Regioselective reactions of *N*-(carboxyalkyl)- and *N*-(aminoethyl)ureas with glyoxal and 1,2-dioxo-1,2-diphenylethane*

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Regioselective reactions of *N*-(carboxyalkyl)ureas (ureido acids) and *N*-(aminoethyl)ureas with 1,2-dioxo-1,2-diphenylethane (benzyl) and glyoxal are studied in detail. The structure of the reactants affects the reaction regioselectivity. Acid-catalyzed reactions of glyoxal with 1-[2-(dimethylamino(acetylamino))ethyl]ureas and benzene with ureido acids result mainly in 2,6-disubstituted glycolurils. The structure of 2,6-di(methoxycarbonylethyl)glycoluril is unambiguously established by X-ray diffraction.

Key words: *N*-(carboxyalkyl)ureas (ureido acids), 1-{2-[dimethylamino(acetylamino)]-ethyl}ureas, glyoxal, benzyl, 2,6- and 2,8-disubstituted glycolurils, regioselective reactions.

Recently, we elaborated synthetic methods to access monofunctional glycolurils bearing aminoalkyl, hydroxyalkyl, and carboxyalkyl groups at the nitrogen atoms.[1—7] Among synthesized compounds, substances exhibiting neurotropic (sedative, anxiolytic), neuroprotective, nootropic (superior than Nootropil) activities were found.[8,9] Glycolurils bearing the 2-acetylaminoethyl[8] and 3-carboxypropyl moieties[9] at the same nitrogen atom turned out to be the most effective. This fact demonstrates the feasibility of search for the new promising compounds in this series; therefore, the introduction of one more acetylaminoethyl and carboxyalkyl groups into glycoluril is of interest. Earlier,[10,11] 2,6- and 2,8-di(carboxyalkyl)glycolurils were synthesized by the reaction of *N*-carbamoylglycine and its esters with glyoxal and 1,2-dioxo-1,2-diphenylethane (benzyl). From the reaction mixture obtained in the reaction of *N*-carbamoylglycine with glyoxal at 100 °C for 0.2 h,[10] some product was isolated in 14% yield. Based on the melting point and elemental analysis, to this compound, the structure of 2,6- and/or 2,8-di(carboxymethyl)glycoluril was ascribed. Predominant formation of 2,8-di(carboxymethyl)-1,5-diphenylglycoluril diesters was demonstrated on the example of several reactions of *N*-cabamoylglycinates with benzyl derivatives.[11] The reactions were carried out in benzene in the presence of trifluoroacetic acid. The obtained glucoluril diesters were hydrolyzed to 2,8-di(carboxymethyl)-1,5-diphenylglucolurils.

With the aim to develop novel regioselective syntheses of 2,6-*trans* (**1**) or 2,8-*cis* difunctionally substituted** (**2**) glycolurils, in the present work we first studied in detail the diastereoselective condensations of glyoxal and benzyl with 1-[2-(dimethylamino(acetylamino))ethyl]ureas **3a**,**b** and *N*-(carboxyalkyl)ureas (ureido acids) **3c—e** (Schemes 1 and 2).

The starting ureas **3a—e** were synthesized by N-carbamoylation of the corresponding ethylenediamines (2-(dimethylamino)ethyl- and 2-(acetylamino)ethylamines) and amino acids (Gly, β-Ala, γ-aminobutyric acid) in the presence of KOCN similarly to earlier developed procedures.[12] 2-(Acetylamino)ethylamine was obtained by ethylenediamine acetylation.[13]

Condensations of glyoxal with 1-[2-(dimethylamino-(acetylamino))ethyl]ureas **3a**,**b** and ureido acids **3c—e** (see Scheme 1) were performed in water under conditions used previously[14] for the synthesis of 2,6-dialkylglycolurils, *i.e.*, pH 1—2, reaction time of 1 h. Regioselectivity of the reactions was estimated by ^{1}H NMR spectroscopy of the reaction mixtures evaporated to dryness. The most informative signals of the compounds synthesized are the signals

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** Since the *cis*-fusing of the imidazolidine rings in glycoluris is well known, the terms 2,8-*cis*- and 2,6-*trans*- are used to describe the orientation of substituents at the cyclic nitrogen atoms.

