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1,3-Dipolar Cycloaddition Reactions in the Series of *N*-Alkynyl-Substituted Uracils

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Abstract—Reactions of 1-(ω-bromoalkyl)-3,6-dimethyluracils and 1,3-bis(ω-bromoalkyl)-6-methyluracils with sodium azide gave the corresponding mono- and bis-azides. 1,3-Dipolar cycloaddition of the latter with prop-2-yn-1-ol, hex-1-yne, and dec-1-yne in the presence of copper(I) ions afforded acyclic and macrocyclic uracil derivatives containing 1,4-disubstituted 1,2,3-triazole fragments, which were subjected to quaternization with propyl iodide and methyl *p*-toluenesulfonate at the 1,2,3-triazole nitrogen atom.

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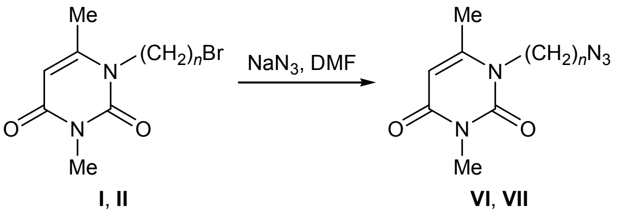
1,3-Dipolar cycloaddition of organic azides to terminal alkynes leads to 1,4- or 1,5-disubstituted 1,2,3-triazoles which are widely used in medicinal chemistry, molecular biology, and materials science [1–3]. These reactions occur both in the absence of a catalyst [4, 5] and in the presence of copper(I) salts [6, 7]. Noncatalytic cycloaddition of azides to alkynes is characterized by low rate and is not selective; as a result, mixtures of isomeric 1,4- and 1,5-disubstituted 1,2,3-triazoles are obtained. The use of Cu(I) as catalyst under both homogeneous [6] and heterogeneous conditions [7] considerably increases the reaction rate, and the corresponding 1,4-disubstituted 1,2,3-triazoles are formed almost exclusively.

Due to aromatic character, 1,2,3-triazole ring is highly resistant to oxidation, reduction, and hydrolysis; it possesses a large dipole moment and can act as hydrogen bond acceptor [8]; in addition, 1,2,3-triazole derivatives exhibit intrinsic diverse biological activity [9–11]. The above properties determine the use of 1,2,3-triazole ring as bridging fragment in the design of new biologically active compounds, bioconjugates, and new materials, e.g., polymers, dendrimers, and various nanostructures [1, 12]. For this purpose, 1,2,3-triazole fragments, in particular 1,4-disubstituted, are generated *in situ* by copper(I)-catalyzed 1,3-dipolar cycloaddition of organic azides to terminal alkynes. In recent years, 1,4-disubstituted 1,2,3-triazole bridges were incorporated into new nucleoside and oligonucleoside analogs [13].

The present communication reports on the synthesis of *N*-alkyl-substituted uracil derivatives having 1,2,3-triazole fragments in the alkyl chains. Nucleic acid bases, in particular uracils, connected to 1,2,3-triazole ring through a hydrocarbon tether attract interest from the viewpoint of biological activity. We anticipated that uracil derivatives containing a 1,2,3-triazole fragment would provide stronger binding to a biological target, which should enhance their physiological effect or even change the kind of biological activity [14–16]. It was also interesting to elucidate the possibility for regioselective synthesis of 1,2,3-triazole derivatives having *N*-alkyl-substituted uracil fragments as substituents with a view to obtain acyclic and macrocyclic structures with three-dimensional architecture.

