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CONTENTS

PHYSICS

Aliuly A., Kaltayev A.

Aliuly A., Kaltayev A. Assessment of the Applicability of Similarity Laws for Centrifugal Pump Scaling Based on Hydrodynamic Modeling.....14

Baratov A.G., Sailaubek A., Serik A.S.

Synthesis and Investigation of a Narrow-Bandgap SrTaO₂N-Based Photocatalyst.....33

Nurbayev B., Dmitriyeva E., Kemelbekova A.

Modern Methods of Selective Lithium Leaching from Spent Lithium-Ion Batteries.....45

Seitov A., Amanzholov T.

Comparative Analysis of One-Dimensional Physical-Hydrodynamic Models of Centrifugal Flow in an Impeller for Mineralized Media.....60

Syzdykova A.M., Serikbayev N.S., Kutum B.B.

Local Kodama-Type Transformations and Integrability Limits of the Extended Fifth-Order Korteweg-de Vries Equation.....83

Ualikhanova U.A., Ussipkyzy T., Altayeva G.S., Razina O.V.

Calculation of the Screened $f(T)$ Gravity Model.....101

Zhadyranova A.A., Tsyba P.Yu., Ismail U.K., Yerzhan B.

Divergence-Free Deceleration Parameter, Kinematic Constraints from DESI DR2 and Cosmic Chronometers.....123

Zhenishan K., Bekov S.S., Syzdykova A.M.

The Influence of Gaussian Process Parameters on Reconstructing the Hubble Constant.....146

CHEMISTRY

Amangeldi B., Zhanikulov N., Taimasov B., Aitureev M., Dauletiyarov M.

Research of the Firing Processes and Whiteness of White Cement Clinkers.....155

Baisalova G.Zh., Bauyrzhanova G.B., Niyaz G.A., Taltenov A.A., Ainabayev A.A.

Study of the Chemical Composition of Ethanol Extracts of Lady's Mantle by Gas Chromatography-Mass Spectrometry.....169

Bishimbaev V.K., Kapsalyamov B.A.

Hydrogeochemical Indicators of Sulfuric-Acid Uranium Leaching Impact on Groundwater in Shieli and Zhanakorgan Districts.....183

Darmenbayeva A.S., Aubakirova R.A. Nurgaliyeva D.A., Abylkassova G.E., Abilmazhinova G.A.

Structural and Morphological Features of Polymer-Metal Functional Materials.....205

Dyusebaeva M.A., Berganayeva A.E., Ibragimova N.A., Utaraliev D.M., Berganayeva G.E.

Green synthesis of silver nanoparticles using the n-butanol fraction of Galega officinalis L.....223

Dyussembekova S.B., Utarova D.A., Kuspanov Zh.B., Daulbayev Ch.B., Abdikarimova U.A. Investigation of the Effect of SrTiO ₃ Heat Treatment on the Photocatalytic Efficiency of the \	
Decomposition of an Amphoteric Antibiotic.....	239
Issayeva U.B., Akhmetova G.S., Praliyev K.D., Malmakova A.E., Seilkhanov T.M. 1-Benzyl-4-(p-Fluorobenzoyloxyimino)Piperidine Hydrochloride as a Candidate for	
an Anti-Infective Agent.....	252
Kamunur K., Yskak M., Mussapyrova L. Effect of Chemical Modification of Sodium Lignosulfonate on Flotation Properties in the	
Barite – Calcite System.....	264
Kononov A., Kamunur K., Mussapyrova L., Assylkhanova D., Batkal A. Obtaining and Studying the Inorganic Flocculant Al–Fe–Mn Based on Modified Bentonite.....	276
Kurmangaliyeva A.1, Akhmetova F.2, Kareshova Zh.1, Iskakov R. PDMA-Modified Tagan Bentonite for Hydrogen Production in Catalytic Conversion	
of Hydrocarbons.....	292
Kurtebayeva A.A., Silvia Álvarez-Torrellas., Noor Haida Mohd Kaus., Gomes H.T., Kalmakhanova M.S. Corn-Cob-Derived Fe-Modified Activated Carbons for Paracetamol and Sulfamethoxazole	
Removal by Adsorption and Oxidative Treatment.....	307
Nadirov R.K., Nurtazina N.D., Ryskaliyeva R.G. Response Surface Modelling and Optimisation of Ilmenite Flotation Using a Modified	
Lignosulphonate Reagent.....	334
Nefedov A.N., Taikenova A.T., Imashev B.K., Nurislamov R.M., Leontyeva X. Quantum Computing in the Modeling of Corrosion Processes.....	350
Nurkenov O.A., Fazylov S.D., Syzdykov A.K., Kabiyeva S.K., Zhaslan R.K. Synthesis and Structural Study of 3,5-Dimethylisoxazole Sulfone Derivatives with Secondary	
Amines.....	365
Orazbekova R.S., Tungatarova S.A., Baizhumanova T.S., Kaumenova G.B., Zhumabek M. Influence of Reaction Mixture Composition in Steam Reforming of Bioethanol on a High-Entropy	
Oxide Catalyst.....	382
Ryskaliyeva R.G., L.K. Beisembayeva, Osserov T.B. Hydrocyclone Classification of Balkhash Processing Plant Tailings.....	398
Sass A.S., Torlopov I.I., Rakhmetova K.S., Kenzin E.N., Zhurinov M. Formation and Maturation of Phosphate Coatings on Steel from an Alcohol-Based	
Phosphating Solution.....	418
Sdikova G.Zh., Dalabayeva N.S., Balkembay A.S., Sarova N.B., Zhaltyrbayeva N.K. Effect of Electrolyte Formulation on the Characteristics of Zinc-Based	
Electroplated Coatings.....	435
Seitkaliyeva N., Kussainova G., Zhursumbayeva M., Mohamad Ibrahim M.N., Abdiyev K. Study of the Flocculation Properties of Itaconic Acid-Based Copolymers.....	448

Sergazina S.M., Nurmukhanbetova N.N., Ostretsova I.B., Kamze A.R., Kassenova N.B. Comprehensive Assessment of Natural Drinking Water Quality and Statistical Analysis of Physicochemical Parameters.....	460
Talgatkyzy A., Nazhipkyzy M., Otenov A., Seitkazinova A., Issanbekova A. Wood Waste-Derived Organosolv Lignin-Based Carbon Nanofibers For Energy Storage Applications.....	475
Toktabayeva A.K., Makhayeva D.N., Rakhmetullayeva R.K., Rvaidarova G.O., Issenova G.D. Synthesis, Structure, and Physicochemical Properties of Sulfur-Containing Composites Based on Aniline, p-Phenylenediamine, Phenol, and Formaldehyde.....	498
Yeshmanova G.B., Smagulov D.U. Effect of Silicon-Based Particles on the Formation and Composition of PEO Coatings.....	517
Zhortarova A.A., Kubicek V., Ibrayev M.K., Panshina S.Y., Seidakhmetova R.B. N-Phosphorylation of Amino-thiazoles and Amino-Thiadiazoles with P(III)- and P(V)-Reagents: Synthesis, Structure, and Biological Activity.....	538
Zhussupova A., Tyumentseva O., Antonyuk V. Comparative Study of the Kinetics and Energy Characteristics of Planetary Milling of Copper Smelting Dump Slag and Granulated Lead-Smelting Slag.....	552

МАЗМҰНЫ

ФИЗИКА

Әлиұлы А., Калтаев А.

Гидродинамикалық модельдеу негізінде ортадан тепкіш сорғыларды масштабтауда ұқсастық заңдарының қолданылуын бағалау.....14

Баратов А.Ғ., Сайлаубек А., Серік А.С.

SrTaO_2N негізіндегі тар тыйым салынған аймақты фотокатализаторды алу және зерттеу.....33

Нұрбаев Б., Дмитриева Е., Кемелбекова А.

Пайдаланылған литий-ионды аккумуляторлардан литийді селективті шаймалаудың заманауи әдістері.....45

Сейтов А.Н., Аманжолов Т.Е.

