LC-ESI-MS analysis of 1,2,4-triazole derivatives with various alkyl and aromatic substituents

Yu. V. Karpenko[1,A-F], M. O. Panasenko[1,B,C], H. I. Kharytonenko[2,B]

[1]Zaporizhzhia State Medical and Pharmaceutical University, Ukraine, [2]Kyiv National University of Technologies and Design, Ukraine

A – research concept and design; B – collection and/or assembly of data; C – data analysis and interpretation; D – writing the article;
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Derivatives of 1,2,4-triazole and related heterocycles continue to attract significant attention due to their diverse biological activities and potential pharmaceutical applications.

The aim of this work is to resynthesize and perform mass spectrometric characterization of a series of 16 organic compounds – derivatives of 1,2,4-triazole and 1,3,4-oxadiazole – containing a 5-mercapto-1,2,4-triazole fragment and various substituents at the N^2 atom. The objective is to investigate their fragmentation patterns and establish analytical markers for these bioactive heterocycles.

Materials and methods. The target compounds were resynthesized according to established procedures, with reagents purchased from Sigma-Aldrich. The preparation involved refluxing 2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carbohydrazide with appropriate isothiocyanates or carbon disulfide, followed by purification. S-alkyl derivatives were prepared via nucleophilic substitution of haloalkanes under basic conditions. Mass spectra were recorded using liquid chromatography coupled with electrospray ionization mass spectrometry (LC-ESI-MS) in both positive and negative ion modes. Chromatographic separation was performed on a Zorbax SB-C18 column under gradient elution.

Results. Protonated molecular ions $[M+H]^+$ were observed for all compounds, with characteristic isotopic peaks confirming the presence of sulfur. Fragmentation primarily involved cleavage at sulfur and N^2 substituents, yielding prominent ions corresponding to loss of alkyl radicals as alkenes. *N*-phenyl derivatives showed additional fragmentation pathways, including cleavage of the phenyl group and deeper degradation of the triazole ring. A consistent fragment corresponding to the protonated 1,2,4-triazole core was identified across most spectra, serving as a useful structural marker. Substitution pattern and alkyl chain length significantly influenced fragmentation intensity and pathways.

Conclusions. LC-ESI-MS analysis revealed reproducible fragmentation trends for these heterocyclic derivatives, providing valuable insights for their structural identification and analytical profiling. These findings facilitate the development and quality control of new bioactive 1,2,4-triazole-based compounds. Further research is recommended to expand chemical diversity and conduct biological evaluations, including antimicrobial and antidiabetic activity assessments.

Keywords: 1,2,4-triazole, LC-ESI-MS analysis, fragmentation, molecular ion, liquid chromatography.

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LC-ESI-MS аналіз похідних 1,2,4-тріазолу з різноманітними алкільними та ароматичними замісниками

Ю. В. Карпенко, М. О. Панасенко, Г. І. Харитоненко

Похідні 1,2,4-тріазолу та споріднених гетероциклів мають важливе значення через широкий спектр біологічної активності, що їм властива, та перспективи фармацевтичного застосування.

Мета роботи – дослідження ресинтезу та мас-спектрометричної характеристики 16 органічних сполук – похідних 1,2,4-тріазолу та 1,3,4-оксадіазолу, що містять 5-меркапто-1,2,4-тріазольний фрагмент і різні замісники при атомі N^2; вивчення їхніх характерних шляхів фрагментації та визначення аналітичних маркерів для цих біоактивних гетероциклів.

Матеріали і методи. Ресинтез сполук здійснено за відомими методиками з використанням реагентів Sigma-Aldrich. Продукти реакції одержано шляхом кип'ятіння 2,6-діоксо-1,2,3,6-тетрагідропіримідин-4-карбогідразиду з відповідними ізотіоціанатами або карбондисульфідом із наступним очищенням. S-алкілпохідні отримували реакцією заміщення галогеналканів у лужному середовищі. Мас-спектри записано методом рідинної хроматографії з електроспрей-іонізацією (LC-ESI-MS) у позитивному та негативному режимах. Хроматографічне розділення здійснено на колонці Zorbax SB-C18 за градієнтних умов.

Результати. Для всіх сполук визначено протоновані молекулярні йони $[M+H]^+$ з характерними ізотопними піками, що підтверджують наявність сірки. Основні шляхи фрагментації – розриви у замісниках при сірці та N^2 з утворенням інтенсивних іонів, що відповідають втраті алкільних радикалів – алкенів. У похідних з N-фенілом додатково виявлено розриви фенільної групи та глибшу деградацію

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тріазольного кільця. В усіх спектрах виявлено стабільний фрагмент, що відповідає протонованому ядру 1,2,4-тріазолу, який може бути структурним маркером. Тип замісника та довжина алкільного ланцюга суттєво впливали на інтенсивність і характер фрагментації.