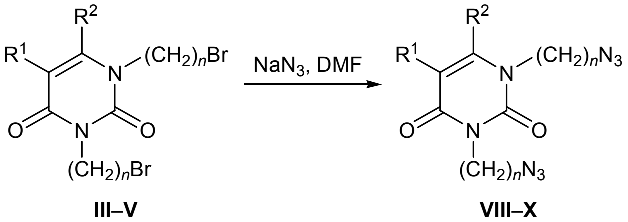
1,2,3-Triazole fragments were introduced into uracil derivatives via 1,3-dipolar cycloaddition of organic azides to terminal acetylenes. The reactions were carried out in aqueous ethanol in the presence of copper(I) ions which were generated *in situ* by reduction of copper(II) sulfate with sodium ascorbate [2, 3, 6]. This procedure ensured selective formation of 1,4-disubstituted 1,2,3-triazoles. As initial uracil derivatives we used 1-(ω-bromoalkyl)- and 1,3-bis(ω-bromoalkyl)-substituted 3,6-dimethyluracil, 6-methyluracil, and 5-bromouracil with different lengths of the alkyl chains (compounds **I**–**V**) [17–19]. By reactions of **I**–**V** with sodium azide in DMF we obtained the corresponding mono- (**VI**, **VII**; Scheme 1) and bis-azides (**VIII**–**X**, Scheme 2).

Scheme 1.



I, VI, $n = 6$; II, VII, $n = 7$.

Scheme 2.



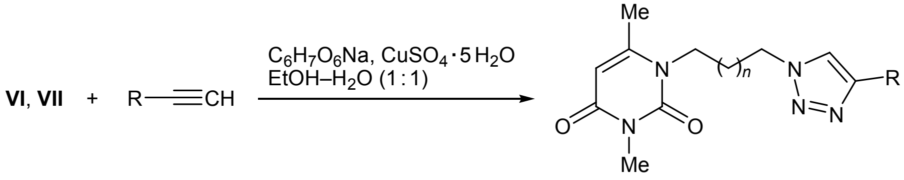
III, VIII, $n = 4$, $R^1 = H$, $R^2 = Me$; IV, IX, $n = 5$, $R^1 = H$, $R^2 = Me$; V, X, $n = 5$, $R^1 = Br$, $R^2 = H$.

Compounds **VI**–**X** were then brought into 1,3-dipolar cycloaddition with terminal alkynes, namely prop-2-yn-1-ol, hex-1-yne, and dec-1-yne. The reactions were carried out in aqueous ethanol in the presence of 1 mol % of $CuSO_4 \cdot 5H_2O$ and 10 mol % of sodium ascorbate ($C_6H_7O_6Na$) as reducing agent for the conversion of Cu(II) to Cu(I). Compounds **XI** and **XII** having one 1,2,3-triazole ring in the alkyl chain attached to N^1 of uracil (Scheme 3) and their analogs **XIII** and **XIV** having two 1,2,3-triazole fragments (Scheme 4) were thus synthesized in 55–100% yield. 1,3-Dipolar cycloaddition to propargyl alcohol with formation of **XI** and **XIII** was characterized by the highest (nearly quantitative) yield. The lowest yield was observed for compound **XIV**, presumably due to poor solubility of initial dec-1-yne in aqueous alcohol.

We also used 1,3-dipolar cycloaddition of azides to terminal alkynes to obtain macrocyclic compounds. The reaction of dibromide **VIII** with diyne **XV** afforded heterocyclophane **XVI** in a poor yield. In addition, acyclic product **XVII** was isolated (Scheme 5). The reaction was carried out in strongly dilute solution, otherwise an insoluble material was obtained, which was likely to be a mixture of oligomers.

The presence of pyridine-type nitrogen atoms in the 1,2,3-triazole ring makes it possible to obtain water-soluble derivatives via quaternization. According to published data, 1-alkyl-1,2,3-triazoles readily undergo quaternization at N^3 by the action of alkyl halides [20, 21]. However, we succeeded in obtaining the corresponding 1,2,3-triazolium salts only by prolonged heating of some 1,4-disubstituted 1,2,3-triazole derivatives with alkylating agent. Compound **XVIII** was synthesized by treatment of compound **XII** with propyl iodide in boiling acetonitrile for a long time (Scheme 6), and heating of **XIV** in methyl *p*-toluenesulfonate for 10 h at 100°C gave the corresponding *N*-methyl derivative **XIX** (Scheme 7).

