарыштық оқиғаларды іздеу.....	78
<b>Коштыбаев Т.Б., Татенов А.М., Алиева М.Е., Тугелбаева Г.Т., Жаналиева Г.Ж.</b> Электромагниттік өрісті термодинамикалық бастамалар тұрғысында зерттеу.....	89
<b>Мукамеденқызы В., Ақбердиев Б.</b> Ar–N <sub>2</sub> бинарлы газ қоспаларындағы механикалық тепе-теңдік тұрақтылығына қиғаш бұрыштың әсерін сандық зерттеу.....	105
<b>Мясникова Л.Н., Узакбаева С.С., Шанина З.К., Бекешев А.З.</b> Хром-шпинельді ұнтақ қосылған жоғары тығыздықты полиэтиленнің кинетикалық қасиеттері.....	119
<b>Нұрбаев Б.М., Дмитриева Е.А., Кемелбекова А.Е.</b> Қалайы негізіндегі перовскитті материалдардың тұрақтылығын арттырудағы төменөлшемді қабатты құрылымдардың рөлі.....	136
<b>Саттинова З., Ермаханова Ф., Асылбеков Б., Таймуратова Л.</b> Бериллий керамикалық бұйымдарын қалыптастыру кезінде әр түрлі салқындату жағдайлары мен жылу беру коэффициенттерінің қатаюға әсері.....	149
<b>Шестакова Л.И., Серебрянский А.В., Спасюк Р.Р., Омаров Ш.Т.</b> Күн жүйесінің ішкі аймағындағы комета-метеорлық тектегі газды іздеу: CaII иондарының жарқырауы.....	165

**Уалиханова У.А., Тұрсынқазы Ф., Сыздықова А.М., Алтаева Г.С., Алтайбаева А.Б.**  
Бессель функцияларын пайдаланып  $f(T)$  гравитациялық толқындардың  
амплитудасын зерттеу.....179

**Жексенбаева Г.А., Насирова Д.М., Айманова Г.К., Шомшекова С.А**  
V725 Тау симбиотикалық объектiсiн фотометрлiк зерттеу.....194

**Жусупова Н.К., Жадыранова А.А.**  
Энергия шарттарын талдауға негiзделген  $f(T, T)$  серпiлiс космологиясы.....205

**Зиятбекова Г.З., Абдиманапова П.Б., Сағынтай О.А., Нұрым А.А., Ильинов Р.А.**  
Жасанды интеллект көмегiмен медициналық деректер бойынша  
ауруларды болжау.....225

### ХИМИЯ

**Алмассов Н.Ж., Жумагалиева А.Н., Дүйсенбеков С.Е., Жакиев Н.К.**  
Қазақстанда сутегi өндiруге арналған гибрирдiк жаңартылатын энергия жүйелерiн  
жобалау және оңтайландыру.....236

**Амангелдi Б., Жаникулов Н., Таймасов Б., Айтүреев М., Даулетияров М.**  
Ақ портландцемент клинкерiн алу үшiн шикiзат шихта құрамын есептеу.....251

**Баешов А., Ташенов Е.А., Атыханова С.Б., Кошкарбаева Ш.Т.**  
Композициялы күкiрт-графит электродын қолдану арқылы кадмий  
сульфидiн электрохимиялық әдiспен алу.....267

**Байсалова Г.Ж., Ажиханова Ж., Талтенов А.А., Құжатова П.**  
Қазақстан флорасындағы көпжылдық шөптесiн өсiмдiктердiң фенолдық  
қосылыстарының жиынтық мөлшерiн анықтау.....277

**Дарменбаева А.С., Rajasekharan R., Жусипназарова Г.М., Мукажанова Ж.Б.,  
Бегенова Б.Е.**  
Хитозан және целлюлоза негiзiндегi композиттер: синтез, қасиеттерi және қолдану  
перспективалары.....287

**Еркасов Р.Ш., Жамкенова А.С., Сергазина С.М., Нурмуханбетова Н.Н.,  
Касенова Н.Б.**  
Mn (II) кешендерiндегi сутектiк байланыстардың энергиясы мен табиғатына  
галогеннiң әсерi: QТАІМ, NCI және энергия декомпозициясы.....304

**Калимолдина Л.М., Шаихова Ж.Е., Калиева Б.К., Бубиш Ш., Аскарова Ш.К.**  
Күмiс нанобөлшектерiнiң бұршақ, лимон, мандарин, авокадо тұқымдарының  
өнуiне әсерi.....320

<b>Қуртебаева А.А., Álvarez-Torrellas S., Gomes Н.Т., Орынбаев С.Ә., Калмаханова М.С.</b> Алаңдаушылық тудыратын ластаушы заттарды тиімді жою үшін белсендірілген көмір полимерлі мембраналар.....	334
<b>Масенова А.Т., Жұмақанова А.С., Торлопов И.И., Рахметова К.С., Абильмагжанов А.З.</b> ZSM-5 иерархиялық цеолитін бумен сілтілі модификациялау арқылы алу процесін онтайландыру.....	350
<b>Мутушев А.Ж., Нұралы Ә.М., Санат А.С., Шаукарова М.А., Есимситова З.Б.</b> Жарық түрлендіретін пленкалардың биоактивті қосылыстардың жинақталуына және жеміс сапасына әсері.....	366
<b>Нефедов А.Н., Тайекенова А.Т.</b> Мұнай өңдеу өнеркәсібінде органикалық коррозия ингибиторларын қолданудың қазіргі жағдайы.....	379
<b>Омаров Б.Т., Алтыбаев Ж.М., Серикбаева Б.С.</b> Органикалық қалдықтарды вермикомпостинг арқылы биогумус өндіру және оның агроэкологиялық тиімділігін зерттеу.....	399
<b>Рахман Д.М., Қаппасұлы Ә., Махаева Д.Н., Қазыбаева Д.С., Ирмухаметова Ғ.С.</b> Геллан–цистеин кешендері негізінде мукоадгезиялық гидрогельдерді әзірлеу және зерттеу.....	414
<b>Сабыржанова А.Е., Болатқызы Н., Берганаева Г.Е., Дюсебаева М.А.</b> Plantago Major жер үсті бөлігінің құрамындағы амин қышқылдары мен май қышқылдарын зерттеу.....	428
<b>Сатаева С., Ахметова Ф., Уразова А., Айтуганова С., Ерниязова К.</b> ЭД-20 эпоксидті желімдерінің физика-механикалық және эксплуатациялық қасиеттеріне ПЭПА концентрациясының ықпалы.....	439
<b>Заманбек А.Ж., Кошкарбаева Ш.Т., Сатаев М.С.</b> Күміс нанобөлшектерінің алыну әдістері мен антибактериалдық қасиеттері.....	450
<b>Жоргарова А.А., Салькева Л.К., Минаева Е.В., Ибраев М.К., Фазылов С.Д.</b> Фосфоносірке қышқылының эфирін синтездеу мен фосфорландырудың жаңа мүмкіндіктері.....	462