Висновки. У результаті LC-ESI-MS досліджень підтверджено сталість шляхів фрагментації похідних гетероциклів, що сприяє їхній структурній ідентифікації та аналітичному контролю. Результати є перспективними для розроблення нових біоактивних сполук на основі 1,2,4-тріазолу. Доцільним є розширення хімічного різноманіття та біологічне тестування сполук, включно з оцінюванням антимікробної та антидіабетичної активності.

Ключові слова: 1,2,4-тріазол, LC-ESI-MS аналіз, фрагментація, молекулярний іон, рідинна хроматографія.

Актуальні питання фармацевтичної і медичної науки та практики. 2025. Т. 18, № 3(49). С. 237-243

Derivatives of 1,2,4-triazole have attracted significant attention in the fields of medicinal, pharmaceutical, and materials chemistry due to their broad spectrum of biological activities and diverse functional applications. It is well established that over fifteen pharmaceutical drugs and numerous candidates for new therapeutic agents contain the 1,2,4-triazole moiety within their molecular structure, which contributes to their efficacy and selectivity. These compounds exhibit antifungal [1,2], antiviral [3], antibacterial [4,5], and anti-inflammatory properties [6,7], and are also widely employed as corrosion inhibitors [8], components of ionic liquids [9], and ligands for metal complexation [10]. This wide-ranging utility underscores the ongoing need to develop new triazole derivatives with improved physicochemical and biological profiles.

In modern organic chemistry, the synthesis of new complex compounds cannot be accomplished without thorough and reliable structural characterization. This is especially true for heterocyclic compounds such as 1,2,4-triazoles, where precise identification is critical for the subsequent evaluation of their properties and applications. In this regard, mass spectrometry, particularly electrospray ionization mass spectrometry (ESI-MS) combined with liquid chromatography (LC), has emerged as one of the most powerful analytical tools. This technique not only allows to determine molecular mass and purity but also provides valuable information on fragmentation pathways, which is key to confirming molecular structure and the nature of functional substituents.

The relevance of LC-ESI-MS in the study of 1,2,4-triazole derivatives [11] stems from its high sensitivity, selectivity, and capability to analyze complex mixtures even at low concentrations [12]. This method enables rapid and accurate identification of synthetic products, detection of side reactions, and differentiation of conformational isomers, which is essential in pharmaceutical chemistry and drug development. Furthermore, mass spectrometric analysis facilitates the elucidation of characteristic fragmentation patterns related to the triazole core structure and the diversity of substituents, enhancing the understanding of the chemical behavior of these compounds.

Thus, the application of mass spectrometry is an indispensable component of contemporary research in the organic synthesis of 1,2,4-triazole derivatives, supporting effective identification, structural characterization, and the advancement of new bioactive compounds.

Aim

The aim of this work is to synthesize and perform mass spectrometric characterization of a series of 31 organic compounds – derivatives of 1,2,4-triazole and 1,3,4-oxadiazole – containing a 5-mercapto-1,2,4-triazole fragment and various substituents at the N^2 atom. The objective is to investigate their fragmentation patterns and establish analytical markers for these bioactive heterocycles.

Materials and methods

Compounds **1.1–1.16** were resynthesized following known procedures described in previous studies [13], with physicochemical properties consistent with literature data. All reagents were purchased from Sigma-Aldrich (Merck).

Objects of study. Thirty-one organic compounds – derivatives of 1,2,4-triazole and 1,3,4-oxadiazole – were analyzed; their general structure is shown in *Fig. 1*.

All compounds contain a 5-mercapto-1,2,4-triazole fragment (a substituent at the 5th position of the triazole ring – the –S–R group) and various substituents at the N^2 atom of the triazole ring. The following variations were made: the alkyl substituent R_2 on sulfur (–S–R) was varied from methyl to decyl; the substituent N^2 was varied from methyl / ethyl to phenyl; and the heteroatom at the 2nd position of the ring was modified (in compound 1.16, the N^2 atom was replaced by oxygen, forming a 1,3,4-oxadiazole fragment).