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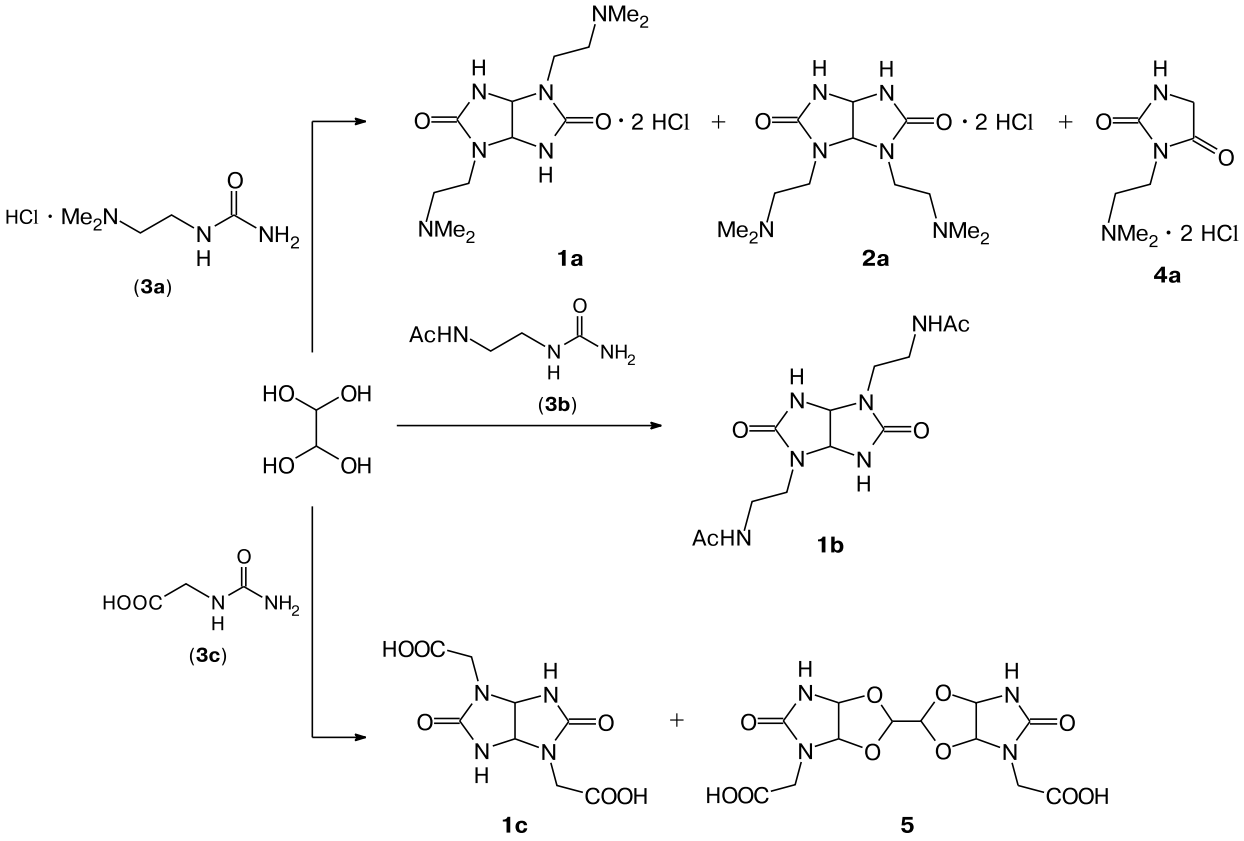
Scheme 1