## СОДЕРЖАНИЕ

## ФИЗИКА

<b>Аймаганбетова З.К., Кулшымбаев Е.А., Жантурина Н.Н., Бекетова Г.К.</b> Расчет по первому принципу электронных свойств двойного галогенидного перовскита Cs <sub>2</sub> Ag <sub>0.2</sub> Na <sub>0.4</sub> In <sub>0.6</sub> Ti <sub>0.4</sub> Cl <sub>6</sub> на основе программы Quantum Espresso.....	14
<b>Амангелдинова С., Жүнісхан С., Калжигитов Н., Курмангалиева В.</b> Исследование кластерной структуры зеркальных ядер <sup>5</sup> He и <sup>5</sup> Li в двухкластерном приближении.....	35
<b>Чокин К., Отунчи Е., Кожрахметова А., Касенова А., Шонгалова А.</b> Разработка и испытания лабораторной пирометаллургической установки для переработки литий-ионных аккумуляторов.....	46
<b>Исаева А.Б., Бейсебаева А.С., Мадыбекова Г.М., Шиназбекова Ш.С., Иса А.Б.</b> Сравнительный анализ физико-химических характеристик питьевой, родниковой и природной воды юга Казахстана.....	65
<b>Ким В.Ю., Аймуратов Е.К.</b> Поиск транзиентных космических событий методом сканирования неба широкоугольными телескопами.....	78
<b>Коштыбаев Т.Б., Татенов А.М., Алиева М.Е., Тугелбаева Г.Т., Жаналиева Г.Ж.</b> Исследование электромагнитного поля на основе термодинамических принципов.....	89
<b>Мукамеденкызы В., Акбердиев Б.</b> Численное исследование влияния угла наклона на устойчивость механического равновесия в бинарной газовой смеси Ar–N <sub>2</sub> .....	105
<b>Мясникова Л.Н., Узакбаева С.С., Шанина З.К., Бекешев А.З.</b> Кинетические свойства высокоплотного полиэтилена с добавлением хром-шпинельного порошка.....	119
<b>Нурбаев Б.М., Дмитриева Е.А., Кемелбекова А.Е.</b> Роль низкоразмерных слоистых структур в повышении стабильности перовскитных материалов на основе олова.....	136
<b>Саттинова З., Ермаханова Ф., Асылбеков Б., Таймуратова Л.</b> Влияние различных условий охлаждения и коэффициентов теплопередачи на затвердевание при формировании бериллиевых керамических изделий.....	149

<b>Шестакова Л.И., Серебрянский А.В., Спасюк Р.Р., Омаров Ш.Т.</b> Поиск газа кометно-метеорного происхождения во внутренней области Солнечной Системы: Свечение ионов СаII.....	165
<b>Уалиханова У.А., Турсынказы Ф., Сыздыкова А.М., Алтаева Г.С., Алтайбаева А.Б.</b> Изучение амплитуды $f(T)$ гравитационных волн с использованием функций Бесселя.....	179
<b>Жексенбаева Г.А., Насирова Д.М., Айманова Г.К., Шомшекеева С.А.</b> Фотометрическое исследование симбиотического объекта V725 Tau.....	194
<b>Жусупова Н.К., Жадыранова А.А.</b> Космология отскока в $f(T, \mathcal{J})$ гравитации на основе анализа энергетических условий.....	205
<b>Зиятбекова Г.З., Абдимананова П.Б., Сағынтай О.А., Нұрым А.А., Ильинов Р.А.</b> Использование искусственного интеллекта для прогнозирования заболеваний на основе медицинских данных.....	225

## ХИМИЯ

<b>Алмассов Н.Ж., Жумагалиева А.Н., Дуйсенбеков С.Е., Жакиев Н.К.</b> Проектирование и оптимизация гибридных возобновляемых источников энергии для производства водорода в Казахстане.....	236
<b>Амангелді Б., Жаникулов Н., Таймасов Б., Айтуреев М., Даулетияров М.</b> Расчёт состава сырьевой шихты для получения белого порландцементного клинкера.....	251
<b>Башов А., Ташенов Е.А., Атыханова С.Б., Кошкарбаева Ш.Т.</b> Получение сульфида кадмия электрохимическим методом с использованием композитного сера-графитового электрода.....	267
<b>Байсалова Г.Ж., Ажиханова Ж., Талтенов А.А., Кужатова П.</b> Определение суммы фенольных соединений в многолетних травянистых растениях флоры Казахстана.....	277
<b>Дарменбаева А.С., Rajasekharan R., Жусиппазарова Г.М., Мукажанова Ж.Б., Бегенова Б.Е.</b> Композиты на основе хитозана и целлюлозы: синтез, свойства и перспективы применения.....	287
<b>Еркасов Р.Ш., Жамкенова А.С., Сергазина С.М., Нурмуханбетова Н.Н., Касенова Н.Б.</b> Влияние галогена на энергетику и природу водородных связей в Mn(II): QTAIM, NCI и энергодекомпозиция.....	304