Mass spectra were acquired using liquid chromatography coupled with electrospray ionization (LC-ESI-MS) on an Agilent 1200 LC/MSD SL system equipped with a single quadrupole mass detector. Analyses were performed in both positive and negative ionization modes. Chromatographic separation was carried out on a Zorbax SB-C18 column (30 × 4.6 mm, 1.8 μm particle size) using a mobile phase consisting of solvent A (water with 0.1 % formic acid) and solvent B (acetonitrile with 0.1 % formic acid) under gradient elution conditions. The ESI source was operated at a fragmentation voltage of 150 V. For each compound, total ion chromatograms (TIC) and mass spectra of the main chromatographic peaks were recorded. In the positive ion mode, protonated molecular ions $[M+H]^+$ were detected, whereas in the negative ion mode, deprotonated molecules $[M–H]^-$ (typical for acids and their salts) as well as characteristic adducts and fragment ions were observed.

Results

To enable standardized identification, we compiled a reference set of LC-MS parameters for 16 compounds *(Table 1)*, including the monoisotopic mass (Da), theoretical m/z values for $[M+H]^+$ and $[M–H]^-$, and the retention time under the selected chromatographic method. For each compound, we

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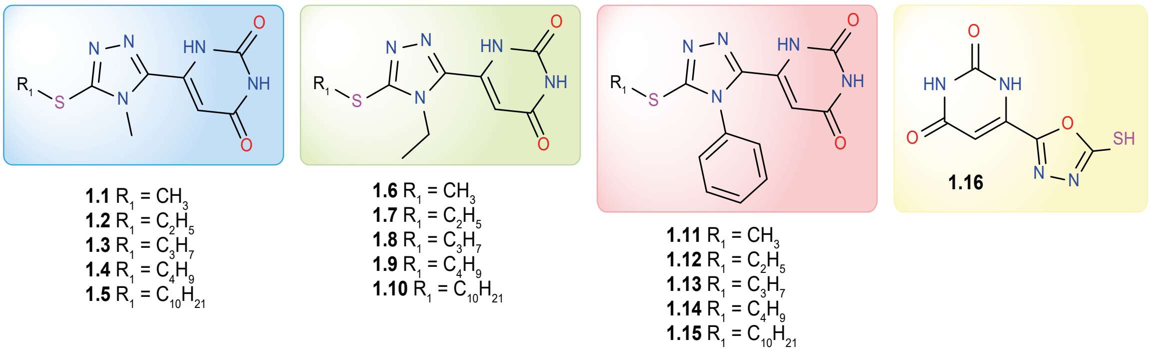

Fig. 1. Chemical structures of the main compounds studied in this work.

Table 1. LC-MS compound parameters of 1,2,4-triazole / 1,3,4-oxadiazole derivatives

No.	Monoisotopic mass, m/z	RT, min	$[M+H]^+$, m/z	$[M\text{-}H2O+H]^+$, m/z	Top 3 fragments
1.1	239.2572	0.516	240.0	–	149.0, 197.0, 464.2 m/z
1.2	253.2843	0.675	254.2	–	149.0, 197.2, 212.2 m/z
1.3	267.3114	0.772	268.2	–	152.0, 196.2, 269.2 m/z
1.4	281.3385	0.865	–	263.2	197.0, 226.2, 290.2 m/z
1.5	365.5010	1.049	366.2	–	226.2, 290.2, 366.2 m/z
1.6	253.2843	0.585	–	–	173.2, 201.2, 237.2 m/z
1.7	267.3114	0.623	268.2	–	201.2, 202.2, 237.2 m/z
1.8	281.3385	0.801	–	–	173.2, 212.0, 240.2 m/z
1.9	295.3656	1.715	–	–	173.2, 174.2, 312.2 m/z
1.10	379.5281	1.648	–	361.2	194.0, 269.2, 312.2 m/z
1.11	301.3289	0.858	–	285.2	194.0, 192.2, 237.2
1.12	315.3560	0.981	–	297.2	102.2, 269.2, 298.2
1.13	329.3831	0.960	–	311.2	269.2, 313.2
1.14	343.4102	1.018	–	325.2	269.2, 327.2
1.15	427.5727	1.242	–	409.2	268.6, 340.6, 395.6
1.16	212.1878	1.018	–	–	102.2, 130.2, 131.4

report the top MS/MS fragments with annotations of plausible neutral losses, allowing the observed fragmentation to be linked to key structural motifs. These characteristics can be used directly to build an internal library, support retention indexing, and enable routine confirmation of target analytes in complex biological and technological matrices.