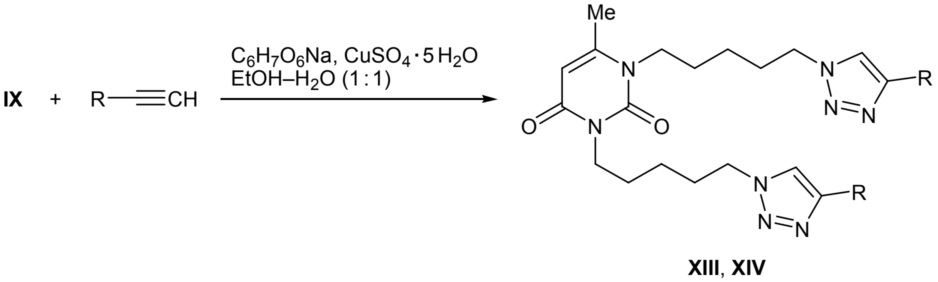
Scheme 3.



XI, XII

XI, $n = 4$, $R = HOCH_2$; XII, $n = 5$, $R = Bu$.

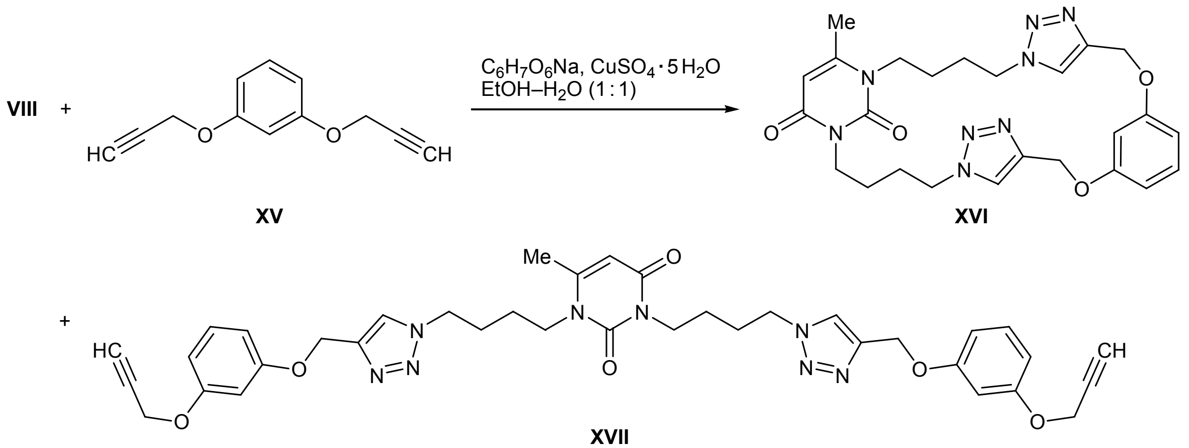
Scheme 4.



XIII, XIV

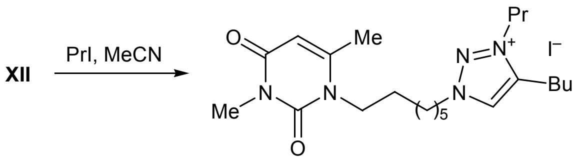
XIII, $R = HOCH_2$; XIV, $R = C_8H_{17}$.

Scheme 5.



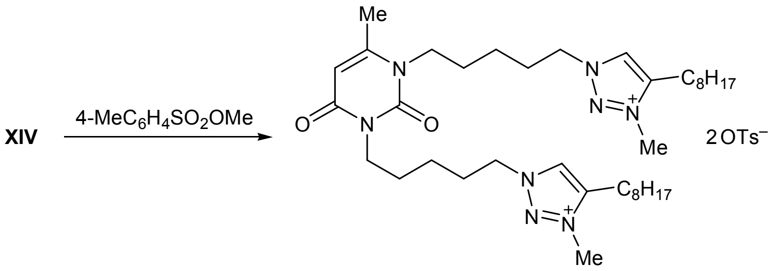
XV XVI XVII

Scheme 6.



XVIII

Scheme 7.



XIX

To conclude, by reaction of *N*-mono- and *N*,*N'*-bis-(ω-azidoalkyl)-6-methyluracils with terminal alkynes we have synthesized acyclic and macrocyclic uracil derivatives containing 1,4-disubstituted 1,2,3-triazole fragments in the alkyl chains. 1,2,3-Triazole fragments in the obtained compounds were subjected to quaternization at N^3 with propyl iodide and methyl *p*-toluenesulfonate.