<b>Калимолдина Л.М., Шаихова Ж.Е., Калиева Б.К., Бубиш Ш., Аскарова Ш.К.</b> Влияние наночастиц серебра на прорастание семян фасоли, лимона, мандарина, авокадо.....	320
<b>Куртебаева А.А., Álvarez-Torrellas S., Gomes Н.Т., Орынбаев С.А., Калмаханова М.С.</b> Полимерные мембраны с активированным углем для эффективного удаления загрязняющих веществ вызывающих обеспокоенность.....	334
<b>Масенова А.Т., Жұмақанова А.С., Торлопов И.И., Рахметова К.С., Абильмагжанов А.З.</b> Оптимизация процесса получения иерархического цеолита ZSM-5 паровой щелочной модификацией.....	350
<b>Мутушев А.Ж., Нуралы А.М., Санат А.С., Шаукарова М.А., Есимсиитова З.Б.</b> Влияние светопреобразующих плёнок на накопление биоактивных соединений и качество плодов.....	366
<b>Нефедов А.Н., Тайекенова А.Т.</b> Современное состояние применения органических ингибиторов коррозии в нефтепереработке.....	379
<b>Омаров Б.Т., Алтыбаев Ж.М., Серикбаева Б.С.</b> Получение биогумуса путем вермикомпостирования органических отходов и исследование его агроэкологической эффективности.....	399
<b>Рахман Д.М., Қаппасұлы Ә., Махаева Д.Н., Казыбаева Д.С., Ирмухаметова Г.С.</b> Разработка и исследование мукоадгезивных гидрогелей на основе комплексов геллан–цистеин.....	414
<b>Сабыржанова А.Е., Болаткызы Н., Берганаева Г.Е., Дюсебаева М.А.</b> Исследование аминокислот и жирных кислот в составе надземной части <i>Plantago Major</i> .....	428
<b>Сатаева С., Ахметова Ф., Уразова А., Айтуганова С., Ерниязова К.</b> Влияние концентрации ПЭПА на физические, механические и эксплуатационные свойства эпоксидных клеев ЭД-20.....	439
<b>Заманбек А.Ж., Кошкарбаева Ш.Т., Сатаев М.С.</b> Методы получения наночастиц серебра и антибактериальные свойства.....	450
<b>Жоргарова А.А., Салькева Л.К., Минаева Е.В., Ибраев М.К., Фазылов С.Д.</b> Новые возможности синтеза и фосфорилирования фосфонуксусного эфира.....	462

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## NEW POSSIBILITIES FOR THE SYNTHESIS AND PHOSPHORYLATION OF PHOSPHONOACETIC ACID ESTER

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**Abstract.** The development of original substances for production of pharmaceuticals based on heterocyclic compounds remains an urgent and sought-after area of research. Effective drugs have been discovered among phosphorylated derivatives of heterocycles, including armin and phosphacol for glaucoma treatment, as well as antitumor agents such as imifos, thiophosphamide, fosfestrol, cyclophosphamide. At the same time, the study of reactions for obtaining phosphorus derivatives of aminothiadiazoles with pronounced pharmacological activity has not received due attention or a comprehensive approach from researchers. Significant interest in phosphonoacetic acid (PAA) and its derivatives is driven by their high antiviral activity, particularly their ability to



inhibit the replication of herpes simplex virus, cytomegalovirus, Epstein-Barr virus, and cowpox virus. Another important feature of PAA is its diverse biological activity, including herbicidal, fungicidal, and insecticidal properties. Additionally, research has explored the potential use of PAA in the treatment of human AIDS. The interest in PAA and its derivatives is related to their availability and possibilities of chemical modification, which can lead to the synthesis of new biologically active compounds. The research aimed to develop and identify effective methods for synthesizing PAA and its derivatives with biologically active properties. This goal was pursued by introducing thiadiazole fragment into the PAA structure, followed by further chemical modification of resulting compounds. The presence of a free amino group in the thiadiazole ring significantly enhances the potential for remodeling reactions using reactive *tert.*-butyltetraethyl diamidophosphite. Additionally, the active *tert.*-butoxyl group facilitates further functionalization through the Arbuzov reaction with a wide range of electrophilic reagents.

**Keywords:** phosphonacetic acid (PAA), thiadiazole, aminothiadiazole, *tert.*-butyltetraethyldiamidophosphite, Arbuzov reaction

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## ФОСФОНОСІРКЕ ҚЫШҚЫЛЫНЫҢ ЭФИРІН СИНТЕЗДЕУ МЕН ФОСФОРЛАНДЫРУДЫҢ ЖАҢА МҮМКІНДІКТЕРІ

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**Аннотация.** Гетероциклдік қосылыстар негізінде дәрілік препараттар жасауға арналған бастапқы субстанцияларды әзірлеу өзекті әрі сұранысқа ие зерттеу саласы болып қала береді. Гетероциклдердің фосфорланған туындыларының қатарында глаукоманы емдеуге қолданылатын армин мен фосфакол, сондай-ақ ісікке қарсы имифос, тиофосфамид, фосфэстрол, циклофосфан және басқа да тиімді дәрілік препараттар белгілі. Сонымен қатар, айқын фармакологиялық белсенділікке ие аминотиадиазолдардың фосфорқұрамды туындыларын алу реакцияларын зерттеуге қатысты кешенді және жүйелік өзқарас жеткіліксіз деңгейде болған. Фосфонсірке қышқылына (ФСҚ) және оның туындыларына деген жоғары қызығушылық олардың айқын вирусқа қарсы белсенділік көрсетуімен, атап айтқанда қарапайым герпес вирусының, цитомегаловирустың, Эпштейн–Барр вирусының, сиыршешегі вирусының және басқа да вирустардың репликациясын тежеу қабілетімен байланысты. ФСҚ-тың тағы бір маңызды ерекшелігі – гербицидтік, фунгицидтік, инсектицидтік және басқа да биологиялық белсенділік түрлерін көрсетуі. Сонымен қатар, ФСҚ-ты адамның ЖИТС-ін емдеуде қолдану бойынша зерттеулер жүргізілгені белгілі. ФСҚ пен оның туындыларына деген қызығушылық олардың қолжетімділігімен және жаңа биологиялық белсенді қосылыстарды синтездеуге мүмкіндік беретін химиялық модификациялау әлеуетімен түсіндіріледі. Осыған байланысты зерттеудің мақсаты биологиялық белсенді қасиеттерге ие ФСҚ пен оның туындыларын алудың тиімді әдістерін әзірлеу және анықтау болды. Қойылған міндет ФСҚ құрамына тиадиазол фрагментін енгізу және түзілген қосылыстарды одан әрі химиялық модификациялау арқылы жүзеге асырылды.

Тиадиазол сақинасындағы бос амин тобының болуы реакцияға қабілетті үшіншілік-бутил-тетраэтилдиамидофосфитті пайдалану арқылы перемидирлеу реакциясының мүмкіндіктерін едәуір кеңейтеді, сондай-ақ көптеген электрофильді реагенттермен Арбузов реакциясына түсе алатын белсенді үшіншілік-бутоксил тобы есебінен кейінгі функционалдандыруға жағдай жасайды.