The molecular ion peak $[M+H]^+$ was observed in positive ESI mode for most of the studied compounds. For example, for compound **1.5** ($N^2 = CH_3$, $R_2 = C_{10}H_{21}$), the protonated molecular ion was detected at m/z ≈366.2. The presence of a sulfur atom in the structure was confirmed by a characteristic isotopic peak at m/z ≈368.2 $[M+H+2]^+$ with an intensity of approximately 4 % relative to the main peak, attributable to the ^{34}S isotope *(Fig. 2)*.

Similarly, for the series of compounds with varying alkyl chain lengths R_1 (**1.7:** $R_1 = C_2H_5$; **1.8:** $R_1 = C_3H_7$; **1.9:** $R_1 = C_4H_9$; **1.10:** $R_1 = C_{10}H_{21}$, all with $N^2 = C_2H_5$), [M+H]+ peaks were observed in the m/z range of approximately 288–410, increasing with molecular weight. For compounds bearing an aromatic substituent $R_1 = C_6H_5$ (series **1.11–1.15**, $R = C_1–C_{10}H_{2n+1}$), the $[M+H]^+$ values ranged from about m/z 283 (for $R_1 = CH_3$) up to ~410 (for $R_1 = C_{10}H_{21}$).

The mass spectra of the compounds revealed consistent fragmentation processes associated with the cleavage of substituents from the 1,2,4-triazole core [14]. The most intense fragments for 5-alkylthio-1,2,4-triazoles result from the heterolytic cleavage of the C–S bond with loss of the alkyl radical R as an alkene. In this process, the charge remains on the heterocycle, while a proton attaches to the sulfur atom (forming a thiol group) – effectively, a neutral alkene molecule (C_nH_{2n}) is lost from the molecular ion.

For example, in compound **1.9** one of the main peaks in the positive spectrum appears at m/z ≈269.2, corresponding to

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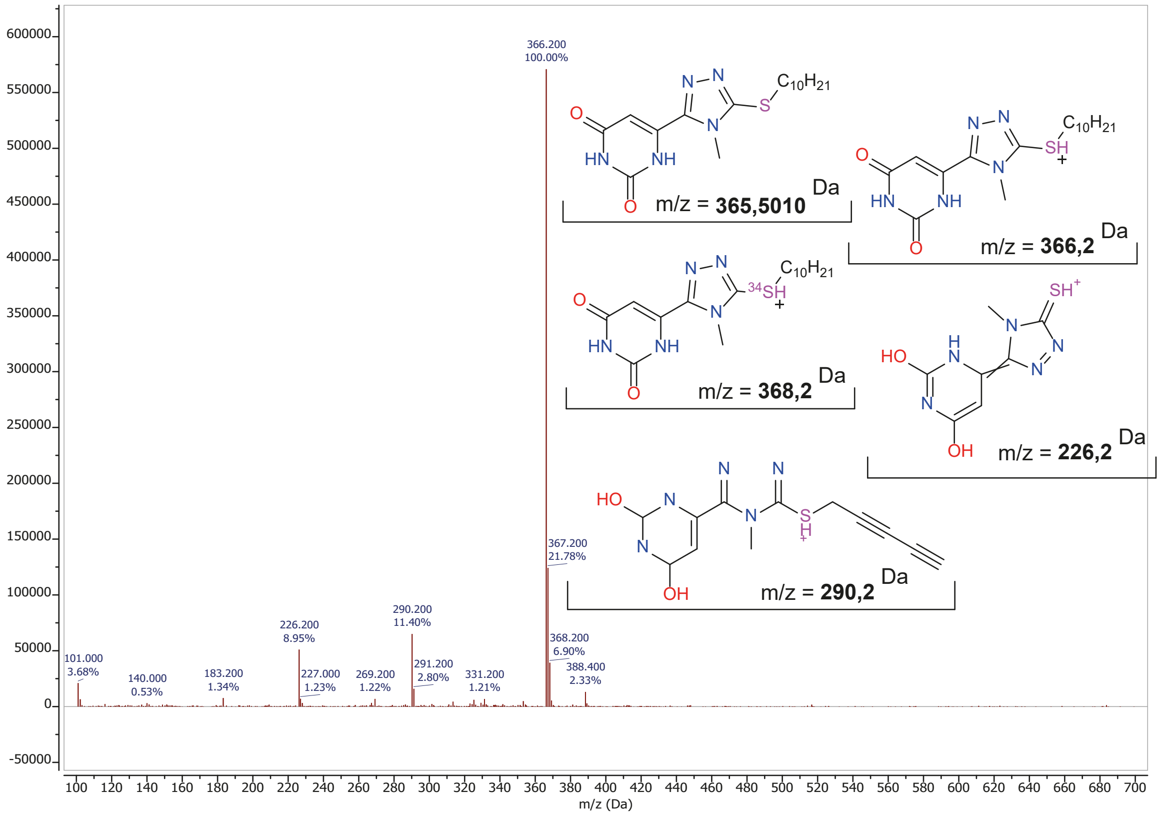