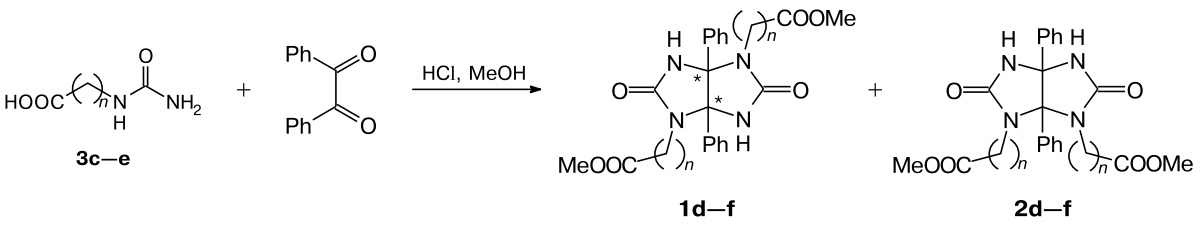
of the protons of the CH—CH glycoluril groups, namely, the doublet of doublets for *cis*-isomers and singlet for *trans*-isomer, and variable chemical shifts of the NH group singlets. It is shown that the reaction of glyoxal with 1-[2-(dimethylamino)ethyl]urea **3a** yields *trans*- (**1a**) and *cis*-glycolurils (**2a**) in an 1 : 1 ratio. The separation of these isomers failed due to the proximity of physico-chemical properties. Moreover, ^{1}H NMR spectrum contains also the signals of the known hydantoin **4a**.[15] Isolated yields of the mixture of isomers **1a** and **2a** and hydantoin **4a** are 49 and 31%, respectively.

It is found that the reactions of glyoxal with both 1-(2-acetylaminoethyl)urea **3b** and ureido acid **3c** are regiospecific and result in *trans*-isomers **1b**,**c** in the yields of 51 and 26%, respectively. Even traces of the corresponding *cis*-isomers **2b**,**c** were not detected. Glyoxal reacts with ureido acid **3c** to give hitherto unknown compound, 3,3′-bi[(1*R**,5*S**)-2,4-dioxa-6,8-diaza-7-oxobicyclo[3.3.0]oct-6-yl)acetic acid] (**5**). The structure of bisbicycle **5** was established by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry taking in account the data for the previously synthesized 3,3′-bi(6,8-dialkyl-2,4-dioxa-7-thia-6,8-diazabicyclo[3.3.0]octane-7,7-dioxides).[16]

Similar reactions between either *N*-carbamoyl-β-alanine (**3d**) or *N*-carbamoyl-γ-butyric acid (**3e**) afford the complex mixtures of the unidentified products.

Acid-catalyzed condensations of benzyl with 1-[2-(dimethylamino(2-acetylamino))ethyl]ureas **3a,b** and ureido acids **3c—e** were carried out in MeOH or Pr^{i}OH because benzyl is insoluble in water. Attempted reaction of benzyl with ureas **3a**,**b** failed and the starting compounds were recovered. Cyclocondensations of ureido acids **3c—e** with benzyl (Scheme 2) were performed in MeOH since in Pr^{i}OH no reaction occurred. Refluxing of the reactants for 1 h yielded methyl esters of *trans*- (**1d—f**) and *cis*- (**2d—f**) glycoluril derivatives. The ratios of the isomers, **1d** : **2d** = = 1 : 2, **1e** : **2e** = 3.3 : 1, and **1f** : **2f** = 4.4 : 1, clearly indicate the regioselectivity of the reactions. The ratios of the 2,6- and 2,8-substituted products were determined by ^{1}H NMR spectroscopy. It is found that the alkyl chain elongation in ureido acids **3c—e** leads to the increase in the content of 2,6-di(methoxycarbonylalkyl)glycolurils **1d—f**. Compounds **1d—f** and **2d—f** were separated by fractional crystallization in the yields of 11—50% for **1d—f** and 8—22% for **2d—f**. Along with glucoluril derivatives, from the reaction mixtures, the following compounds were isolated: benzyl, ureido acid **3e**, and known products of

Scheme 2



n = 1 (**1d**, **2d**, **3c**), 2 (**1e**, **2e**, **3d**), 3 (**1f**, **2f**, **3e**)

ureido acid cyclization, namely, hydantoin **4b** (in the case of ureido acid **3c**)[1] and dihydropyrimidine-2,4(1*H*,3*H*)-dione **4c** (in the case of ureido acid **3d**).[17]