Минералданған орталарға арналған жұмыс дөңгелегіндегі ортадан тепкіш ағыстың бірөлшемді физикалық–гидродинамикалық модельдерін салыстырмалы талдау.....60

Сыздыкова А.М., Серикбаев Н.С., Кутум Б.Б.

Кенетейлген бесінші ретті Кортевег-де Фриз тендеуінің локалды кодам типті түрлендіруі мен интегралдану шектері.....83

Уалиханова У.А., Үсіпқызы Т., Алтаева Г.С., Разина О.В.

Экрандалған $f(T)$ – гравитация моделінің есебі.....101

Жадыранова А.А., Цыба П.Ю., Исмаил Ү.Қ., Ержан Б.

Дивергенциясыз бәсеңдеу параметрі, DESI DR2 және космикалық хронометрлер деректері бойынша кинематикалық шектеулер.....123

Жеңіскан Қ., Беков С.С., Сыздыкова А.М.

Хаббл тұрақтысын реконструкциялауға Гаусстық процестер параметрлерінің әсері.....146

ХИМИЯ

Амангелді Б., Жаникулов Н., Таймасов Б., Айтүреев М., Даулетияров М.

Ақ цемент клинкерлерінің күйдіру процестерін және ақтығын зерттеу.....155

Байсалова Г.Ж., Бауыржанова Г.Б., Нияз Г.А., Талтенов А.А., Айнабаев А.А.

Газ хроматография-масс-спектрометрия әдісімен кәдімгі теңгежапырақ өсімдігінің этанолды сығындыларының химиялық құрамын зерттеу.....169

Бишимбаев В.К., Капсаямов Б.А.

Шиелі және Жаңақорған аудандарындағы уранды күкірт қышқылымен шаймалаудың жер асты суларына әсерінің гидрогеохимиялық көрсеткіштері.....183

Дарменбаева А.С., Аубакирова Р.А., Нурғалиева Д.А., Абылкасова Г.Е., Абильмажинова Г.А.

Полимер-металл функционалдық материалдардың құрылымдық-морфологиялық ерекшеліктері.....205

Дюсебаева М.А., Берганаева А.Е., Ибрагимова Н.А., Утаралиев Д.М., Берганаева Г.Е.

Galega officinalis L. өсімдігінің N-бутанолдық фракциясы арқылы күміс нанобөлшектерін жасыл синтездеу.....223

Дюсембекова С.Б., Утарова Д.А., Құспанов Ж.Б., Даулбаев Ч.Б., Әбдікәрімова Ұ.Ә. Термиялық өңделген SrTiO ₃ фотокатализаторларының екідайлы антибиотикті тиімді ыдыратуын зерттеу.....	239
Исаева Ұ.Б., Ахметова Г.С., Пірәлиев Қ.Ж., Малмакова А.Е., Сейлханов Т.М. Жұқпалы ауруларға қарсы кандидат ретінде 1-бензил-4-(П-фторбензоилоксиимино) пиперидин гидрохлориді.....	252
Қамұнұр Қ., Ысқақ М., Мусапирова Л. Барит–кальцит жүйесіндегі натрий лигносульфонатының флотациялық қасиеттеріне химиялық модификацияның әсері.....	264
Кононов А., Қамұнұр Қ., Мусапирова Л., Асылханова Д., Батқал А. Модификацияланған бентонит негізіндегі Al–Fe–Mn бейорганикалық флокулянтын алу және зерттеу.....	276
Қурманғалиева А.1, Ахметова Ф., Карешова Ж., Исаков Р. Көмірсутектердің каталитикалық конверсиясы арқылы сутек алуға арналған ПДМА-модификацияланған таған бентониті.....	292
Қуртебаева А.А., Álvarez-Torrellas S., Noor Haida Mohd Kaus., Gomes H.T., Калмаханова М.С. Жүгері собықтарынан алынған темірмен модификацияланған белсендірілген көмірлермен парацетамол мен сульфаметоксазолды адсорбциялық-тотығу жолымен жою.....	307
Надиров Р.К., Нуртазина Н.Д., Рыскалиева Р.Г. Модификацияланған лигносульфонатты реагентті қолдану арқылы ильменит флотациясының жауап бетін модельдеу және оңтайландыру.....	334
Нефедов А.Н., Тайекенова А.Т., Имашев Б.К., Нурисламов Р.М., Леонтьева К.А. Коррозиялық процестерді модельдеудегі кванттық есептеулер.....	350
Нүркенов О.А., Фазылов С.Д., Сыздықов А.К., Қабиева С.Қ., Жаслан Р.К. Екіншілік аминдермен 3,5-диметилизоксазолдың сульфотуындыларын синтездеу және құрылымдық зерттеу.....	365
Оразбекова Р.С., Тунгатарова С.А., Байжұманова Т.С., Кауменова Г.Б., Жұмабек М. Жоғары энтропиялық оксид катализаторы қатысында биоэтанолдың бу риформингісіне реакциялық қоспа құрамының әсері.....	382
Рыскалиева Р.Г., Бейсембаева Л.К., Осеров Т.Б. Балқаш байыту фабрикасының байыту қалдықтарын гидроциклондық классификациялау.....	398
Сасс А.С., Торлопов И.И., Рахметова К.С., Кензин Э.Н., Жұрынов М. Спирт негізіндегі фосфаттау ерітіндісінен болат бетінде фосфатты жабындардың қалыптасуы және жетілуі.....	418
Сдикова Г.Ж., Далабаева Н.С., Балкембай А.С., Сарова Н.Б., Жалтырбаева Н.К. Мырыш негізіндегі гальваникалық қаптамалардың қасиеттеріне электролит құрамының әсері.....	435

Сейтқалиева Н., Құсаинова Г., Жүрсімбаева М., Мохамад Ибрагим М.Н., Әбдиев Қ. Итакон қышылы негізіндегі сополимерлердің флокуляциялық қасиеттерін зерттеу.....	448
Сергазина С.М., Нұрмұханбетова Н.Н., Острцова И.Б., Камзе А.Р., Касенова Н.Б. Табиғи ауыз су сапасын кешенді бағалау және физика-химиялық көрсеткіштерге статистикалық талдау.....	460
Талгатқызы Ә., Нажипқызы М., Өтенов Ә., Сейтқазинаева Ә., Исанбекова А. Ағаш қалдықтарынан алынған органосольв лигнин негізіндегі көміртеккі талшықтарды энергия сақтау жүйелерінде қолдану.....	475
Тоқтабаева Ә.Қ., Махаева Д.Н., Рахметуллаева Р.Қ., Рвайдарова Г.О., Исенова Г.Д. Анилин, п-фенилендиамин, фенол және формальдегид негізіндегі күкіртқұрамды композиттердің синтезі, құрылымы және физика-химиялық қасиеттері.....	498
Ешманова Г.Б., Смағұлов Д.У. Кремний негізіндегі бөлшектердің ПЭО жабындарының қалыптасуы мен құрамына әсері.....	517
Жортарова А.А., Kubicek V., Ибраев М.Қ., Паньшина С.Ю., Сейдахметова Р.Б. P(III) және P(V) реагенттерімен аминотиазолдар мен аминок-тиадиазолдарды N-фосфорлирлеу: синтезі, құрылымы және биологиялық белсенділігі.....	538
Жусупова А., Тюменцева О., Антонюк В. Үйінді мыс балқыту шлагы мен қорғасын балқытудың түйіршіктелген шлагын планетарлық ұнтақтау кинетикасы мен энергетикасын салыстырмалы зерттеу.....	552

СОДЕРЖАНИЕ

ФИЗИКА

Әлиұлы А., Калтаев А.