EXPERIMENTAL

The ^1H NMR spectra were recorded on a Bruker Avance-400 spectrometer with Fourier transform (400 MHz, $CDCl_3$, 30°C) using tetramethylsilane as internal reference. The mass spectra (MALDI-TOF) were recorded on a Bruker Ultraflex instrument using *p*-nitroaniline as matrix. The melting points were measured on a Boetius melting point apparatus and are uncorrected. Dimethylformamide was kept first over alkali and then over P_2O_5 and distilled twice over P_2O_5. Chloroform, ethyl acetate, acetonitrile, diethyl ether, and petroleum ether were distilled over P_2O_5; methanol was distilled over sodium. Silica gel (0.04–0.06 mm, Acros Organics) was used for column chromatography. Sodium azide, sodium ascorbate, and copper(II) sulfate pentahydrate were commercial reagents (from Acros Organics). 1-(6-Bromohexyl)-3,6-dimethyluracil (**I**), 1-(7-bromoheptyl)-3,6-dimethyluracil (**II**), 1,3-bis(4-bromobutyl)-6-methyluracil (**III**), 1,3-bis(5-bromopentyl)-6-methyl-uracil (**IV**), 5-bromo-1,3-bis(5-bromopentyl)uracil (**V**) [17–19], and 1,3-bis(prop-2-yn-1-yloxy)benzene (**XV**) [22] were synthesized according to known methods.

Azides VI and VII and bis-azides VIII–X (*general procedure***).** Sodium azide, 1.5 or 3 equiv, was added to 1 equiv of bromide **I** or **II** or dibromide **III**–**V**, respectively, and a catalytic amount of tetrabutylammonium hydrogen sulfate in DMF. The mixture was stirred for 10 h at 70°C, the progress of the reaction being monitored by TLC. The mixture was cooled, the solvent was distilled off, 100–200 ml of chloroform was added to the residue, the precipitate was filtered off, and the filtrate was evaporated to obtain azide **VI** or **VII** or bis-azide **VIII**–**X**.

1-(6-Azidohexyl)-3,6-dimethyluracil (VI) was synthesized from 2.5 g (8 mmol) of **I** and 0.78 g (12 mmol) of NaN_3 in 100 ml of DMF. Yield quantitative, mp 68°C. ^1H NMR spectrum, δ, ppm: 1.40–1.44 m (4H, 3′-H, 4′-H), 1.60–1.66 m (4H, 2′-H, 5′-H), 2.25 s (3H, 6-CH_3), 3.26–3.32 t (2H, 6′-H, $J = 6.8$ Hz), 3.32 s (3H, 3-CH_3), 3.80–3.83 t (2H, 1′-H, $J = 7.5$ Hz), 5.59 s (1H, 5-H). Found, %: C 54.26; H 7.25; N 26.33. $C_{12}H_{19}N_5O_2$. Calculated, %: C 54.32; H 7.22; N 26.40.

1-(7-Azidoheptyl)-3,6-dimethyluracil (VII) was synthesized from 2.0 g (6 mmol) of **II** and 0.59 g (9 mmol) of NaN_3 in 80 ml of DMF. Yield quantitative, mp 73°C. ^1H NMR spectrum, δ, ppm: 1.38 m (6H, 3′-H, 4′-H, 5′-H), 1.60–1.67 m (4H, 2′-H, 6′-H), 2.25 s (3H, 6-CH_3), 3.25–3.28 t (2H, 7′-H, $J = 7.0$ Hz), 3.32 s (3H, 3-CH_3), 3.78–3.82 t (2H, 1′-H, $J = 7.9$ Hz), 5.59 s (1H, 5-H). Found, %: C 55.82; H 7.54; N 24.96. $C_{13}H_{21}N_5O_2$. Calculated, %: C 55.90; H 7.58; N 25.07.