The structures of the synthesized compounds were established by microanalysis data, ^{1}H and ^{13}C NMR spectroscopy, and mass spectrometry. The structure of the major isomer **1e** was also confirmed by X-ray diffraction (Fig. 1). According to X-ray data, in crystal **1e**, one and a half molecules are crystallographically independent with the slightly different geometrical parameters.* Thus, the heterocycle conformation in both cases is an *envelope* with a deviation from the mean plane of 0.33(1)—0.35(1) Å for the C(1) and C(3) atoms and the angles between these planes of 69.9(3)° and 70.6(3)°. Therefore, the mutual imidazolidine cycle arrangement characteristic of these type of compounds[2—4,7,14] can be regarded as "half-open book". The C(17)N(2)N(4)C(21) and C(18)C(17)C(21)C(22) dihedral angles describing the mutual orientation of the ester groups are 101.4(3)/38.2(3)° and 108.8(3)/45.3(3)° in two molecules, respectively. Like the previously studied glycolurils,[7] the phenyl groups at the bridgehead carbons adopt *cis* orientation.

The crystals of compound **1e** contain the endless chains formed by the N—H...O hydrogen bonds (the NO distance is 2.805(3)—2.826(3) Å, the NHO angle is 171.0(3)—172.8(3)°). The C—H...O, C—H...π, and weak interactions connect these chains into a 3D network (Fig. 2).

In summary, the detail study of the reactions of aminoethyl- and carboxyalkylureas with glyoxal and benzyl reveals the effect of the reactant structure on regioselectivity of formation of 2,6- and 2,8-disubstituted glycolurils. It is shown that both 2-acetylaminoethylureas and *N*-carbamoylglycine regiospecifically react with glyoxal to give exclusively 2,6-disubstituted glycolurils, while 2-dimethylaminoethylureas react with glyoxal to yield the mixture of 2,6- and 2,8-isomers in an 1 : 1 ratio. Condensation of benzyl with ureido acids regioselectively produces methyl esters of 2,6- and 2,8-isomers; wherein the longer the alkyl chain of the ureido acid, the higher the content of 2,6-di(methoxycarbonylalkyl)glycolurils.

Experimental

Commercially available (Acros) amino acids, *N*,*N*-(dimethyl)ethylamine hydrochloride, glyoxal trimer dihydrate, and 40% aqueous glyoxal were used. Ureido acids **3a**—**e** were synthesized by treatment of the corresponding amines with KOCN as earlier described.[12]

NMR spectra were run on Bruker AM-250 (^{1}H, 250 MHz) and Bruker AM-300 (^{13}C, 75.5 MHz) instruments in DMSO-d_6, the chemical shifts are given in the δ scale relative to Me_4Si (internal standard). The melting points were determined on a GALLENKAMP apparatus (Sanyo).

* The numbering scheme for glycolurils in the X-ray experiment differs from the IUPAC numbering scheme.

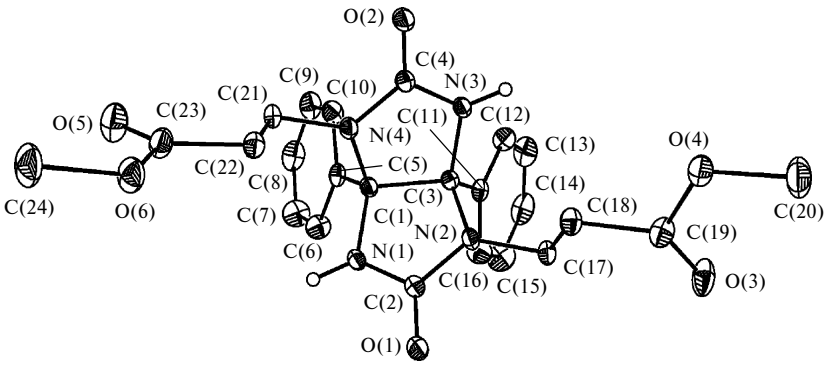


Fig. 1. Molecular structure of compound **1e**, displacement ellipsoids are given with 30% probability.