Оценка применимости законов подобия при масштабировании центробежных насосов на основе гидродинамического моделирования.....14

Баратов А.Г., Сайлаубек А., Серік А.С.Получение и исследование узкозонного фотокатализатора на основе SrTaO_2N33**Нұрбаев Б., Дмитриева Е., Кемелбекова А.**

Современные методы селективного выщелачивания лития из отработанных литий-ионных аккумуляторов.....45

Сейтов А.Н., Аманжолов Т.Е.

Сравнительный анализ одномерных физико-гидродинамических моделей центробежного течения в рабочем колесе для минерализованных сред.....60

Сыздыкова А.М., Серикбаев Н.С., Кутум Б.Б.

Локальные преобразование типа кодамы и пределы интегрируемости расширенного уравнения Кортевега-де Фриза пятого порядка.....83

Уалиханова У.А., Усипкызы Т., Алтаева Г.С., Разина О.В.Расчёт экранированной модели $f(T)$ – гравитации.....101**Жадыранова А.А., Цыба П.Ю., Исмаил У.Қ., Ержан Б.**

Дивергентно-свободный параметр замедления, кинематические ограничения по данным DESI DR2 и космических хронометров.....123

Женискан К., Беков С.С., Сыздыкова А.М.

Влияние параметров Гауссового процесса на реконструкцию постоянной Хаббла.....146

ХИМИЯ

Амангелди Б., Жаникулов Н., Таймасов Б., Айтурсев М., Даулетияров М.

Исследование процессов обжига и белизны клинкеров белых цементов.....155

Байсалова Г.Ж., Бауыржанова Г.Б., Нияз Г.А., Талтенов А.А., Айнабаев А.А.

Изучение химического состава этанольных экстрактов манжетки обыкновенной методом газ хроматографии-масс-спектрометрии.....169

Бишимбаев В.К., Капсалямов Б.А.

Гидрогеохимические индикаторы воздействия сернокислотного выщелачивания урана на подземные воды районов Шиели и Жанакоргана.....183

Дарменбаева А.С., Аубакирова Р.А., Нургалиева Д.А., Абылкасова Г.Е., Абилямажинова Г.А.

Структурно-морфологические особенности полимер-металлических функциональных материалов.....205

Дюсебаева М.А., Берганаева А.Е., Ибрагимова Н.А., Утаралиев Д.М., Берганаева Г.Е. Зеленый синтез серебряных наночастиц с использованием N-бутанольной фракции Galega Officinalis L.....	223
Дюсембекова С.Б., Утарова Д.А., Куспанов Ж.Б., Даулбаев Ч.Б., Абдикаримова У.А. Исследование влияния термической обработки SrTiO ₃ на фотокаталитической эффективности разложения амфотерного антибиотика.....	239
Исаева У.Б., Ахметова Г.С., Пралиев К.Д., Малмакова А.Е., Сейлханов Т.М. Гидрохлорид 1-бензил-4-(п-фторбензоилоксиимино) пиперидина в качестве кандидата в противомикробное средство.....	252
Қамұнұр Қ., Ысқақ М., Мұсапирова Л. Влияние химической модификации лигносульфоната натрия на его флотационные свойства в системе барит–кальцит.....	264
Кононов А., Қамұнұр Қ., Мұсапирова Л., Асылханова Д., Батқал А. Получение и исследование неорганического флокулянта Al–Fe–Mn на основе модифицированного бентонита.....	276
Курмангалиева А., Ахметова Ф., Карешова Ж., Исаков Р. ПДМА-модифицированный таганский бентонит для получения водорода при каталитической конверсии углеводородов.....	292
Куртебаева А.А., Álvarez-Torrellas S., Noor Haida Mohd Kaus., Gomes H.T., Калмаханова М.С. Модифицированные железом активированные угли из кукурузных початков для адсорбционно-окислительного удаления парацетамола и сульфаметоксазола.....	307
Надиров Р.К., Нуртазина Н.Д., Рыскалиева Р.Г. Моделирование поверхности отклика и оптимизация флотации ильменита с использованием модифицированного лигносульфонатного реагента.....	334
Нефедов А.Н., Тайекенова А.Т., Имашев Б.К., Нурисламов Р.М., Леонтьева К.А. Квантовые вычисления в моделировании коррозионных процессов.....	350
Нуркенов О.А., Фазылов С.Д., Сыздыков А.К., Кабиева С.К., Жаслан Р.К. Синтез и структурное исследование сульфопроизводных 3,5-диметилизоксазола совторичными аминами.....	365
Оразбекова Р.С., Тунгатарова С.А., Байжұманова Т.С., Кауменова Г.Б., Жұмабек М. Влияние состава реакционной смеси в паровом риформинге биоэтанола на высокоэнтропийном оксидном катализаторе.....	382
Рыскалиева Р.Г., Бейсембаева Л.К., Осеров Т.Б. Гидроциклонная классификация хвостов обогащения Балхашской обогажительной фабрики.....	398
Сасс А.С., Торлопов И.И., Рахметова К.С., Кензин Э.Н., Журинов М. Формирование и созревание фосфатных покрытий на стали из фосфатирующего раствора на основе спирта.....	418

Сдикова Г.Ж., Далабаева Н.С., Балкембай А.С., Сарова Н.Б., Жалтырбаева Н.К. Влияние состава электролита на свойства гальванических покрытий на основе цинка.....	435
Сейткалиева Н., Кусаинова Г., Журсумбаева М., Мохамад Ибрагим М.Н., Абдиев К. Исследование флокулирующих свойств сополимеров на основе итаконовой кислоты.....	448
Сергазина С.М., Нурмуханбетова Н.Н., Острцова Н.Б., Камзе А.Р., Касенова Н.Б. Комплексная оценка качества природной питьевой воды и статистический анализ физико-химических показателей.....	460
Талгаткызы А., Нажибкизы М., Отенов А., Сейтказинова А., Исанбекова А. Углеродные волокна на основе органосольв лигнина, полученного из древесных отходов, для применения в системах хранения энергии.....	475
Токтабаева А.К., Махаева Д.Н., Рахметуллаева Р.К., Рвайдарова Г.О., Исенова Г.Д. Синтез, структура и физико-химические свойства серосодержащих композитов на основе анилина, п-фенилендиамина, фенола и формальдегида.....	498
Ешманова Г.Б., Смагулов Д.У. Влияние частиц на основе кремния на формирование и состав ПЭО покрытий.....	517
Жортарова А.А., Kubicek V., Ибраев М.К., Панышина С.Ю., Сейдахметова Р.Б. N-фосфорилирование аминотиазолов и аминок-тиадиазолов с помощью реагентов Р(III) и Р(V): синтез, структура и биологическая активность.....	538
Жусупова А., Тюменцева О., Антонюк В. Сравнительное исследование кинетики и энергетики планетарного измельчения отвального медеплавильного шлака и гранулированного шлака свинцовой плавки.....	553

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N-PHOSPHORYLATION OF AMINOTHIAZOLES AND AMINO- THIADIAZOLES WITH P(III)- AND P(V)-REAGENTS: SYNTHESIS, STRUCTURE, AND BIOLOGICAL ACTIVITY

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Abstract. This study investigates the N-phosphorylation of key mono- and diaminoheterocycles within the thiazole and thiadiazole series using dimethyl chlorophosphate (P(V)) and 1-tert-butoxy-N,N,N',N'-tetraethylphosphanediamine (P(III)) reagents. Eight novel derivatives were successfully synthesized and isolated. Reaction conditions were optimized, employing triethylamine in acetonitrile at 80 °C for P(V) agents, and ethyl acetate at 80 °C via diethylamine elimination for P(III) agents. Diamino substrates underwent efficient, symmetric bis-phosphorylation at both exocyclic amino positions. Due to the electron-withdrawing effect of the

second endocyclic nitrogen in the thiadiazole core, its amino groups showed lower nucleophilicity, resulting in lower yields (31–41%) compared to thiazole counterparts (65–83%). Structural frameworks were confirmed by ^{31}P NMR spectroscopy, appearing at δ 5.85–5.92 ppm for phosphoramidates and δ 124.66–128.48 ppm for phosphoramidites.