1,3-Bis(4-azidobutyl)-6-methyluracil (VIII) was synthesized from 2.0 g (5 mmol) of **III** and 1.00 g (15.4 mmol) of NaN_3 in 100 ml of DMF. Yield quantitative, oily substance. ^1H NMR spectrum, δ, ppm: 1.64–1.74 m (8H, 2′-H, 3′-H), 2.25 s (3H, 6-CH_3), 3.29–3.40 m (4H, 4′-H), 3.82–3.86 t (2H, 1-CH_2, $J = 7.2$ Hz), 3.93–3.97 t (2H, 3-CH_2, $J = 7.2$ Hz), 5.58 s (1H, 5-H). Found, %: C 48.72; H 6.24; N 34.96. $C_{13}H_{20}N_8O_2$. Calculated, %: C 48.74; H 6.29; N 34.98.

1,3-Bis(5-azidopentyl)-6-methyluracil (IX) was synthesized from 2.5 g (6 mmol) of **IV** and 1.17 g (18.0 mmol) of NaN_3 in 100 ml of DMF. Yield 2.05 g (100%), oily substance. ^1H NMR spectrum, δ, ppm: 1.44–1.48 m (4H, 3′-H), 1.64–1.68 m (8H, 2′-H, 4′-H), 2.25 s (3H, 6-CH_3), 3.25–3.31 m (4H, 5′-H), 3.79–3.83 t (2H, 1-CH_2, $J = 7.5$Hz), 3.90–3.94 t (2H, 3-CH_2, $J = 7.5$ Hz), 5.57 s (1H, 5-H). Found, %: C 51.62; H 6.87; N 32.18. $C_{15}H_{24}N_8O_2$. Calculated, %: C 51.71; H 6.94; N 32.16.

1,3-Bis(5-azidopentyl)-5-bromouracil (X) was synthesized from 1.5 g (3 mmol) of **V** and 0.59 g (9.0 mmol) of NaN_3 in 60 ml of DMF. Yield 1.22 g (100%), oily substance. ^1H NMR spectrum, δ, ppm: 1.44–1.48 m (4H, 3′-H), 1.64–1.70 m (8H, 2-H, 4′-H), 3.29–3.32 m (4H, 5′-H), 3.76–3.80 t (2H, 1-CH_2, $J = 7.3$ Hz), 3.99–4.03 t (2H, 3-CH_2, $J = 7.3$ Hz), 7.51 s (1H, 6-H). Mass spectrum: m/z 412.1 $[M]^+$. Found, %: C 40.65; H 5.13; Br 19.24; N 27.04. $C_{14}H_{21}BrN_8O_2$. Calculated, %: C 40.69; H 5.12; Br 19.33; N 27.11. M 412.10.

Reaction of azides VI and VII and bis-azides VIII–X with alkynes (*general procedure*). Azide **VI** or **VII** or bis-azide **VIII**–**X**, 1 equiv, was dissolved in aqueous ethanol (1:1), and 1 or 2 equiv of the corresponding alkyne, an aqueous solution of 0.1 equiv of sodium ascorbate, and an aqueous solution of 0.01 equiv of $CuSO_4 \cdot 5H_2O$ were added in succession under stirring. The mixture was evaporated, the residue was treated with 100–150 ml of chloroform, the precipitate was filtered off, the filtrate was evaporated under reduced pressure, 50–70 ml of diethyl ether was added to the residue, the solvent was separated by decanting, and the residue (compound **XI**–**XIV**) was dried.

1-[6-(4-Hydroxymethyl-1*H*-1,2,3-triazol-1-yl)-hexyl]-3,6-dimethyluracil (XI) was synthesized from 1.11 g (4.2 mmol) of **VI** and 0.23 g (4.1 mmol) of prop-2-yn-1-ol in a mixture of 10 ml of water with 10 ml of EtOH using 0.72 ml (0.4 mmol) of a freshly prepared 0.56 M aqueous solution of $C_6H_7O_6Na$ and 0.1 ml (0.04 mmol) of 0.4 M aqueous $CuSO_4 \cdot 5H_2O$. Yield 1.20 g (91%), mp 107°C. ^1H NMR spectrum, δ, ppm: 1.38 m (4H, 3′-H, 4′-H), 1.62–1.65 m (2H, 2′-H), 1.92–1.95 m (2H, 5′-H), 2.23 s (3H, 6-CH_3), 3.31 s (3H, 3-CH_3), 3.75–3.79 t (2H, 1′-H, $J = 7.6$ Hz), 4.34–4.38 t (2H, 6′-H, $J = 7$Hz), 4.81 s (2H, 4″-CH_2), 5.59 s (1H, 5-H), 7.54 s (1H, 5″-H). Mass spectrum: m/z 321.2 $[M]^+$. Found, %: C 55.98; H 7.23; N 21.67. $C_{15}H_{23}N_5O_3$. Calculated, %: C 56.06; H 7.21; N 21.79. M 321.18.