**Түйін сөздер:** фосфонсірке қышқылы (ФСҚ), тиадиазол, аминотиадиазол, трет-бутилтетраэтилдиамидофосфит, Арбузов реакциясы

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## НОВЫЕ ВОЗМОЖНОСТИ СИНТЕЗА И ФОСФОРИЛИРОВАНИЯ ФОСФОНУКСУСНОГО ЭФИРА

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**Аннотация.** Разработка оригинальных субстанций для создания лекарственных препаратов на основе гетероциклических соединений остается актуальным и востребованным направлением исследований. Среди фосфорилированных производных гетероциклов выявлены эффективные лекарственные средства, такие как армин и фосфакол, применяемые для лечения глаукомы, а также противоопухолевые препараты имифос, тиофосфамид, фосфэстрол, циклофосфан и другие. В то же время исследованию реакций получения фосфорсодержащих производных аминотиадиазолов, обладающих выраженной фармакологической активностью, до настоящего времени не уделялось достаточного внимания, а комплексный подход к их изучению остается недостаточно разработанным. Значительный интерес к фосфонуксусной кислоте (ФУК) и ее производным обусловлен их высокой антивирусной активностью, в частности способностью подавлять репликацию вируса простого герпеса, цитомегаловируса, вируса Эпштейна-Барр, вируса коровьей оспы и других. Другой важной особенностью ФУК является проявление различных видов биологической активности, включая гербицидную, фунгицидную и инсектицидную. Имеются также сведения о возможностях применения ФУК при лечении СПИДа. Интерес к ФУК и ее производным связан не только с их биологической активностью, но и с доступностью исходных соединений и широкими возможностями их химической

модификации, способствующими синтезу новых биологически активных веществ. В связи с этим целью исследования явилась разработка и выявление эффективных методов получения ФУК и ее производных, обладающих биологически активными свойствами. Решение поставленной задачи осуществлялось путем введения тиadiaзольного фрагмента в структуру ФУК с последующей химической модификацией образующихся соединений. Наличие свободной аминогруппы в тиadiaзольном кольце существенно расширяет возможности реакций переамидирования с использованием реакционноспособного трет-бутилтетраэтилдиамидофосфита, а также последующей функционализации за счет активной трет-бутоксильной группы, способной вступать в реакцию Арбузова с широким кругом электрофильных реагентов.

**Ключевые слова:** фосфонуксусная кислота (ФУК), тиadiaзол, аминотиadiaзол, трет.-бутилтетраэтилдиамидофосфит, реакция Арбузова

**Introduction.** Thiadiazole and its functional derivatives play a crucial role in the development of potent medicines, which are an integral part of modern pharmacotherapy (Hu et al., 2014). The incorporation of the thiadiazole ring as an effective pharmacophore into organic molecules can significantly enhance or modify their biological activity (Asadullina et al., 2016). Consequently, numerous compounds containing the thiadiazole ring with diverse biological properties have been widely reported in the literature (Hemanth et al., 2022).

On the other hand, organic phosphorus compounds continue to attract significant scientific interest, particularly in the incorporation of various phosphorus derivatives into drug molecules, which can lead to the development of new pharmacophore groups (Yao et al., 2019). In this context, organic phosphorus compounds, especially phosphonoacetic acid (PAA) and its derivatives, have recently regained prominence. Notably, PAA esters are well known as pyrophosphate antimetabolites with broad inhibitory activity against various viral infections (Rodriguez et al., 2019).

Various methods for synthesizing PAA and its derivatives, particularly those based on phosphoric acid derivatives such as dialkyl and trialkylphosphites, have been well documented in the literature. For instance, studies describe the synthesis of PAA via acid hydrolysis of the trimethyl ester of phosphonoacetic acid in an acidic medium. This reaction, traditionally performed by boiling in concentrated hydrochloric acid, requires more than three days to complete. Building upon this work, further research was carried out to optimize the process, leading to the successful application of microwave irradiation. This advancement significantly reduced the reaction time while simultaneously increasing the yield of the desired product (Sokruta et al., 2017).

Continuing the research towards improving the synthesis of PAA and its derivatives and their further use in the synthesis of phosphorylated thiadiazole derivatives, the purpose of the work was to carry out a series of syntheses of PAA and its derivatives and analyzed their efficiency in further chemical modification.

A method for synthesizing phosphorylated thiadiazoles based on chloroethylphosphonates and thiosemicarbazide has been reported in the literature (Egorova

et al., 2019), noted for its simplicity and mild reaction conditions. However, in this study, we propose a broader range of experimental approaches to efficiently obtain phosphorylated thiadiazoles via different synthetic routes using readily available starting materials.

**Materials and methods.** All chemicals were of analytical grade and purchased from Sigma-Aldrich without requiring further purification. Reaction progress was monitored using TLC on Merck F254 silica gel-coated plates. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on JEOL 500 MHz FT-NMR Spectrometer in  $\text{CDCl}_3$ , with TMS as the internal standard.

Mass spectra were recorded using a Shimadzu mass spectrometer, while IR spectra were obtained using a Thermo Scientific Nicolet 6700 FTIR spectrometer (Madison, WI, USA). The melting point was determined using a Buchi Melting point M-560 instrument.

Diethyl ((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) (Figure 1).