In vitro screening demonstrated a strong, dose-dependent antimicrobial profile, with Gram-negative strains displaying enhanced susceptibility. Trivalent phosphorus derivative emerged as the most potent broad-spectrum candidate. Against *P. aeruginosa*, 1-tert-butoxy-N,N-diethyl-N'-(1,3,4-thiadiazol-2-yl)phosphanediamine exhibited a 27–33 mm inhibition zone, outperforming streptomycin (MIC = 6.25, MBC = 12.5 $\mu\text{g}/\text{mL}$). Against *T. viride*, it outclassed clotrimazole with a 30–39 mm zone (MIC = 12.5, MFC = 25 $\mu\text{g}/\text{mL}$). The results obtained open up broad prospects for the development of new, highly effective antibacterial and antifungal agents based on phosphorylated heterocycles.

Keywords: aminothiazole, aminothiadiazole, N-phosphorylation, phosphonamides, dimethylchlorophosphate, amidophosphite, P(III)/P(V), antibacterial and antifungal activity

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Р(III) ЖӘНЕ Р(V) РЕАГЕНТТЕРІМЕН АМИНОТИАЗОЛДАР МЕН АМИНО-ТИАДИАЗОЛДАРДЫ N-ФОСФОРЛИРЛЕУ: СИНТЕЗІ, ҚҰРЫЛЫМЫ ЖӘНЕ БИОЛОГИЯЛЫҚ БЕЛСЕНДІЛІГІ

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Аннотация. Бұл зерттеу тиазол және тиadiaзол қатарындағы негізгі моно- және диаминогетероциклдердің N-фосфорлануын диметилхлорфосфат (P(V) реагенті) және 1-трет-бутоксид-N,N,N',N'-тетраэтилфосфандиамин (P(III) реагенті) көмегімен зерттеуге арналған. Сегіз жаңа туынды сәтті синтезделіп, бөлініп алынды. Реакция шарттары оңтайландырылды: P(V) реагенттері үшін ацетонитрил ортасында, триэтиламин қатысында, 80 °C температурада; P(III) реагенттері үшін этилацетат ортасында, 80 °C температурада, диэтиламиннің элиминациялануы арқылы жүргізілді. Диамин субстраттары екі экзоциклді амин тобы бойынша да тиімді, симметриялы бис-фосфорлануға ұшырады. Тиadiaзол ядросындағы екінші эндоциклді азот атомының электрон тартқыш әсеріне байланысты оның амин топтарының нуклеофильдігі төмендеді, нәтижесінде тиазол туындыларымен (65–83%) салыстырғанда шығым төмен болды (31–41%). Қосылыстардың құрылымы ³¹P ЯМР спектроскопиясы әдісімен расталды: фосфорамидаттардың сигналдары δ 5.85–5.92 м.б. аймағында, фосфорамидиттердің сигналдары δ 124.66–128.48 м.б. аймағында байқалды.

In vitro скринингі күшті, дозаға тәуелді антимикробтық профильді көрсетті, грамтеріс штаммдар жоғары сезімталдық танытты. Үшвалентті фосфор туындысы кең спектрлі әсер ететін ең белсенді кандидат болып шықты. *P. aeruginosa* штаммына қарсы 1-трет-бутоксид-N,N-диэтил-N'-(1,3,4-тиadiaзол-2-ил) фосфанедиамин қосылысы 27–33 мм тежелу аймағын көрсетіп, стрептомициннен басым түсті (МИК = 6.25, МБК = 12.5 мкг/мл). *T. viride* саңырауқұлағына қарсы ол клотримазолдан басым болып, 30–39 мм тежелу аймағын көрсетті (МИК = 12.5, МФК = 25 мкг/мл). Алынған нәтижелер фосфорланған гетероциклдер негізіндегі жаңа тиімділігі жоғары бактерияларға және саңырауқұлақтарға қарсы дәрі-дәрмектерді әзірлеу үшін кең мүмкіншіліктерді ашады.

Түйін сөздер: аминотиазол, аминотиadiaзол, N-фосфорлану, фосфонамидтер, диметилхлорфосфат, амидофосфит, P(III)/P(V), антибактериалды және антисаңырауқұлақтық белсенділік

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Н-ФОСФОРИЛИРОВАНИЕ АМИНОТИАЗОЛОВ И АМИНО- ТИАДИАЗОЛОВ С ПОМОЩЬЮ РЕАГЕНТОВ P(III) И P(V): СИНТЕЗ, СТРУКТУРА И БИОЛОГИЧЕСКАЯ АКТИВНОСТЬ

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Аннотация. Настоящее исследование посвящено N-фосфорилированию ключевых моно- и диаминогетероциклов ряда тиазола и тиадiazола с использованием диметилхлорфосфата (реагент P(V)) и 1-трет-бутоксi-N,N,N',N'-тетраэтилфосфандиамина (реагент P(III)). Успешно синтезированы и выделены восемь новых производных. Условия реакции были оптимизированы: для реагентов P(V) — с использованием триэтиламина в ацетонитриле при 80 °C, для реагентов P(III) — в среде этилацетата при 80 °C с элиминированием диэтиламина. Диаминосубстраты подвергались эффективному симметричному бис-фосфорилированию по обоим экзоциклическим аминогруппам. Вследствие электроноакцепторного эффекта второго эндоциклического атома азота в тиадiazольном ядре, его аминогруппы проявляли пониженную нуклеофильность, что приводило к более низким выходам (31–41%) по сравнению с тиазольными аналогами (65–83%). Структуры соединений были подтверждены методом спектроскопии ЯМР 31P: сигналы фосфорамидатов наблюдались в области δ 5.85–5.92 м.д., фосфорамидитов — в области δ 124.66–128.48 м.д.

Скрининг *in vitro* продемонстрировал выраженный, дозозависимый антимикробный профиль, при этом грамотрицательные штаммы проявляли повышенную чувствительность. Производное трёхвалентного фосфора показало

себя наиболее активным кандидатом широкого спектра действия. В отношении *P. aeruginosa* соединение 1-трет-бутоксид-N,N-диэтил-N'-(1,3,4-тиадиазол-2-ил)фосфанедиамин проявило зону ингибирования 27–33 мм, превзойдя стрептомицин (МИК = 6.25, МБК = 12.5 мкг/мл). В отношении *T. viride* оно превзошло клотримазол с зоной ингибирования 30–39 мм (МИК = 12.5, МФК = 25 мкг/мл). Полученные результаты открывают широкие перспективы для разработки новых высокоэффективных антибактериальных и противогрибковых средств на основе фосфорилированных гетероциклов.

Ключевые слова: аминотиазол, аминотиадиазол, N-фосфорилирование, фосфонамиды, диметилхлорфосфат, амидофосфит, P(III)/P(V), антибактериальная и противогрибковая активность

Introduction. Heterocyclic systems of the thiazole and thiadiazole series are among the priority areas of modern medicinal and organoelemental chemistry (Das et al., 2016, Chhabria et al., 2021). The thiazole moiety is found in natural compounds — for example, thiamine — and in numerous medicinal products, whilst the 2-aminothiazole synthon is one of the most sought-after pharmacophores in the design of biologically active molecules (Das et al., 2016, Chhabria et al., 2021). Numerous reviews (Das et al., 2016, Chhabria et al., 2021, Makam et al., 2014, Alizadeh et al., 2021) in recent years have systematised data on the antitumour, antimicrobial, antitubercular and anti-inflammatory activities of 2-aminothiazole derivatives, whilst the 2-aminothiazole moiety itself is present in the structure of a number of clinically used drugs.