Fig. 2. Mass spectrum of 6-(5-(decylthio)-4-methyl-4*H*-1,2,4-triazol-3-yl)pyrimidine-2,4(1*H*,3*H*)-dione (**1.5**).

the ion $[M+H–C_4H_9]^+$ – the protonated molecule (m/z 343.2) has lost butyl (57 Da). Similar processes were observed throughout the series: the fragment $[M+H–R–H]^+$ (loss of alkane C_nH_{2n+2} or alkene C_nH_{2n}) appears for every value of n. For instance, in compound **1.8** ($R_1 = C_3H_7$), the fragment resulting from propene loss (42 Da) corresponds to an ion at m/z ~240 (M+H 282 → 240), while in **1.7** ($R_2 = C_2H_5$), the fragment $[M+H–C_2H_4]^+$ is also observed near m/z ~240. Due to the close masses of ethene and propene, these values partially overlap. In all cases, cleavage of the alkyl group is accompanied by the attachment of a hydrogen atom to sulfur, i. e., restoration of the thiol group at the 5th position of the triazole.

For compounds bearing a substituent at N^2, cleavage of this substituent is also characteristic. In particular, for *N*-ethyl derivatives (**1.6–1.10**), a fragment corresponding to the loss of ethylene (28 Da) forming the ion $[M+H–C_2H_4]^+$ was observed. Often, the cleavage of substituents at N^2 and sulfur occurs sequentially or even simultaneously.

As a result, many spectra exhibit an ion corresponding to the "naked" triazole core – that is, the protonated molecule lacking substituents at both N^2 and sulfur. For 5-alkylthio-*N*-ethyl-1,2,4-triazoles, this «core» corresponds to a protonated 5-mercapto-1,2,4-triazolyl-aminoacyl fragment (a structure with a restored thiol group and a reduced secondary amine at N^2).

Its mass is approximately constant (~240.2 Da for the indicated skeletal fragment), regardless of N^2 and R_1. For compound **1.7** (with a shorter R chain), a similar ion is observed at m/z ~240.2, while for longer chains (**1.1, 1.6**), the intensity of the ~240.2 ion is somewhat lower, as the multistep loss of substituents competes with other fragmentation pathways.

In the presence of an aryl substituent (*N*-phenyl, series **1.11-1.15**), additional fragmentation pathways are observed. Besides the cleavage of the alkyl group R_1 from sulfur (yielding ions $[M+H–CnH2n]^+$ similar to those in *N*-alkyl analogs), cleavage of the phenyl radical from the N^2 atom also occurs. This results in a fragment ion corresponding to the loss of C_6H_5 (77 Da) from the protonated molecule.

Overall, phenyl-containing triazoles are characterized by the presence of an intense fragment at m/z ~269–270 (corresponding to the loss of an alkene from $[M+H]^+$, similar to *N*-alkyl series) and a fragment at ~192–194. The latter is formed through deeper degradation: sequential loss of the alkyl radical and the phenyl group, as well as partial breakdown of the triazole ring itself (possibly involving the loss of HNCO or CO fragments).

For example, in the spectrum of compound **1.11** *(Fig. 3)*, the fragment at m/z 192.2 is one of the main peaks – likely a product of cleavage of both the C–S bond and the $N^2–C_6H_5$ bond, followed by the loss of CO from the uracil (dioxo-dihydropyrimidine) ring. Thus, the phenyl substituent promotes deeper fragmentation of the triazole core compared to alkyl analogs.