Sodium diethyl phosphite was prepared by reacting 6.9 g (0.05 mol) of diethyl phosphite with 1.15 g (0.05 mol) of metallic sodium in dry benzene. The resulting mixture was placed in a reaction flask, and with constant stirring, 6.13 g (0.05 mol) of ethyl monochloroacetate was added at room temperature following the procedure described in (Kormachev and Fedoseev, 1992). The precipitated NaCl was filtered off, and the solvent was evaporated. The residue was then distilled under reduced pressure, yielding 7.3 g (65%) of phosphonoacetic acid ester (III) with a boiling point of 141-143°C (10 mmHg) and a refractive index of  $n_D^{20}$  1.4320. The obtained compound (III) was subsequently subjected to alkaline hydrolysis, resulting in the formation of PAA as a light-yellow oil. The crude PAA was then reacted with 4.6 g (0.05 mol) of thiosemicarbazide in the presence of concentrated  $\text{H}_2\text{SO}_4$  and PPA at 60-70°C. This resulted in the isolation of 9.04 g (72%) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI), which is white crystals with mp of 128-130 °C, IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3255 ( $\text{NH}_2$ ), 3181 (NH), 1254 (P=O), P-O-C (1035), 1540 (C=N). Mass spectrum,  $m/z$ : 252 [ $\text{M}+\text{H}$ ] $^+$  (calculated for  $\text{C}_7\text{H}_{14}\text{N}_3\text{O}_3\text{PS}$ : 251).  $^{31}\text{P}$  NMR spectrum ( $\text{CD}_3\text{OD}$ ):  $\delta_p$  22 ppm.  $^1\text{H}$  NMR spectrum,  $\delta$ , ppm (J, Hz): 1.36 t (6H,  $\text{OCH}_2\text{CH}_3$ ,  $^3J_{\text{H-NH}} = 7.1$  Hz), 3.03 d (2H,  $\text{PCH}_2$ ,  $^2J_{\text{H-NR}} = 21.0$  Hz), 4.19 d.q (4H,  $\text{OCH}_2\text{CH}_3$ ,  $^3J_{\text{H-NH}} = 7.3$ ,  $^3J_{\text{H-NR}} = 12.3$  Hz), 6.86 s (2H).  $\delta_c$ , ppm: 15.36 d ( $\text{CH}_3\text{CH}_2$ ,  $^3J_{\text{PC}} = 5.4$  Hz), 27.61 d ( $\text{PCH}_2$ ,  $^1J_{\text{PC}} = 142.3$  Hz), 63.06 d ( $\text{CH}_3\text{CH}_2\text{OP}$ ,  $^2J_{\text{PC}} = 6.8$  Hz), 149.84 d ( $\text{CH}_2\text{C}=\text{N}$ ,  $^2J_{\text{PC}} = 10.1$  Hz). The results are in agreement with the literature data [16].

Diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) (Figure 2).

Sodium diethyl phosphite, prepared from 6.9 g (0.05 mol) of diethyl phosphite and 1.15 g (0.05 mol) of sodium metal in a dry benzene medium, was placed in a reaction flask. With constant stirring, 4.7 g (0.05 mol) of monochloroacetic acid was added at room temperature. The precipitated NaCl was filtered off, and the resulting phosphonoacetic acid (PAA) was obtained as a light-yellow oil. The crude PAA was then reacted with 4.6 g (0.05 mol) of thiosemicarbazide in the presence of concentrated  $\text{H}_2\text{SO}_4$  and polyphosphoric acid (PPA) at 60-70°C. As a result, 10.3 g (82%) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) was isolated, with a melting point of 128-130°C.

Diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) (Figure 3).

A solution of 4.3 g of 2-amino-5-methyl-1,3,4-thiadiazole, synthesized from 3.0 g (0.05 mol) of acetic acid and 4.6 g (0.05 mol) of thiosemicarbazide in dichloroethane, was prepared. To this solution, 1.12 g of paraformaldehyde and 1.3 g of freshly calcined zinc chloride were added with vigorous stirring. Hydrogen chloride gas was then bubbled through the reaction mixture, leading to an exothermic reaction that increased the temperature from 15°C to 30°C. Once the heat evolution ceased, the reaction mixture was further heated to 55°C and maintained at this temperature for 2 hours, with a weak stream of hydrogen chloride continuously passed through to ensure solution saturation. The resulting mixture was washed with water (2 × 15 mL) and dried over calcium chloride. Dichloroethane was removed under reduced pressure, and the residue was recrystallized from alcohol, yielding 6.8 g (68%) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) with a melting point of 128-130°C.

Diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) (Figure 4) – Method A.

To the sodium salt prepared from 8.0 g (0.05 mol) of malonic ester and 1.2 g (0.05 mol) of sodium in a dry benzene medium, 8.6 g (0.05 mol) of diethyl chlorophosphate was added at room temperature. The precipitated NaCl was filtered off, and the residue was distilled under vacuum, yielding 12.9 g (87%) of phosphonmalonic ester with a boiling point of 159-160°C at 10 mmHg and a refractive index of  $n_D^{20}$  1.4458. The obtained phosphonmalonic ester was treated with a saturated KOH solution, and the resulting phosphonmalonic acid was heated to 80°C. Dehydration and decarboxylation yielded phosphonoacetic acid (PAA), which was then reacted with 4.6 g (0.05 mol) of thiosemicarbazide, following the previously described procedure. This resulted in the formation of 8.2 g (65%) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) with a melting point of 129-130°C.

Diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) (Figure 5) – Method B

A solution of sodium diethylphosphite was prepared by reacting 6.9 g (0.05 mol) of diethyl phosphite with 1.15 g (0.05 g atom) of metallic sodium in a dry benzene medium. Simultaneously, 8.0 g (0.05 mol) of malonic ester and 8.0 g (0.05 mol) of bromine were dissolved in dry benzene. The solution of sodium diethylphosphite was then added gradually while maintaining the temperature between 20-25°C. The precipitated NaBr was filtered off, and the solvent was removed under reduced pressure. The obtained residue was treated with a saturated KOH solution to yield phosphonmalonic acid, which was further heated to 80°C, leading to dehydration and decarboxylation to obtain phosphonoacetic acid (PAA). The resulting PAA was subsequently reacted with 4.6 g (0.05 mol) of thiosemicarbazide, following the previously described procedure. As a result, 7.5 g (60%) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) was obtained, with a melting point of 129-130°C.

Diethyl ((7-oxido-4-thia-1,2,6-triazo-7-phosphobicyclo [3.2.0] hepta-2,5-dien-3yl) methyl) phosphonate (VIIIe)

In a reaction flask, 2.48 g (0.01 mol) of tetraethyl diamidotert.-butyl phosphite (VII) and 2.51 g (0.01 mol) of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate

(VI) were mixed in ethyl acetate medium and heated to the boiling point of the solvent, at which time it was observed that diethylamine was distilled off in the solvent mixture. The amount of diethylamine released was determined by passing dry HCl through the distillate of the mixture with the solvent and measuring the mass of the resulting hydrochloride, which corresponds to the stoichiometry of the reaction (1:1), and amounted to 2.0 g (92%). The melting point of  $(C_2H_5)_2NH \cdot HCl$  corresponds to the literature value of 221 °C. Isobutylene gas was simultaneously observed and collected by the water displacement method. The completion of the reaction was monitored by measuring the amount of diethylamine hydrochloride formed. The reaction yielded 2.23 g (75%) of diethyl ((7-oxido-4-thia-1,2,6-triazo-7-phosphobicyclo [3.2.0] hepta-2,5-dien-3-yl) methyl) phosphonate (VIIIe).