Equally significant as a heterocyclic platform are thiadiazole derivatives, which combine two nitrogen atoms and a ‘bridging’ sulphur atom (=N–C(SR)=N– fragment) within the ring, which provides them with pronounced meso-ion stabilisation and the ability to form hydrogen bonds with biological targets. According to comprehensive reviews (Jain et al., 2013, Górecki et al., 2025, Hemanth et al., 2022), thiadiazole derivatives exhibit a broad spectrum of biological activity—including antimicrobial, antifungal, antiviral, antitumour, anti-inflammatory and CNS activity (Janovska et al., 2003). In particular, one of the most recent review article (Górecki et al., 2025) notes that, among 79 new thiadiazoles tested against 19 bacterial strains, a significant proportion of the compounds exhibited activity comparable to or exceeding that of the reference compounds. Similar results were also recorded for 75 compounds tested against 25 species of fungi (Janovska et al., 2003).

A separate area of aminoheterocycle modification involves their conversion into phosphoric acid derivatives (phosphonamides, phosphoramidates) by replacing the hydrogen atoms of the exocyclic amino group with a phosphoryl or phosphite moiety; phosphonates and phosphoramidates, as analogues of natural phosphates, are described in detail in a fundamental review (Engel et al., 1977). The introduction of a P–N bond into a biologically active molecule is a well-known technique in medicinal chemistry: the ProTide technology, which is based on the introduction of a phosphoramidate group into nucleoside and nucleotide substrates, has made it possible to overcome the problem of low cellular permeability and insufficient intracellular phosphorylation of nucleoside

analogues, and has formed the basis for a number of approved antiviral and antitumour drugs (Dehmchi et al., 2024, Slusarczyk et al., 2018), including phosphoramidate prodrugs against HIV (Mehellou et al., 2009) and the hepatitis C virus (Perrone et al., 2007). In addition to synthetic prodrugs, the P–N bond has also been identified in a number of naturally occurring biologically active compounds — the phosphoramidate antibiotic agrocin 84 (Roberts et al., 1977), the nucleotide antibiotic fosmidisin (Phillips et al., 1993) and the peptide-nucleotide antibiotic microcin C7 (Guijarro et al., 1995). Extending this approach to heteroaromatic amines—in particular, aminothiazoles and aminothiadiazoles — is of interest both as a means of modifying the pharmacokinetic properties of known pharmacophores and as a route to new classes of physiologically active organophosphorus compounds (IUPAC et al., 2025).

From the perspective of synthetic methodology, the N-phosphorylation of heterocyclic amines can be achieved via two fundamentally different routes: (a) reaction with chloranhydrides of pentavalent phosphorus P(V) (dialkyl chlorophosphates) in the presence of a base-acceptor HCl, leading directly to stable phosphoramidates; and (b) reaction with amidophosphites of trivalent phosphorus P (III) (in particular, diamidophosphites of the general formula $R_2N-P(NR_2)-OR'$), the reaction with which proceeds via the elimination of a secondary amine and the formation of a P(III)–N bond without a change in the oxidation state of phosphorus. A comparison of the reactivity of the same series of amino-heterocycles towards these two types of agents allows an assessment of the relative contribution of the heterocycle's electronic and steric factors to the regioselectivity and efficiency of N-phosphorylation, which was the aim of this work, which continues the systematic study of the phosphorylation of aminothiazole and aminothiadiazole substrates previously initiated by the authors (Zhortarova et al., 2026, Zhortarova et al., 2026)

Thus, in this work, we present the first direct comparative study on the P–N phosphorylation of key mono- and diaminoheterocycles within the thiazole and thiadiazole series: 2-aminothiazole (1a), 2-aminothiadiazole (1b) (Scheme 1), 2,4-diaminothiazole (1c), and 2,5-diaminothiadiazole (1d) (Scheme 2). Using dimethyl chlorophosphate (P(V), 2a) and 1-tert-butoxy-N,N,N',N'-tetraethylphosphanediamine (P(III), 2b) as reagents, we investigated how the electronic and steric features of the substrates influence the regioselectivity and efficiency of the reaction. This insight enabled the development of selective methods for the synthesis of novel phosphoramidates 3a-d and phosphoramidites 4a-d.

Materials and Methods. Reactions sensitive to moisture were carried out in a dry argon atmosphere. All reagents and starting materials were of analytical grade, were purchased from Sigma-Aldrich, and were used as received without further purification. The progress of the reactions was monitored by thin-layer chromatography (TLC) on plates coated with Merck silica gel F 254. Melting and boiling points were determined in open capillaries using a Buchi M560 apparatus. IR spectra were registered using an FSM 1201 FT-IR spectrometer in the frequency range $4000-400\text{ cm}^{-1}$, using KBr pellets. ^1H , ^{13}C and ^{31}P NMR spectra were recorded on a Bruker Avance 400 spectrometer at operating frequencies of 400, 100 and 162 MHz, respectively. The

studies were carried out in CDCl_3 solution. Chemical shifts (δ) are given in parts per million (ppm) relative to tetramethylsilane (TMS) as the internal standard for ^1H and ^{13}C NMR, and 85% H_3PO_4 as the external standard for ^{31}P NMR. Splitting is denoted as s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad peak, and spin-spin interaction constants are given in Hz.

General procedure for the preparation of compounds 3a-d (reaction with dimethyl chlorophosphate, 2a)

To a solution of 0.01 mol of the corresponding amino-heterocycle (1a-d; for diamines 1c, d — 0.01 mol based on 2 equivalents of reagent 2a) and 0.01–0.02 mol of triethylamine in 120 mL of absolute acetonitrile; whilst stirring and cooling, 0.01 mol (or 0.02 mol for diamines) of dimethyl chlorophosphate (2a) was added dropwise. The reaction mixture was heated at 80 °C for 4 h, monitoring the progress of the reaction by TLC. Upon completion of the reaction, the triethylamine hydrochloride precipitate was filtered off and the solvent was evaporated under reduced pressure.

Compound 3a — dimethyl thiazol-2-ylphosphoramidate. Yield: 2.5 g. 83%. Melting point: 158–161 °C. IR (KBr, cm^{-1}): 3340 (N–H), 1610 (C=N), 1490 (C=C), 1520 (N–H bend), 1245 (P=O), 1030 (P–O–C), 940 (P–N), 730 (C–S). ^1H NMR (CDCl_3) δ 3.72 (d, J = 11.0, 6H), 6.68 (d, J = 4.5, 1H), 7.22 (s, 1H), 9.66 (s, 1H). ^{13}C NMR (CDCl_3) δ 54.42, 54.34, 112.03, 136.71, 171.80. ^{31}P NMR (CDCl_3) δ 5.86

Compound 3b — dimethyl (1,3,4-thiadiazol-2-yl)phosphoramidate. Yield: 2.09 g. 40%. Melting point: 146–149 °C. IR (KBr, cm^{-1}): 3335 (N–H), 1605 (C=N), 1485 (C=C/N=N), 1515 (N–H bend), 1250 (P=O), 1035 (P–O–C), 945 (P–N), 725 (C–S). ^1H NMR (CDCl_3) δ 3.72 (d, J = 11.0, 6H), 8.91 (s, 1H), 9.16 (s, 1H). ^{13}C NMR (CDCl_3) δ 54.33, 54.41, 157.20, 173.86. ^{31}P NMR (CDCl_3) δ 5.92.

Compound 3c — tetramethyl thiazole-2,4-diylbis(phosphoramidate). Yield: 2.71 g. 82%. Melting point: 174–177 °C. IR (KBr, cm^{-1}): 3320, 3300 ($2\times\text{N–H}$), 1615 (C=N), 1495 (C=C), 1525 (N–H bend), 1250, 1235 ($2\times\text{P=O}$), 1040, 1020 ($2\times\text{P–O–C}$), 950, 930 ($2\times\text{P–N}$), 730 (C–S). ^1H NMR (CDCl_3) δ 3.72 (m, 12H), 5.62 (s, 1H), 8.13 (s, 1H), 9.29 (s, 1H). ^{13}C NMR (CDCl_3) δ 52.80, 52.70, 110.50, 142.05, 166.1. ^{31}P NMR (CDCl_3) δ 5.85.