1-[7-(4-Butyl-1*H*-1,2,3-triazol-1-yl)heptyl]-3,6-dimethyluracil (XII) was synthesized from 0.70 g (2.5 mmol) of **VII** and 0.21 g (2.5 mmol) of hex-1-yne in a mixture of 10 ml of water with 10 ml of EtOH using 0.45 ml (0.25 mmol) of a freshly prepared 0.56 M aqueous solution of $C_6H_7O_6Na$ and 0.1 ml (0.025 mmol) of 0.25 M aqueous $CuSO_4 \cdot 5H_2O$. Yield 0.60 g (66 %), mp 62°C. ^1H NMR spectrum, δ, ppm: 0.93 t (3H, CH_3, $J = 7.3$ Hz), 1.36–1.41 m (8H, 3′-H, 4′-H, 5′-H, 3‴-H), 1.61–1.67 m (4H, 2′-H, 2‴-H), 1.87–1.91 t (2H, 6′-H, $J = 7.0$ Hz), 2.23 s (3H, 6-CH_3), 2.69–2.73 t (2H, 4″-CH_2, $J = 7.7$ Hz), 3.32 s (3H, 3-CH_3), 3.76–3.80 t (2H, 1-CH_2, $J = 7.7$ Hz), 4.29–4.32 t (2H, 7′-H, $J = 7.0$ Hz), 5.59 s (1H, 5-H), 7.54 s

(1H, 5″-H). Mass spectrum: *m*/*z* 361.9 [*M*]$^+$. Found, %: C 63.15; H 8.58; N 19.32. $C_{19}H_{31}N_5O_2$. Calculated, %: C 63.12; H 8.64; N 19.37. *M* 361.25.

1,3-Bis[5-(4-hydroxymethyl-1*H*-1,2,3-triazol-1-yl)pentyl]-6-methyluracil (XIII) was synthesized from 0.5 g (1.4 mmol) of **IX** and 0.16 g (2.8 mmol) of prop-2-yn-2-ol in a mixture of 5 ml of water with 5 ml of EtOH using 0.50 ml (0.28 mmol) of a freshly prepared 0.56 M aqueous solution of $C_6H_7O_6Na$ and 0.1 ml (0.025 mmol) of 0.25 M aqueous $CuSO_4 \cdot 5H_2O$. Yield 0.65 g (100%), oily substance. ^{1}H NMR spectrum, δ, ppm: 1.33–1.37 m (4H, 3′-H), 1.63–1.67 m (4H, 2′-H), 1.93–1.99 m (4H, 4′-H), 2.22 s (3H, 6-CH_3), 3.74–3.78 t (2H, 1-CH_2, *J* = 7.9 Hz), 3.86–3.90 t (2H, 3-CH_2, *J* = 7.5 Hz), 4.33–4.39 m (4H, 5′-H), 4.76 s and 4.78 s (2H each, 4″-CH_2), 5.55 s (1H, 5-H), 7.60 s and 7.62 s (1H each, 5″-H). Mass spectrum: *m*/*z* 461.2 [*M* + H]$^+$. Found, %: C 54.73; H 6.91; N 24.35. $C_{21}H_{32}N_8O_4$. Calculated, %: C 54.77; H 7.00; N 24.33. *M* 460.25.