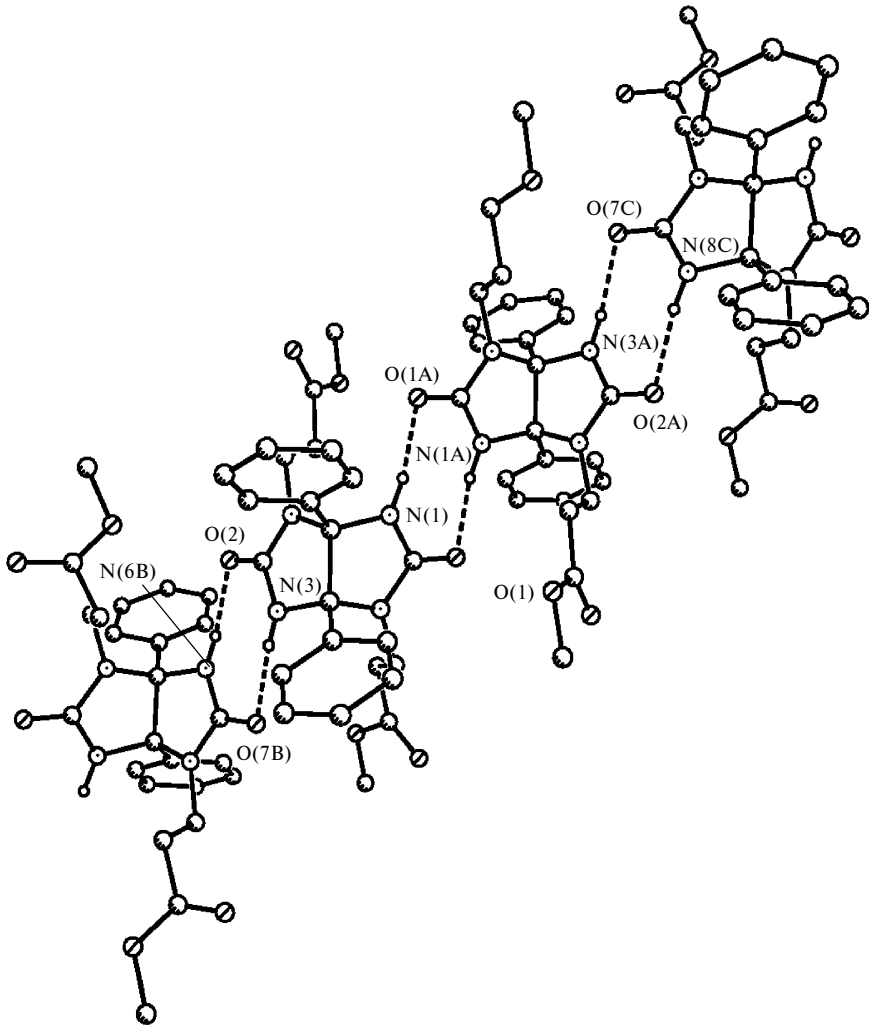


Fig. 2. H-Bonded chain in crystal **1e**.

X-ray diffraction study of compound 1e was performed on a SMART 1000 CCD diffractometer (MoKα radiation, ω scanning mode). The structure was solved by the direct methods and refined using the full-matrix least squares on F^2_{hkl} in anisotropic approximation. Hydrogen atoms of the NH groups were localized from difference Fourier syntheses of electron density, other hydrogen atoms were positioned geometrically. The positions of all hydrogen atoms were refined isotropically using the riding model. The X-ray data collection and refinement statistic are given in Table 1. All calculations were performed using SHELXTL PLUS program package.[18]

Synthesis of 2,6(2,8)-di[2-(dimethylamino)ethyl]- (1a and 2a) and 2,6-di(2-acetylaminoethyl)-2,4,6,8-tetraazabicyclo[3.3.0]-octane-3,7-diones (1b) (general procedure). To a solution of glyoxal trimer dihydrate (0.0033 mol) or 40% aqueous glyoxal (0.01 mol, 1.15 mL, d = 1.265) in water (10 mL), 1-[2-(dimethylamino)ethyl]- (**3a**) or 1-(2-acetylaminoethyl)urea (**3b**) (0.02 mol) was added followed by addition of concentrated HCl to pH 1, and the reaction mixture was heated at 80 °C for 1 h. The solvent was removed *in vacuo* to give the oily residue. The residue was treated with isopropyl alcohol and methanol, the resulted precipitate of glycolurils **1a**, **2a** or **1b** was collected by filtration. Slow concentration of the filtrate afforded crystalline compound **4a**.