Compound 3d — tetramethyl (1,2,4-thiadiazole-3,5-diyl)bis(phosphoramidate). Yield: 1.36 g. 41%. Melting point: 148–151 °C. IR (KBr, cm^{-1}): 3330 (N–H), 1600 (C=N), 1480 (C=C/N=N), 1510 (N–H bend), 1240 (P=O), 1025 (P–O–C), 935 (P–N), 720 (C–S). ^1H NMR (CDCl_3) δ 3.72 (m, 12H), 8.39 (s, 1H), 9.43 (s, 1H). ^{13}C NMR (CDCl_3) δ 52.70, 52.72, 152.11, 173.08. ^{31}P NMR (CDCl_3) δ 5.90

General procedure for the preparation of compounds 4a-d (reaction with 1-tert-butoxy-N,N,N',N'-tetraethylphosphanediamine, 2b)

To a solution of 0.01 mol of the corresponding amino-heterocycle (1a-d; for diamines 1c, d — calculated on the basis of 2 equivalents of reagent 2b) in 150 ml of absolute ethyl acetate, whilst stirring at +50°C, 0.01 mol (or 0.02 mol for diamines, respectively) 1-tert-butoxy-N,N,N',N'-tetraethylphosphanediamine (2b). The reaction mixture was stirred at 80 °C for 8 hours, whilst the evolving diethylamine was gradually distilled off. The solvent was evaporated under vacuum.

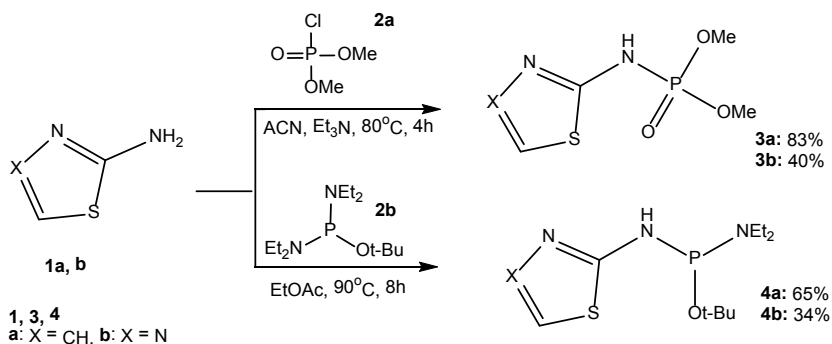
Compound 4a — *1-tert-butoxy-N,N-diethyl-N'-(thiazol-2-yl)phosphanediamine*. Yield: 1.78 g. 65%. Melting point: 167–170 °C. IR (KBr, cm⁻¹): 3345 (N–H), 1615 (C=N), 1495 (C=C), 1525 (N–H bend), 1040 (P–O–C), 950 (P–N), 735 (C–S). ¹H NMR (CDCl₃) δ 0.94 (td, *J* = 1.0, 8.1, 6H), 1.04 (s, 9H), 3.19 (pent, *J* = 8.1, 4H), 6.00 (s, 1H), 8.64 (d, *J* = 4.5, 1H). ¹³C NMR (CDCl₃) δ 14.34, 30.86, 39.79, 68.52, 112.71, 137.60, 171.85. ³¹P NMR (CDCl₃) δ 124.66.

Compound 4b — *1-tert-butoxy-N,N-diethyl-N'-(1,3,4-thiadiazol-2-yl)phosphanediamine*. Yield: 0.93 g. 34%. Melting point: 160–163 °C. IR (KBr, cm⁻¹): 3340 (N–H), 1610 (C=N), 1490 (C=C/N=N), 1520 (N–H bend), 1045 (P–O–C), 955 (P–N), 730 (C–S). ¹H NMR (CDCl₃) δ 0.91 (td, *J* = 1.0, 8.1, 6H), 1.04 (s, 9H), 3.19 (pent, *J* = 8.1, 4H), 5.68 (s, 1H), 8.89 (s, 1H). ¹³C NMR (CDCl₃) δ 14.24, 30.67, 39.93, 69.52, 152.6, 173.5. ³¹P NMR (CDCl₃) δ 126.28.

Compound 4c — *N,N-(thiazole-2,4-diyl)bis(1-tert-butoxy-N,N-diethylphosphanediamine)*. Yield: 3.63 g. 78%. Melting point: 167–169 °C. IR (KBr, cm⁻¹): 3325, 3305 (2×N–H), 1618 (C=N), 1498 (C=C), 1528 (N–H bend), 1045, 1030 (2×P–O–C), 960, 940 (2×P–N), 735 (C–S). ¹H NMR (CDCl₃) δ 0.91 (td, *J* = 1.0, 8.1, 12H), 1.04 (s, 18H), 3.19 (pent, *J* = 8.1, 8H), 5.19 (s, 1H), 10.55 (s, 2H). ¹³C NMR (CDCl₃) δ 14.24, 30.96, 39.89, 68.82, 111.55, 142.50, 166.45. ³¹P NMR (CDCl₃) δ 124.79.

Compound 4d — *N,N-(1,2,4-thiadiazole-3,5-diyl)bis(1-tert-butoxy-N,N-diethylphosphanediamine)*. Yield: 1.44 g. 31%. Melting point: 152–154 °C. IR (KBr, cm⁻¹): 3320, 3300 (2×N–H), 1612 (C=N), 1492 (C=C/N=N), 1522 (N–H bend), 1040, 1025 (2×P–O–C), 955, 935 (2×P–N), 725 (C–S). ¹H NMR (CDCl₃) δ 0.91 (td, *J* = 1.0, 8.2, 12H), 1.04 (s, 18H), 3.19 (pent, *J* = 8.1, 8H), 10.19 (s, 2H). ¹³C NMR (CDCl₃) δ 14.67, 30.86, 39.97, 69.02, 152.69, 173.57. ³¹P NMR (CDCl₃) δ 128.48.

Results and Discussion. The study of reactivity began with the least sterically hindered monoamino-substituted substrates 1a, b. It was found that their reactions with both pentavalent **2a** and trivalent 2b phosphorus derivatives proceed exclusively via the exocyclic nitrogen atom, leading to the corresponding monophosphorylated products 3a, b, 4a, b in high yields (Scheme 1).

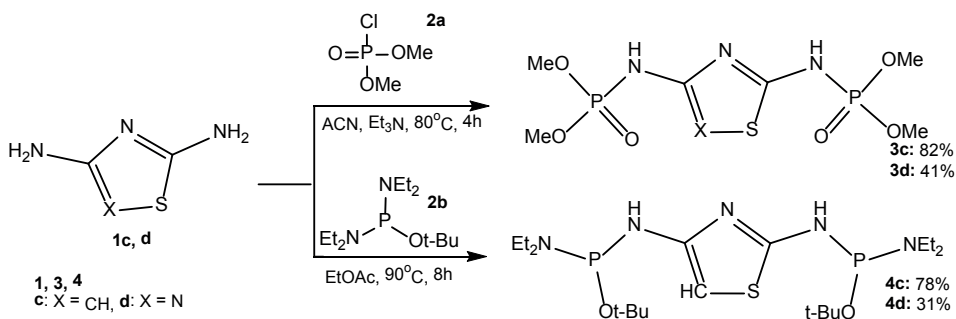


Scheme 1. N-phosphorylation of monoaminoheterocycles 1a and 1b using pentavalent and trivalent phosphorus reagents.

The reactions of substrates 1a and 1b with chlorophosphate 2a were carried out in acetonitrile in the presence of triethylamine as an HCl acceptor (80 °C, 4 h). Under these conditions, stable phosphonamidates 3a and 3b are formed, with the oxidation state of phosphorus (P(V)) being retained. A similar strategy of direct acylation of an exocyclic amino group with dialkyl chlorophosphates has previously been successfully employed to modify a number of bioactive heterocyclic amines, including benzothiazole derivatives (Nayab Rasool et al., 2018).