Oil. IR spectrum ( $\nu$ ,  $cm^{-1}$ ): 1254, 1278 (P=O), P-O-C (1045), 1545 (C=N).  $^{31}P$  NMR spectrum ( $CD_3OD$ ):  $\delta_p$  5.5ppm, P(O)H; 40.15 ppm P(O)CH<sub>2</sub>.  $^1H$  NMR spectrum,  $\delta$ , ppm (J, Hz): 1.38 t (6H, OCH<sub>2</sub>CH<sub>3</sub>,  $^3J_{HH} = 7.1$  Hz), 4.2 d.q (4H, OCH<sub>2</sub>CH<sub>3</sub>,  $^3J_{HH} = 7.0$ , 2.61 d (2H, PCH<sub>2</sub>,  $^2J_{HP} = 14.3$  Hz),  $\delta_c$ , ppm: 16.3 d (CH<sub>3</sub>CH<sub>2</sub>,  $^3J_{PC} = 9.1$  Hz), 34.2 d (PCH<sub>2</sub>,  $^1J_{PC} = 142.3$  Hz), 61.9 d (CH<sub>3</sub>CH<sub>2</sub>OP,  $^2J_{PC} = 9.1$  Hz), 148.2 d (CH<sub>2</sub>C=N,  $^2J_{PC} = 10.1$  Hz), 154.7 s (SC=N). Mass spectrum, m/z: 296 [M+H]<sup>+</sup> (calculated for C<sub>7</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>P<sub>2</sub>S: 297).

**Results and discussion.** We carried out the classical synthesis of diethyl phosphonoacetate (III) from sodium diethyl phosphite (I) and ethyl chloroacetate (II). The alkaline hydrolysis of this intermediate yields diethyl phosphonoacetic acid (IV), which, upon further functionalization with thiosemicarbazide, leads to the formation of phosphono-substituted thiadiazole (VI). Obviously, the reaction proceeds according to the scheme presented in Figure 1:

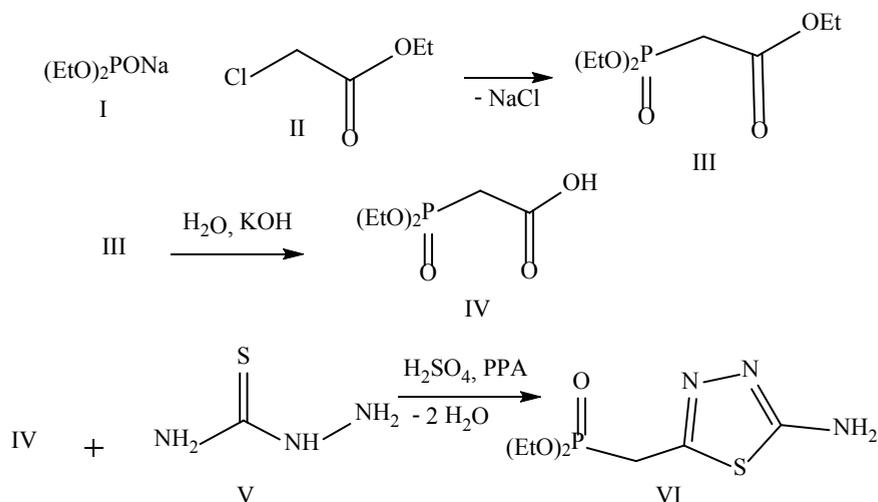


Figure 1 - Synthesis of diethyl((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) from ethyl chloroacetate

The obtained ester (III) underwent alkaline hydrolysis, yielding PAA as an oily product (IV), which was subsequently reacted with thiosemicarbazide without prior

purification. This reaction efficiently produced diethyl((5-amino-1,3,4-thiadiazol-2-yl)methyl) phosphonate (VI) in good yield.

Another method for synthesizing PAA involves the direct reaction of sodium diethyl phosphite with monochloroacetic acid. This approach demonstrated high efficiency, leading to a significant increase in the yield of the target product (Figure 2).

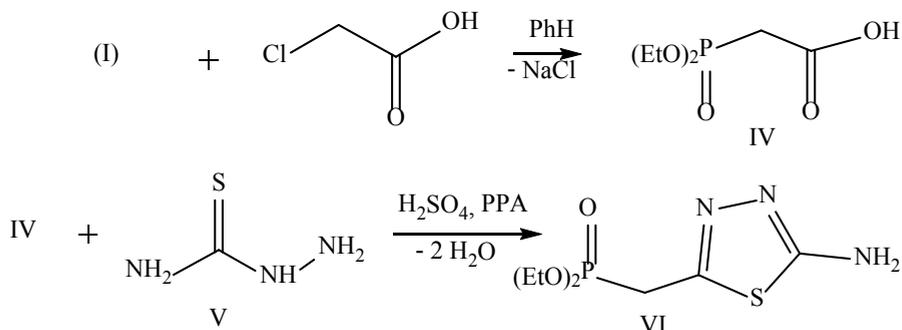


Figure 2 – Synthesis of diethyl ((5-amino-1,3,4-thiadiazol-2-yl)methyl) phosphonate (VI) from monochloroacetic acid

This reaction proved to be significantly more efficient than using ester (II), as it eliminated the need for hydrolysis of the obtained product. In all cases, the reactions were monitored using thin-layer chromatography (TLC).

The classical reaction of the previously synthesized 2-amino-5-methylthiadiazole, followed by chloromethylation using hydrochloric acid and paraformaldehyde in the presence of anhydrous ZnCl<sub>2</sub>, is also an equally efficient method for forming the thiadiazole ring (Figure 3).