6-Methyl-1,3-Bis[5-(4-octyl-1*H*-1,2,3-triazol-1-yl)pentyl]uracil (XIV) was synthesized from 0.8 g (2.3 mmol) of **IX** and 0.63 g (4.6 mmol) of dec-1-yne in a mixture of 10 ml of water and 10 ml of EtOH using 0.82 ml (0.46 mmol) of a freshly prepared 0.56 M aqueous solution of $C_6H_7O_6Na$ and 0.1 ml (0.046 mmol) of 0.46 M aqueous $CuSO_4 \cdot 5H_2O$. Yield 0.79 g (55%), oily substance. ^{1}H NMR spectrum ($CDCl_3$), δ, ppm: 0.86–0.89 m (6H, CH_3), 1.25–1.40 m (24H, 3′-H, 3‴-H–7‴-H), 1.58–1.70 m (8H, 2′-H, 2‴-H), 1.85–1.95 m (4H, 4′-H), 2.22 s (3H, 6-CH_3), 2.65–2.70 m (4H, 4″-CH_2), 3.74–3.78 t (2H, 1-CH_2, *J* = 7.9 Hz), 3.89–3.93 t (2H, 3-CH_2, *J* = 7.5 Hz), 4.32–4.36 m (4H, 1″-CH_2), 5.56 s (1H, 5-H), 7.50 s and 7.53 s (1H each, 5″-H). Mass spectrum: *m*/*z* 625.6 [*M* + H]$^+$. Found, %: C 67.30; H 9.73; N 17.95. $C_{35}H_{60}N_8O_2$. Calculated, %: C 67.27; H 9.68; N 17.93. *M* 624.48.

1^6-Methyl-6^1*H*,12^1*H*--8,10-dioxa-1(1,3)-pyrimidina-6(1,4),12(4,1)-bis(1,2,3-triazola)-9(1,3)-benzenahexadecaphane-1^2,1^4(1^1*H*,1^3*H*)-dione (XVI) and 6-methyl-1,3-bis(4-{4-[3-(prop-2-yn-1-yloxy)phenoxymethyl]-1*H*-1,2,3-triazol-1-yl}butyl)uracil (XVII). A solution of 1.37 g (4.3 mmol) of **VIII** in 75 ml of ethanol and a solution of 0.81 g (4.3 mmol) of **XV** in 75 ml of ethanol were simultaneously added dropwise over a period of 4 h under stirring to a solution of 0.18 g (0.9 mmol) of sodium ascorbate and 0.02 g (0.08 mmol) of $CuSO_4 \cdot 5H_2O$ in a mixture of 100 ml of water and 100 ml of ethanol. The mixture was stirred for 8 h at room temperature and evaporated under reduced pressure, 100 ml of chloroform was added to the residue, the precipitate was filtered off, and the filtrate was concentrated and subjected to column chromatography on silica gel. The column was eluted in succession with petroleum ether, EtOAc–MeOH (50 : 1), and EtOAc–MeOH (30 : 1). Evaporation of the second fraction gave 0.12 g (5%) of compound **XVI** as an oily substance. ^{1}H NMR spectrum, δ, ppm: 1.65 m (4H, CH_2), 1.72 m (4H, CH_2), 2.25 s (3H, 6-CH_3), 3.82–3.86 t (2H, 1-CH_2, *J* = 7.6 Hz), 3.94–3.97 t (2H, 3-CH_2, *J* = 7.5 Hz), 4.40–4.43 m (4H, 1″-CH_2), 5.18 br.s (4H, 4″-CH_2), 5.59 s (1H, 5-H), 6.62 m (3H, C_6H_4), 7.18 m (1H, C_6H_4), 7.64 s and 7.66 s (1H each, 5″-H). Mass spectrum: *m*/*z* 507.3 [*M* + H]$^+$. Found, %: C 59.30; H 5.93; N 22.15. $C_{25}H_{30}N_8O_4$. Calculated, %: C 59.28; H 5.97; N 22.12. *M* 506.24.