The reaction of substrates 1a and 1b with amidophosphite 2b was carried out in ethyl acetate without the addition of an external base (90 °C, 8 h). The driving force behind this process is the substitution of the diethylamide group at the P(III) atom by a weaker basic heteroaromatic amine, accompanied by the formation and removal of low-boiling diethylamine. The reaction yields the corresponding amidophosphites 4a and 4b.

For both monofunctional substrates, 1a and 1b, phosphorylation proceeds exclusively via the exocyclic nitrogen atom. In this context, the yields of products derived from the thiazole precursor 1a are consistently higher than those for its thiadiazole analogue 1b: 83% (3a) versus 40% (3b) in the case of reagent 2a, and 65% (4a) versus 34% (4b) for reagent 2b. The observed difference is due to the strong electronic influence of the second endocyclic nitrogen atom in the thiadiazole ring: as a result of its acceptor action, the unshared electron pair of the exocyclic amino group is more strongly delocalised, which significantly reduces its nucleophilicity compared with aminothiazole.



Scheme 2. N-phosphorylation of diaminoheterocycles 1c and 1b using pentavalent and trivalent phosphorus reagents.

For the bifunctional substrates 1c and 1d, which contain two exocyclic amino groups, complete N-phosphorylation occurs at both reaction centres when a two-fold molar excess of the phosphorylating agent is used. This results in the formation, in good yields, of symmetrical bis-phosphonamidates 3c, d and bis-phosphoramidites (or amidophosphites) 4c, d. As with the series of monofunctional analogues, the yields of products based on the thiazole-containing diamine 1c are consistently higher than those for the thiadiazole derivative 1d: 82% (for 3c) versus 41% (for 3d) upon reaction with reagent 2a; and 78% (for 4c) versus 31% (for 4d) when using reagent 2b. These

results fully replicate the previously observed trend of decreasing reactivity of the amino group upon transition from the electron-rich thiazole ring to the electron-deficient thiadiazole ring. (Scheme 2).

The structures of the compounds obtained were confirmed using a physicochemical methods: IR and ^1H , ^{13}C , ^{31}P NMR spectroscopy; detailed spectral data are presented in the experimental section. The assignment of signals in the ^{31}P NMR spectra is the most informative diagnostic criterion for the course of N-phosphorylation: for the products of the P(V) series (3a-d), chemical shifts are characteristic of the region typical of phosphoramides ($\delta^{31}\text{P}$ 5.85 – 5.92 m.d.), whereas for the products of the P(III) series (4a-d), they are characteristic of the region typical of triamidophosphites ($\delta^{31}\text{P}$ 124.66 – 128.48 m.d.). The ^{31}P NMR spectra of the compounds obtained are presented in Table 1.

Table 1. ^{31}P NMR chemical shifts (CDCl_3) of the synthesized phosphorylated derivatives 3a-d, 4a-d.

Entry	Compound	Phosphorylating agent	$\delta^{31}\text{P}$ NMR (CDCl_3 , ppm)
1	dimethyl thiazol-2-ylphosphoramidate 3a	P(V), 2a (1 equiv.)	5.86
2	1-tert-butoxy-N,N-diethyl-N'-(thiazol-2-yl)phosphanediamine 4a	P(III), 2b (1 equiv.)	124.66
3	dimethyl (1,3,4-thiadiazol-2-yl)phosphoramidate 3b	P(V), 2a (1 equiv.)	5.92
4	1-tert-butoxy-N,N-diethyl-N'-(1,3,4-thiadiazol-2-yl)phosphanediamine 4b	P(III), 2b (1 equiv.)	126.28
5	tetramethyl thiazole-2,4-diylbis(phosphoramidate) 3c	P(V), 2a (2 equiv.)	5.85
6	N,N-(thiazole-2,4-diyl)bis(1-tert-butoxy-N,N-diethylphosphanediamine) 4c	P(III), 2b (2 equiv.)	124.79
7	tetramethyl (1,2,4-thiadiazole-3,5-diyl)bis(phosphoramidate) 3d	P(V), 2a (2 equiv.)	5.90
8	N,N-(1,2,4-thiadiazole-3,5-diyl)bis(1-tert-butoxy-N,N-diethylphosphanediamine) 4d	P(III), 2b (2 equiv.)	128.48

Biological activity. Compounds 3a-d, 4a-d tested for antibacterial activity at four different concentrations — 12.5, 25, 50 and 100 $\mu\text{g/ml}$ — against *Staphylococcus aureus*, *Bacillus subtilis*, *Pseudomonas aeruginosa*, *Klebsiella pneumoniae* and the fungi *Aspergillus niger* and *Trichoderma viride*.

Antibacterial activity. The results of the antibacterial activity study, presented in Table 2, showed that Gram-negative bacteria were more sensitive to the compounds under investigation than Gram-positive bacteria. It was noted that compounds 4a, 3b and 4b exhibited higher activity than the other compounds 3a, 3c, 3d, 4c, and 4d.

This may be due to the fact that compounds 4a, 3b and 4b are monophosphorylated derivatives with a lower molecular weight compared with their bis-phosphorylated analogues (3c, 4c, 3d, 4d), which facilitates their penetration through the bacterial cell wall; furthermore, compounds 4a and 4b, containing a P(III) centre with lipophilic tert-butoxy and diethylamino groups, possess higher lipophilicity compared with P(V) derivatives. In fact, compound 4b demonstrated slightly higher activity against *Pseudomonas aeruginosa* compared with the standard preparation of streptomycin.

This may be due to the combination of compound 4b's moderate molecular weight and the mesoionic nature of the thiadiazole ring, which provide a favourable balance between permeability through the porin channels of Gram-negative bacteria and binding to the target.

Table 2. Screening of the *in vitro* antibacterial activity of synthesized compounds 3a–d and 4a–d (zone of inhibition, mm).

Compound	Gram-positive bacteria							
	<i>Staphylococcus aureus</i>				<i>Bacillus subtilis</i>			
	12.5 μg/ mL	25 μg/ mL	50 μg/ mL	100 μg/ mL	12.5 μg/ mL	25 μg/ mL	50 μg/ mL	100 μg/ mL
3a	-	-	-	-	-	-	-	-
4a	24±1	26±1	28±3	30±1	27±3	29±3	31±3	33±3
3b	29±1	30±1	32±3	33±1	31±3	33±3	35±3	36±3
4b	32±3	33±1	35±3	37±1	34±2	35±2	36±3	38±3
3c	12±3	14±3	16±3	20±1	13±3	14±1	15±3	17±1
4c	11±2	13±3	15±1	18±3	12±2	13±1	14±3	16±2
3d	10±1	12±1	14±1	17±2	11±3	12±1	13±3	14±1
4d	07±2	08±1	09±3	12±1	-	-	11±1	13±3
Streptomycin	30±1	32±2	35±2	37±1	32±3	34±2	36±1	40±1
Compound	Gram-negative bacteria							
	<i>Pseudomonas aeruginosa</i>				<i>Klebsiella pneumoniae</i>			
	08	10	12	14	-	-	13	15
3a	08	10	12	14	-	-	13	15
4a	19±3	21±3	23±1	25±1	34±2	35±2	36±2	37±2
3b	24±3	25±3	26±1	28±1	36±2	37±2	38±2	39±2
4b	27±1	28±2	30±1	33±2	37±1	38±1	39±2	40±1
3c	15±1	17±2	19±1	21±2	16±3	18±1	20±3	22±3
4c	14±1	16±3	18±2	20±1	15±2	17±3	19±2	21±1
3d	13±3	15±2	17±1	19±3	14±1	16±2	18±2	20±2
4d	08±3	10±2	12±2	14±1	09±2	11±1	13±2	15±1
Streptomycin	25±2	27±2	29±2	32±1	38±2	40±2	42±1	44±2
Control (DMSO)	-	-	-	-	-	-	-	-

(-) No activity, (±) Standard deviation.