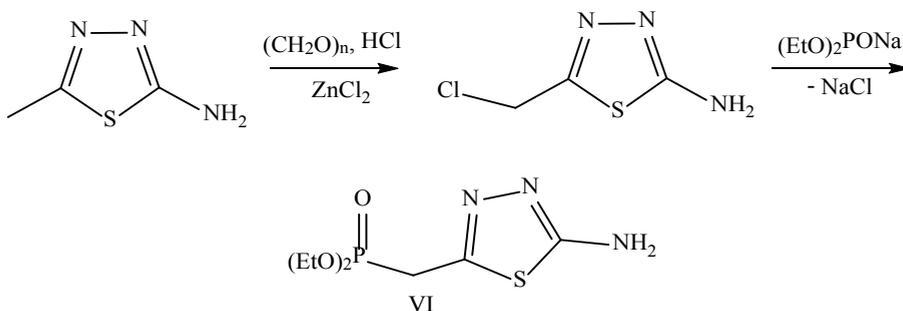


Figure 3 - Synthesis of diethyl ((5-amino-1,3,4-thiadiazol-2-yl)methyl) phosphonate (VI) via the chloromethylation of 2-amino-5-methyl-1,3,4-thiadiazole

Another synthetically valuable approach to obtaining the target product (VI) involves the reaction of sodium malonic ester with chlorophosphate, as well as the reaction of the sodium ester of diethylphosphoric acid (I) with bromomalonic ester. The reaction is expected to proceed according to the proposed scheme (Method A and B), as shown in Figures 4 and 5.

Both methods (A) and (B) proceed under relatively mild conditions and result in a high yield of the desired product (VI). However, Method A offers certain advantages, including a shorter synthetic route that eliminates the need for isolating the intermediate PAA allowing for its direct use in subsequent reactions. In the reaction between the sodium salt of diethyl phosphite and bromomalonic ester, a significant side elimination reaction occurs due to the relatively high basicity of the diethyl phosphonate anion. This leads to the formation of the tetraethyl ester of ethylenetetracarboxylic acid, which has a melting point of 53-54°C. A substantial reduction in the formation of this byproduct was achieved by employing a reverse addition technique, where the reagents were mixed in the opposite order. This approach effectively lowered the concentration of sodium diethyl phosphite, thereby minimizing unwanted side reactions.

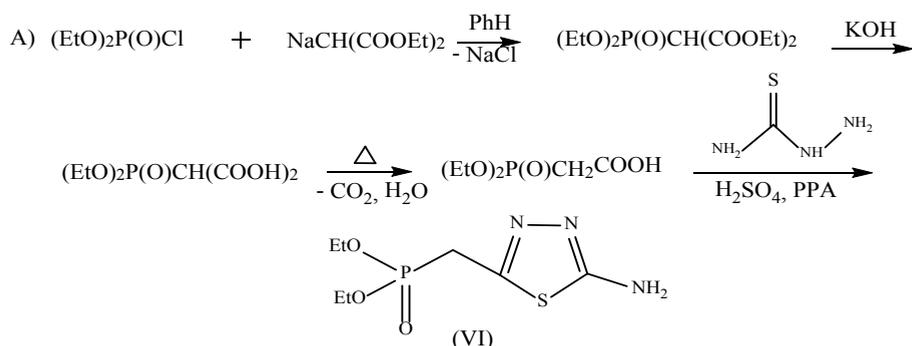


Figure 4 - Synthesis of diethyl ((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) using bromo- and sodium malonic esters. Method A

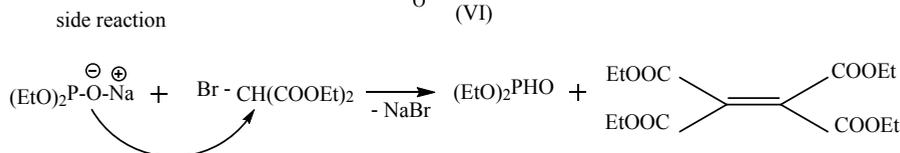
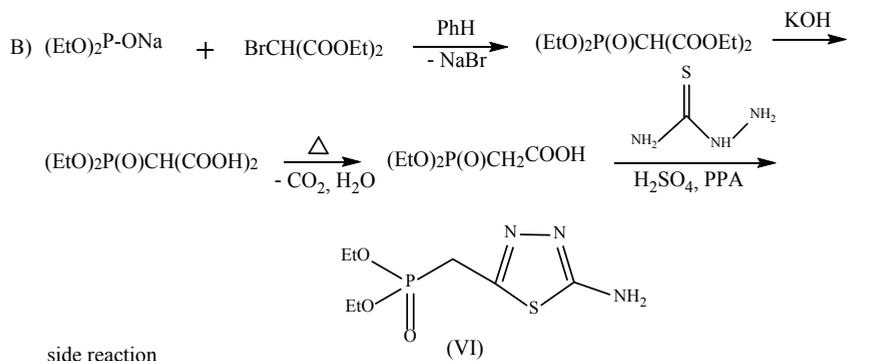


Figure 5 – Synthesis of diethyl ((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) using bromo- and sodium malonic esters. Method B

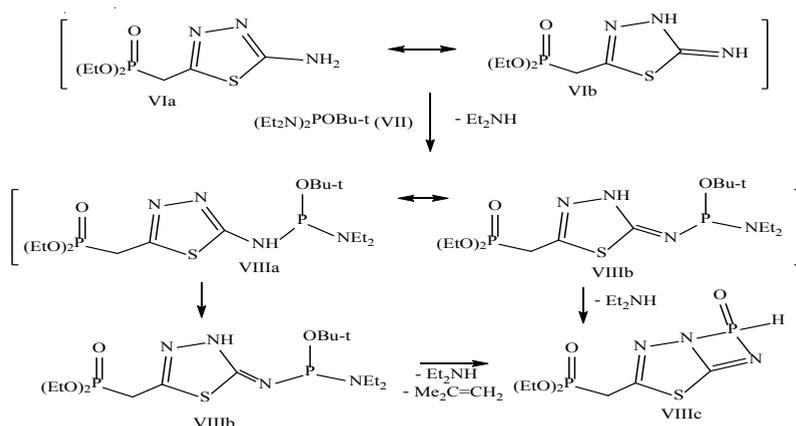
Analysis of the synthesis results for the preparation of (VI) revealed that the most efficient method, in preparative terms, is the approach based on compound

(IV), as outlined in Figure 2. This method allows for the direct reaction of (IV) with thiosemicarbazide without the need for its isolation in free form. The process is characterized by its simplicity, high yield, and excellent purity of the final product.