Mixture of isomers **1a** and **2a**. Yield 49%. ^{1}H NMR, δ: 2.79 (s, 12 H, NMe_2); 2.81 (s, 12 H, NMe_2); 3.00—3.09 (m, 1 H, NCH_2); 3.13—3.41 (m, 12 H, NCH_2); 3.46—3.57 (m, 2 H, NCH_2); 3.72—3.83 (m, 1 H, NCH_2); 5.30 (d, 1 H, CH, J = 8.2 Hz); 5.40 (s, 2 CH); 5.62 (d, 1 H, CH, J = 8.2 Hz); 7.73 (s, 2 H, 2 NH); 7.87 (s, 2 H, 2 NH). Found (%): C, 50.64; H, 8.48; N, 29.58. $C_{12}H_{24}N_6O_2$. Calculated (%): C, 50.69; H, 8.51; N, 29.55.

Compound **1b**. Yield 51%, m.p. 255—257 °C. ^{1}H NMR, δ: 1.78 (s, 6 H, 2 Ac); 2.94—2.98 (m, 2 H, NCH_2); 3.05—3.09 (m, 2 H, NCH_2); 3.20—3.28 (m, 4 H, 2 NCH_2); 5.25 (s, 2 H, 2 CH); 7.49 (s, 2 H, 2 NH); 7.83 (t, 2 H, 2 NHAc, J = 4.9 Hz). ^{13}C NMR, δ: 169.41 (CONH), 159.17 (CO), 65.42 (CH), 39.93 (NCH_2), 36.53 (NCH_2), 22.64 (CH_3). MS, m/z (I_{rel} (%)): 253 $[M - NH_2Ac]^+$ (21.94), 211 (28.39), 169 (58.06), 126 (88.39), 114 (50.32), 110 (50.32), 85 (100), 73 (61.94), 56 (58.71), 43 (84.52). Found (%): C, 46.05; H, 6.49; N, 26.88. $C_{12}H_{20}N_6O_4$. Calculated (%): C, 46.15; H, 6.45; N, 26.91.

Compound **4a**. Yield 31%, m.p. 237—239 °C (*cf.* Ref. 15: 238—239 °C). ^{1}H NMR spectral data are in agreement with those published previously.[15]

Synthesis of (6-carboxymethyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl)acetic acid (1c) and 3,3′-bi(7-oxo-2,4-

Table 1. Crystallographic characteristic, X-ray data collection, and refinement parameters for compound **1e**

Parameter	Value
Molecular formula	$C_{24}H_{26}N_4O_6$
Molecular weight	466.49
T/K	296
Crystal system	Monoclinic
Space group	$C2/c$
Z	12
a/Å	22.444(5)
b/Å	11.080(3)
c/Å	30.118(7)
α/deg	90.00
β/deg	94.29(2)
γ/deg	90.00
V/Å^3	7469(3)
d_{calc}/g cm^{-3}	1.245
μ/cm^{-1}	0.91
F(000)	2952
$2\theta_{max}$/deg	56
Number of measured reflections	37952
Number of independent reflections	9022
Number of reflections with $I > 2\sigma(I)$	4857
Number of refined parameters	468
R_1	0.0764
wR_2	0.2063
GOF	1.042
Residual electron density/e Å^{-3} (ρ_{min}/ρ_{max})	−0.528/1.029

dioxa-6,8-diazabicyclo[3,3,0]octan-6-yl)acetic acid (5). To a solution of glyoxal trimer dehydrate (0.033 mol) or 40% aqueous glyoxal (0.01 mol, d = 1.265) in water (10 mL), *N*-carbamoyl glycine (0.02 mol) was added followed by dropwise addition of concentrated HCl (0.1 mL). The reaction mixture was heated at 80 °C for 1 h. After cooling down, precipitated compound **5** was collected by filtration and washed with water. The filtrate was concentrated to 1/4 of its initial volume and precipitated compound **1c** was collected.