Evaporation of the third fraction gave 0.1 g (3%) of compound **XVII** as an oily substance. ^{1}H NMR spectrum, δ, ppm: 1.64–1.70 m (4H, CH_2), 1.91–1.99 m (4H, CH_2), 2.19 s (3H, 6-CH_3), 2.52 t (2H, ≡CH, *J* = 2.4 Hz), 3.79–3.83 t (2H, 1-CH_2, *J* = 7.2 Hz), 3.95–3.98 t (2H, 3-CH_2, *J* = 7.2 Hz), 4.38–4.44 m (4H, 1″-CH_2), 4.66 d (4H, OCH_2, *J* = 2.4 Hz), 5.17 s and 5.18 s (2H each, 4″-CH_2O), 5.56 s (1H, 5-H), 6.58–6.64 m (6H, C_6H_4), 7.17–7.21 m (2H, C_6H_4), 7.64 s (2H, 5″-H). Mass spectrum: *m*/*z* 693.3 [*M* + H]$^+$. Found, %: C 64.11; H 5.87; N 16.15. $C_{37}H_{40}N_8O_6$. Calculated, %: C 64.15; H 5.82; N 16.17. *M* 623.91.

3,4-Dibutyl-1-[7-(3,6-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)heptyl]-1*H*-1,2,3-triazol-3-ium iodide (XVIII). Propyl iodide, 1.30 g (7 mmol), was added to a solution of 0.5 g (1.4 mmol) of **XII** in 30 ml of acetonitrile, and the mixture was stirred for 30 h on heating under reflux. The mixture was cooled and evaporated, and the residue was washed with three portions of diethyl ether, the solvent being separated each time by decanting. Yield 0.62 g (83%). ^{1}H NMR spectrum, δ, ppm: 1.00 t [3H, 4″-$(CH_2)_3C\mathbf{H}_3$, *J* = 7.4 Hz], 1.06 t [3H, 3″-$(CH_2)_2C\mathbf{H}_3$, *J* = 7.4 Hz), 1.44–1.66 m (12H, 2′-H–5′-H, 4″-$CH_2(C\mathbf{H}_2)_2$), 1.84 t (2H, 6′-H, *J* = 7.0 Hz), 2.06 t (2H, 3″-$CH_2C\mathbf{H}_2$, *J* = 7.4 Hz), 2.28 s (3H, 6-CH_3), 2.84–2.88 t (2H, 4″-CH_2, *J* = 7.8 Hz), 3.32 s (3H, 3-CH_3), 3.79–3.83 t (2H, 1-CH_2, *J* = 7.8 Hz), 4.39–4.43 t (2H, 1″-CH_2, *J* = 7.4 Hz), 4.77–4.81 t (2H, 3″-CH_2, *J* = 7.4 Hz), 5.59 s (1H, 5-H), 9.44 s (1H, 5″-H). Mass spectrum: *m*/*z* 404.6 [*M* – I]$^+$. Found, %: C 49.77; H 7.18; I 23.95; N 13.22; $C_{22}H_{38}IN_5O_2$. Calculated, %: C 49.72; H 7.21; I 23.88; N 13.18. *M* 531.21.

1,1′-[(6-Methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidine-1,3-diyl)bis(pentane-5,1-diyl)]bis(3-methyl-4-octyl-1*H*-1,2,3-triazol-3-ium) bis(4-toluenesulfonate) (XIX). A mixture of 0.4 g (0.6 mmol) of compound **XIV** and 1.2 g (6.5 mmol) of methyl *p*-toluenesulfonate was stirred for 10 h on heating at 90–100°C. The mixture was cooled to room temperature, 20 ml of diethyl ether was added, and the solvent was separated by decanting. This procedure was repeated five times. Yield 0.48 g (80%), oily substance. ^{1}H NMR spectrum, δ, ppm: 0.88 m (6H, CH$_3$), 1.26–1.66 m (32H, 2′-H, 3′-H, 2‴-H–7‴-H), 2.03 m (4H, 4′-H), 2.17 s (3H, 6-CH$_3$), 2.76 m (4H, 4″-CH$_2$), 3.74–3.82 m (2H, 1-CH$_2$), 3.88 m (2H, 3-CH$_2$), 4.18 br.s (6H, 3″-CH$_3$), 4.62 m and 4.68 m (2H each, 1″-CH$_2$), 5.53 s (1H, 5-H), 8.94 s and 9.05 s (1H, 5-H). Mass spectrum: *m/z* 825.5 $[M - \text{OTs}]^+$. Found, %: C 61.40; H 8.03; N 11.25; S 6.49. $C_{51}H_{80}N_8O_8S_2$. Calculated, %: C 61.42; H 8.08; N 11.24: S 6.43. *M* 996.55.

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