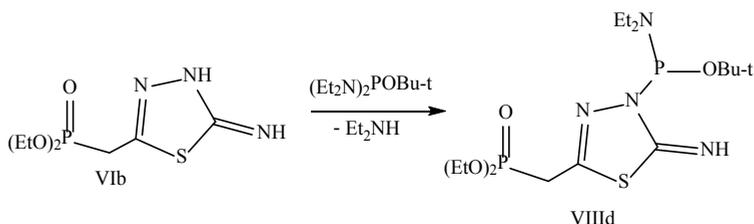
The structure of diethyl ((5-amino-1,3,4-thiadiazol-2-yl) methyl) phosphonate (VI) implies significant reactivity associated with the presence of a free amino group, which exists in the amino–imine tautomeric forms of the thiadiazole ring (Danilova et al., 2010). These structural features are particularly relevant in the study of chemical modification reactions, notably phosphorylation with amidophosphoric acid esters, which readily undergo transamidation with the more nucleophilic diethylamino group.

A considerable number of phosphorylation reactions involving a wide range of amino and oxy compounds using full and partial esters of amidophosphoric acid have been reported in the literature. In particular, we have previously explored the efficiency of tetraethyl diamido-*tert.*-butyl phosphite (VII), which features a highly nucleophilic P(III) atom capable of readily phosphorylating various amino compounds (Sal'keeva et al., 2014). Another advantage of (VII) is the presence of a *tert.*-butyl group, which can be easily eliminated, facilitating the formation of a stable P=O bond. These characteristics make (VII) an attractive reagent for the design of new structures incorporating effective pharmacophore groups.

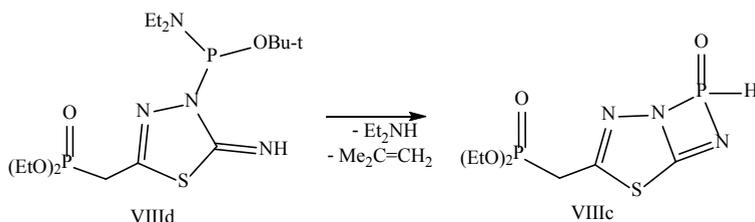
The obtained product (VI) presents an interesting opportunity for further functionalization, particularly involving its free amino group. We propose that a transamidation reaction can be achieved using a highly effective reagent tetraethyl diamido-*tert.*-butyl phosphite (VII). This reaction serves a dual purpose: firstly, it introduces a reactive phosphorus (III) atom, enabling further chemical modifications; secondly, it facilitates the substitution of the amino group's nitrogen in the thiadiazole ring with the more basic diethylamino group from (VII). The reaction is carried out by prolonged heating of (VI) and (VII) in an ethyl acetate medium, with continuous distillation of the solvent mixture and the concurrent release of diethylamine. Completion of the reaction was confirmed by isolating diethylamine as diethylamine hydrochloride and determining its mass. The final product was precipitated from the reaction mixture, separated via filtration, and purified through recrystallization from alcohol.



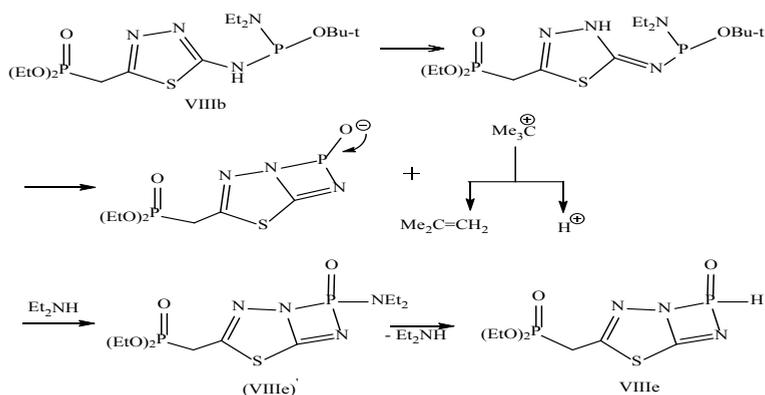
The structure of compound (VI) suggests the existence of two tautomeric forms, (VIa) and (VIb), in which the nitrogen atoms exhibit different basicities, implying different pathways for transamidation reactions. This observation aligns with literature data, which indicate that the nitrogen atoms in 2-amino-1,3,4-thiadiazoles exist in resonance equilibrium, as demonstrated by X-ray diffraction analysis (Asadullina et al., 2016). In this context, another plausible reaction pathway involves phosphorylation at the nitrogen atom of the thiadiazole ring. A similar approach was adopted by Danilova et al. (Danilova et al., 2010) in the case of the alkylation reaction of thiadiazoles.



We believe that the formed product (VIIIId) can readily release the diethylamine molecule due to its spatial arrangement and the high nucleophilicity of the nitrogen atom in the diethylamino group. This transformation subsequently leads to the formation of product (VIIIc).



The evolved isobutylene was collected, and its volume was measured by the water displacement method.



Evidently, the reaction proceeds due to the high lability of the *tert.*-butoxy group, which under the reaction conditions at the boiling point of ethyl acetate readily undergoes elimination of a stable *tert.*-butyl cation, leading to the formation of a stable phosphoryl group (P=O) and, consequently, to the formation of compound (VIIIe). The reaction progress was monitored by TLC and by recording the  $^{31}\text{P}$  NMR spectrum after 10–15 minutes. The formation of structure VIIIa was observed, manifested by a signal at 181.55 ppm, corresponding to a trivalent P(III) species; additionally, a signal of a tetraordinated phosphorus atom, presumably an acidic species, appeared at 40.15 ppm. The initially formed trivalent phosphorus compound is unstable due to the presence of an easily eliminable *tert.*-butoxy group and ultimately converts into the final product VIIIe. It should also be noted, in support of the proposed reaction pathway, that the mass spectrum of (VIIIe) exhibits a peak at  $m/z$  369, corresponding to the structure (VIIIe)' with a molecular weight of 368, which is evidently formed as a result of attack by diethylamine present in the reaction medium followed by substitution with a proton.

**Conclusions.** In conclusion, it should be emphasized that we carried out an experimental evaluation of various methods for the synthesis of phosphonoacetic acid, which was subsequently employed in the preparation of amino-thiadiazole derivatives. These compounds are of particular interest for the generation of new derivatives via functionalization at the free amino group. In this context, the phosphorylation of the obtained phosphono-substituted thiadiazoles was accomplished through transamidation reaction with *tert.*-butyl tetraethylamidophosphite, which readily undergoes substitution of the diethylamino group and enables further modification according to the Arbuzov reaction scheme. The synthesized compounds demonstrate the feasibility of facile phosphorylation of substituted amino-thiadiazoles, representing an efficient approach to the generation of new potential synthons for the synthesis of pharmaceutically active substances.

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