For the 1,3,4-oxadiazole compound **1.16**, in which one of the nitrogen atoms in the triazole ring is replaced by oxygen,

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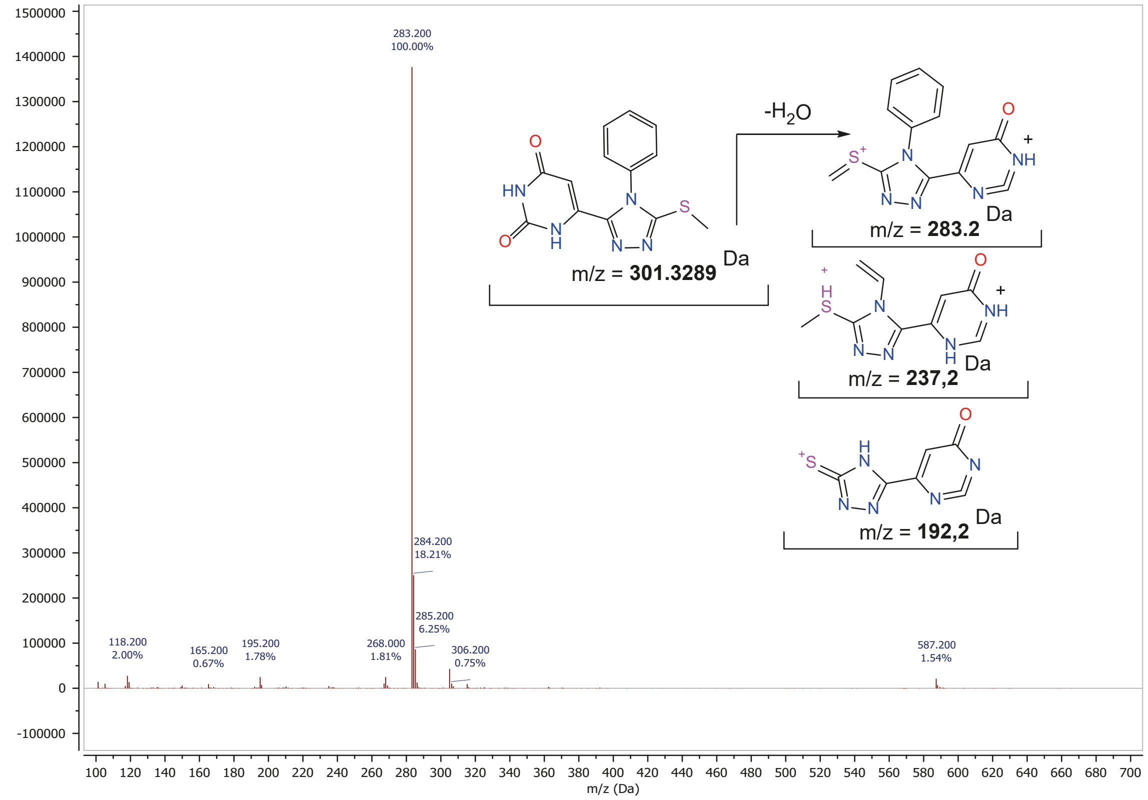

Fig. 3. Mass spectrum of 6-(5-(methylthio)-4-phenyl-4*H*-1,2,4-triazol-3-yl)pyrimidine-2,4(1*H*,3*H*)-dione (**1.11**).

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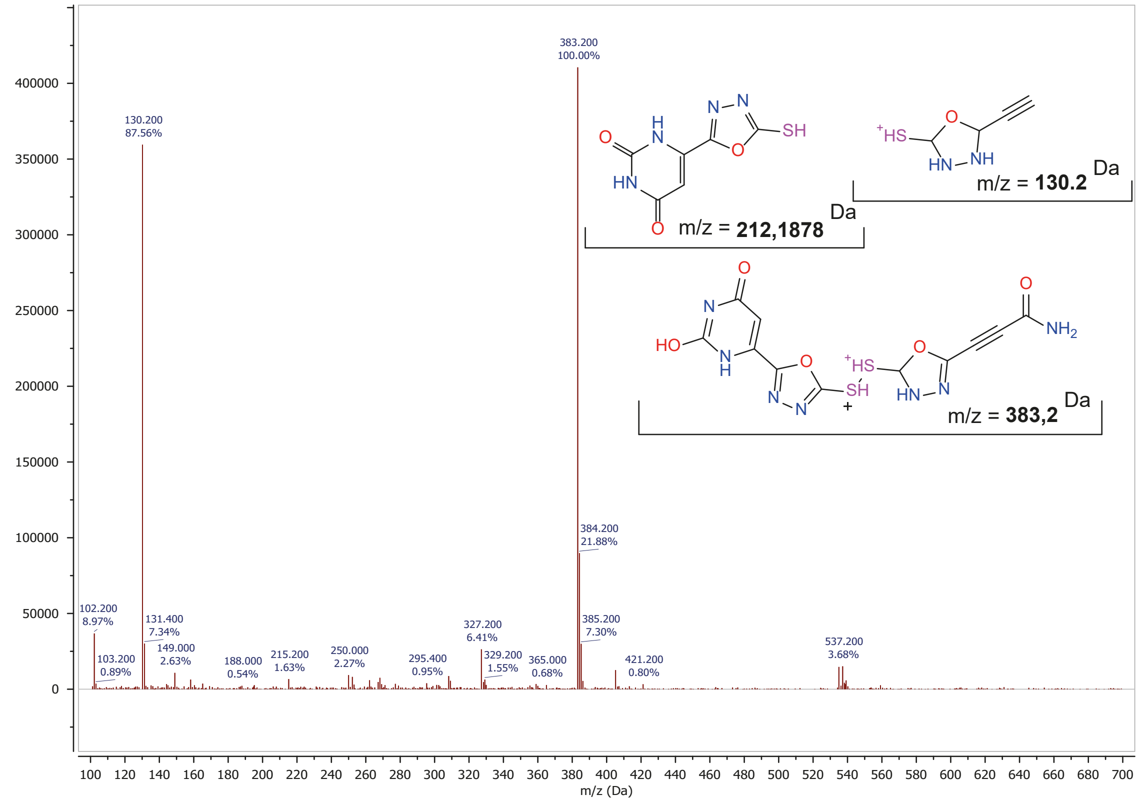