Antifungal activity. All the compounds studied inhibited the germination of spores from the test fungi *Aspergillus niger* and *Trichoderma viride*. Overall, most compounds exhibited higher antifungal activity against *Trichoderma viride* than against *Aspergillus niger*. Among all the compounds, compound 4b demonstrated higher inhibitory activity, particularly against *Trichoderma viride*, compared with the standard drug clotrimazole, as shown in Table 3. Furthermore, compounds 4a and 3b demonstrated good activity compared with the other compounds 3a, 3c, 3d, 4c and 4d.

Table 3. The *in vitro* antifungal activity of compounds 3a-d, 4a-d (zone of inhibition, mm).

Compound	<i>Aspergillus niger</i>				<i>Trichoderma viride</i>			
	12.5 $\mu\text{g}/\text{mL}$	25 $\mu\text{g}/\text{mL}$	50 $\mu\text{g}/\text{mL}$	100 $\mu\text{g}/\text{mL}$	12.5 $\mu\text{g}/\text{mL}$	25 $\mu\text{g}/\text{mL}$	50 $\mu\text{g}/\text{mL}$	100 $\mu\text{g}/\text{mL}$
3a	-	-	-	-	-	-	07 $\pm$ 2	09 $\pm$ 3
4a	23 $\pm$ 1	25 $\pm$ 1	27 $\pm$ 3	29 $\pm$ 1	26 $\pm$ 3	28 $\pm$ 3	30 $\pm$ 3	32 $\pm$ 3
3b	27 $\pm$ 1	28 $\pm$ 1	30 $\pm$ 3	32 $\pm$ 1	29 $\pm$ 3	31 $\pm$ 3	32 $\pm$ 3	34 $\pm$ 3
4b	30 $\pm$ 3	32 $\pm$ 2	33 $\pm$ 1	35 $\pm$ 3	34 $\pm$ 1	36 $\pm$ 2	37 $\pm$ 1	39 $\pm$ 2
3c	20 $\pm$ 1	22 $\pm$ 3	24 $\pm$ 2	25 $\pm$ 2	27 $\pm$ 2	29 $\pm$ 3	32 $\pm$ 2	33 $\pm$ 3
4c	19 $\pm$ 3	21 $\pm$ 2	23 $\pm$ 1	25 $\pm$ 3	26 $\pm$ 1	28 $\pm$ 2	31 $\pm$ 1	32 $\pm$ 2
3d	18 $\pm$ 1	20 $\pm$ 1	21 $\pm$ 2	23 $\pm$ 1	25 $\pm$ 3	27 $\pm$ 3	29 $\pm$ 3	31 $\pm$ 1
4d	-	-	-	-	13 $\pm$ 2	15 $\pm$ 1	17 $\pm$ 1	19 $\pm$ 2
Clotrimazole	31 $\pm$ 3	33 $\pm$ 2	36 $\pm$ 1	39 $\pm$ 1	32 $\pm$ 1	35 $\pm$ 1	36 $\pm$ 2	38 $\pm$ 2
Control (DMSO)	-	-	-	-	-	-	-	-

(-) No activity, ($\pm$) Standard deviation.

MIC, MBC and MFC values for compounds 4a, 3b and 4b. The minimum inhibitory concentration (MIC), minimum bactericidal concentration (MBC) and minimum fungicidal concentration (MFC) values for the compounds under investigation are given in Table 4.

Table 4. MIC, MBC and MFC of compounds 4a, 3b, 4b.

Compound	Minimum inhibitory concentration MIC (MBC / MFC) m					
	<i>S. aureus</i>	<i>B. subtilis</i>	<i>P. aeruginosa</i>	<i>K.pneumoniae</i>	<i>A. niger</i>	<i>T.viride</i>
4a	50(>200)	50(>200)	25(100)	25(>100)	50(>200)	25(100)
3b	50(>200)	50(200)	25(100)	25(>100)	25(100)	50(>200)
4b	25(>100)	25(>100)	6.25(12.5)	12.5(50)	12.5(50)	12.5(25)
Streptomycin	6.25	6.25	6.25	12.5	-	-
Clotrimazole	-	-	-	-	6.25	12.5

The MIC is the lowest concentration of an antimicrobial agent that inhibits the visible growth of a microorganism. (However, it is not known whether the microorganisms are completely destroyed.) MBC/MFC is the lowest concentration of an antibiotic required to kill a specific bacterium or fungus. Determining the MBC/MFC involves an additional set of steps carried out after the minimum inhibitory concentration (MIC) has been determined. Antimicrobial agents are generally considered bactericidal/fungicidal if the MBC/MFC value does not exceed the MIC by more than a factor of four. Compound 4b exhibited low MIC values compared with 4a and 3b. Furthermore, the MBC value for 4b is $2 \times \text{MIC}$ against *P. aeruginosa*, whilst the MFC value is $2 \times \text{MIC}$ against *T. viride*. However, the other compounds exhibited bactericidal and fungicidal activity exceeding $2 \times \text{MIC}$.

Thus, compound 4b demonstrated excellent antibacterial activity against *P. aeruginosa*, showing an inhibition zone of 39 mm at a concentration of 100 $\mu\text{g}/\text{mL}$, with MIC and MBC values of 6.25 $\mu\text{g}/\text{mL}$ and 12.5 $\mu\text{g}/\text{mL}$, respectively. Compounds 4a and 3b also exhibited strong antifungal activity against *T. viride*, with inhibition

zones of 32 mm and 34 mm, respectively, at 100 $\mu\text{g/mL}$, and MIC and MFC values of 12.5 $\mu\text{g/mL}$ and 25 $\mu\text{g/mL}$, respectively.

Conclusion. In summary, we have established a direct synthetic approach for the N-phosphorylation of mono- and diaminoheterocycles within the thiazole and thiadiazole series using P(V) (dimethyl chlorophosphate) and P(III) (1-tert-butoxy-N,N,N',N'-tetraethylphosphanediamine) electrophilic reagents. Eight novel organophosphorus derivatives (3a–d and 4a–d) were isolated and fully characterized. The nucleophilic reactivity of the exocyclic amino groups was found to be highly dependent on the heterocycle architecture, systematically decreasing from the electron-rich thiazoles to the electron-deficient thiadiazoles, resulting in higher yields for thiazole derivatives (65–83% for 3a, 3c, 4a, 4c) compared to their thiadiazole analogues (31–41% for 3b, 3d, 4b, 4d). For bifunctional diamines 1c and 1d, complete and symmetric bis-phosphorylation was successfully achieved at both reaction centers. The structural differences between the P(V) and P(III) derivatives were distinctively confirmed by ^{31}P NMR spectroscopy, showing sharp singlets at δ 5.85–5.92 ppm for the phosphoramidate core and significant downfield shifts at δ 124.66–128.48 ppm for the trivalent phosphoramidite framework.

The *in vitro* screening revealed that the synthesized compounds exhibit high, dose-dependent antibacterial and antifungal profiles, with Gram-negative strains (*P. aeruginosa* and *K. pneumoniae*) showing enhanced susceptibility. Monophosphorylated compounds (4a, 3b, and 4b) possess superior potency over their bulky bis-phosphorylated counterparts, demonstrating that a lower molecular weight facilitates cell wall penetration. The trivalent phosphorus derivative 4b emerged as the most effective broad-spectrum agent: Against *P. aeruginosa*, compound 4b exhibited a prominent zone of inhibition of 27–33 mm (at 100 $\mu\text{g/mL}$), outperforming the standard drug streptomycin (32 mm), with exceptionally low MIC and MBC values of 6.25 and 12.5 $\mu\text{g/mL}$, respectively; Against *T. viride*, compound 4b showed a high zone of inhibition of 34–39 mm (at 100 $\mu\text{g/mL}$) and outclassed the reference drug clotrimazole, demonstrating strict fungicidal parameters with MIC and MFC values of 12.5 and 25 $\mu\text{g/mL}$.

These rigorous experimental and quantitative findings provide a solid basis for further structural optimization and investigation of these novel P–N coupled platforms as potential antimicrobial drug candidates.

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