Fig. 4. Mass spectrum of 6-(5-mercapto-1,3,4-oxadiazol-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione (**1.16**).

similar fragmentation pathways were observed – cleavage of the C–S bond and loss of substituents – however, the cationic fragments were less stable, and most ions were detected in negative mode *(Fig. 4)*. In particular, 6-(5-mercapto-1,3,4-oxadiazol-2-yl)pyrimidine-2,4(1*H*,3*H*)-dione in positive mode showed a weak [M+H+2]$^+$ ion at m/z ≈215.2 and a more intense ion [2M+H–42]$^+$, corresponding to the dimer formation via a diprotonated sulfonium bridge and opening of one pyrimidine ring. Thus, the introduction of an oxygen atom into the ring (N→O substitution) reduces cation stability and complicates fragmentation along the typical pathways seen in triazoles [15].

Discussion

Analysis of the mass spectra of the studied 1,2,4-triazole derivatives revealed that their fragmentation in the ESI source follows certain established patterns sensitive to the substituent structure [16]. The primary fragmentation pathways for 5-alkylthio-1,2,4-triazoles involve the cleavage of the alkyl substituent at sulfur and, to a lesser extent, the loss of the substituent at N^2.

The loss of the alkyl group (especially a long chain) is an energetically favorable process; therefore, for compounds with large R_2 substituents, the intensity of the [M+H]$^+$ peak decreases, while the fragment [M+H–R]$^+$ can become the base peak. For example, in the compound with the longest chain (**1.10**, $R_2 = C_{10}H_{21}$), the fragment corresponding to the loss of decene ([M+H–$C_{10}H_{20}$]$^+$) is expected to have an intensity comparable to or greater than that of the molecular ion, consistent with the general trend that longer radicals detach more readily, forming more stable carbocations or neutral alkenes. Accordingly, the molecular ion peak [M+H]$^+$ may decrease in intensity as the chain length n in R_2 increases.

The substituent at the nitrogen atom (N^2) also influences the fragmentation pattern. *N*-alkyl derivatives typically exhibit similar spectral features, differing mainly in the mass of the fragments. For example, *N*-methyl (**1.1–1.5**) and *N*-ethyl triazoles (**1.6–1.10**) produce a related series of ions differing by approximately 14 Da between corresponding peaks, which corresponds to the mass difference between –CH_3 and –C_2H_5 groups.

In contrast, the presence of an aromatic substituent (phenyl) at N^2 significantly alters the fragmentation pattern: unique fragmentation pathways emerge, involving the cleavage of the phenyl radical and subsequent charge rearrangement. The phenyl substituent evidently stabilizes the charge in the intermediate ion, facilitating additional cleavages within the triazole ring (e. g., loss of CO, ring breakdown).

Therefore, fragmentation of *N*-phenyl derivatives is deeper: besides ions arising from substituent loss, fragmentation products of the heterocyclic core itself are observed (e. g., an ion at m/z ~192 in the **1.11–1.15** series).

This fact can be exploited analytically to differentiate *N*-phenyl from *N*-alkyl 1,2,4-triazoles: the spectra of the former show characteristic fragments from phenyl group loss and ring cleavage, which are absent in the latter.

An interesting fact is that the mass spectra of all studied compounds share common features – in particular, the presence of peaks attributable to the preserved triazole core. Despite the variety of substituents, a fragment with approximately the same mass (around 230 Da in positive mode for the cation and 210–230 Da in negative mode for the anion) appears in the spectra of many compounds. This indicates that the 1,2,4-triazole core together with the attached carbonyl fragment (formed by the cyclic amide residue) is a relatively stable ion formed after the loss of peripheral parts of the molecule. This fragment essentially corresponds to the protonated (or deprotonated) 5-mercapto-3-alkyl-1,2,4-triazole (in positive mode – with the cationic center on the endocyclic nitrogen). It can serve as a marker ion for the identification of certain types of 1,2,4-triazole derivatives.

The general fragmentation pathways can be summarized as follows:

– [M–H]$^-$ → [M–H–H_2O]$^-$ – dehydration of the compound at the uracil core, the most common route leading to major peaks;

– [M+H]$^+$ → [M+H–R_alkene]$^+$ → [M+H–R_alkene – N_2_alkene]$^+$ – sequential loss of the alkyl substituent at sulfur as an alkene, followed by loss of the alkyl substituent at N^2;

– [M+H]$^+$ → [M+H–C_6H_5]$^+$ – cleavage of the phenyl substituent (for aromatic derivatives);

A comparative analysis of the mass spectra of a series of 5-alkylthio-1,2,4-triazoles with *N*-alkyl and *N*-phenyl substituents showed that increasing the length of the alkyl chain R facilitates its cleavage (reflected by an increase in the relative intensity of the fragment [M+H–R]$^+$), while the introduction of an aromatic substituent at N^2 promotes the formation of products resulting from deeper heterocycle degradation. The obtained results are useful for the identification of new 1,2,4-triazole derivatives based on their mass spectrometric "fingerprints" and for understanding the relationship between molecular structure and ion fragmentation pathways.

Conclusions

1. The conducted LC-ESI-MS analysis of 1,2,4-triazole derivatives with various substituents revealed characteristic fragmentation patterns of these compounds.

2. It was established that protonated molecules [M+H]$^+$ are observed for all compounds, and the presence of a sulfur atom in the structure is confirmed by the isotopic peak [M+2] with a relative intensity of approximately 4 %. The main fragmentation pathways of the molecular ions involve cleavage of substituents at the sulfur and N^2 atoms. The cleavage of the C–S bond with loss of an alkyl radical as an alkene leads to the formation of intense fragments [M+H–R]$^+$, which can dominate the spectrum for long-chain substituents.

3. The cleavage of the substituent at N^2 (alkyl or phenyl) produces corresponding ions [M+H–R_1]$^+$ with somewhat lower intensity; however, in the case of phenyl derivatives, this process promotes deeper fragmentation of the triazole ring. It was found that the final fragment corresponding to the 1,2,4-triazole core (after removal of peripheral groups) has a consistent mass and is observed in the spectra of most compounds, which can serve as a structural marker.

Prospects for further research. Further research on these 6-(5-mercapto-1,2,4-triazol-3-yl)pyrimidine-2,4-dione derivatives should focus on expanding their chemical diversity through advanced functionalization techniques and optimizing reaction conditions to improve selectivity and yields. Comprehensive biological evaluations, including *in vitro* and *in vivo* studies, are necessary to fully assess their antimicrobial, anti-inflammatory, and antidiabetic potentials.

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Information about authors:
Karpenko Yu. V., PhD, Associate Professor of the Department of Toxicological and Inorganic Chemistry, Zaporizhzhia State Medical and Pharmaceutical University, Ukraine.
ORCID ID: 0000-0002-4390-9949
Panasenko M. O., MD, Assistant of the Department of Internal Medicine 3, Zaporizhzhia State Medical and Pharmaceutical University, Ukraine.
ORCID ID: 0000-0002-2619-3846
Kharytonenko H. I., PhD, Associate Professor of the Department of Industrial Pharmacy, Kyiv National University of Technologies and Design, Ukraine.
ORCID ID: 0000-0001-9642-5334

Відомості про авторів:
Карпенко Ю. В., канд. хім. наук, доцент каф. токсикологічної та неорганічної хімії, Запорізький державний медико-фармацевтичний університет, Україна.
Панасенко М. О., асистент каф. внутрішніх хвороб 3, Запорізький державний медико-фармацевтичний університет, Україна.
Харитоненко Г. І., канд. біол. наук, доцент каф. промислової фармації, Київський національний університет технологій та дизайну, м. Київ, Україна.

Yurii Karpenko (Юрій Карпенко)
karpenko.y.v@gmail.com

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