2-((1*S,5*S**)-6-Carboxymethyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl)acetic acid (1c).** Yield 26%, m.p. 288—289 °C. ^{1}H NMR, δ: 3.66 (d, 2 H, CH_2, ^3J = 18.1 Hz); 3.96 (d, 2 H, CH_2, ^3J = 18.1 Hz); 5.30 (br.s, 2 H, 2 CH); 7.61 (s, 2 H, 2 NH); 12.75 (br.s, 2 H, 2 CH). Found (%): C, 37.25; H, 3.91; N, 21.65. $C_8H_{10}N_4O_6$. Calculated (%): C, 37.22; H, 3.90; N, 21.70.

3,3´-Bi[((1*R,5*S**)-2,4-dioxa-6,8-diaza-7-oxobicyclo[3.3.0]-octan-6-yl)acetic acid] (5).** Yield 20%, m.p. 330—332 °C (decomp.). ^{1}H NMR, δ: 3.77 (d, 2 H, CH_2, ^3J = 17.7 Hz); 3.92 (d, 2 H, CH_2, ^3J = 17.7 Hz); 4.88 (s, 2 H, 2 CH); 5.71 (s, 4 H, 4 CH); 8.08 (s, 2 H, 2 NH); 12.80 (br.s, 2 OH, 2 COOH). MS, m/z (I_{rel} (%)): 187 1/2[M]$^+$ (6.91), 158 (5.91), 114 (26.83), 113 (32.63), 85 (24.92), 56 (45.25), 44 (71.77), 43 (32.96), 42 (100). Found (%): C, 38.48; H, 3.79; N, 14.97. $C_{12}H_{14}N_4O_{10}$. Calculated (%): C, 38.51; H, 3.77; N, 14.97.

Synthesis of methyl esters of 2,6- (1d—f) and 2,8-di(carboxyalkyl)glycolurils (2d—f) (general procedure). To a solution of benzyl (0.005 mol) and the corresponding ureido acid **3c—e** (0.01 mol) in MeOH (15—25 mL), HCl (1.8 mL) was added, and the stirred mixture was refluxed for 2 h and then kept for 3 days. The precipitate formed was filtered and washed with diethyl ether. 2,6- and 2,8-Disubstituted glycolurils were separated by crystallization from MeOH.

Methyl 2-[6-(methoxycarbonyl)methyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]acetate (1d). Yield 11%, m.p. 279—281 °C. ^{1}H NMR, δ: 3.50 (d, 2 H, CH_2, J = 17.6 Hz); 3.59 (s, 6 H, OMe); 3.92 (d, 2 H, CH_2, J = 17.7 Hz); 6.98—7.15 (m, 10 H, Ph); 8.28 (s, 2 H, NH). ^{13}C NMR, δ: 41.90 (CH_2); 51.63 (OMe); 83.70 (C<u>C</u>Ph); 127.19, 127.66, 128.37 (Ph); 135.22 (C(Ph)); 158.69 (CO); 169.14 (COO). Found (%): C, 60.24; H, 5.05; N, 12.83. $C_{22}H_{22}N_4O_6$. Calculated (%): C, 60.27; H, 5.06; N, 12.78.

Methyl 2-[8-(methoxycarbonyl)methyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]acetate (2d). Yield 22%, m.p. 322—324 °C. ^{1}H NMR, δ: 3.05 (d, 2 H, CH_2, J = 17.5 Hz); 3.66 (s, 6 H, OMe); 3.72 (d, 2 H, CH_2, J = 17.7 Hz); 6.98—7.15 (m, 10 H, Ph); 8.29 (s, 2 H, NH). ^{13}C NMR, δ: 42.78 (CH_2); 51.80 (OMe); 79.95, 88.28 (C<u>C</u>Ph); 127.17, 127.32, 127.75, 128.13, 128.54, 129.46 (Ph); 133.35, 137.28 (C(Ph)); 159.00 (CO); 169.79 (COO). Found (%): C, 60.29; H, 5.07; N, 12.74. $C_{22}H_{22}N_4O_6$. Calculated (%): C, 60.27; H, 5.06; N, 12.78.

Methyl 3-[6-(2-methoxycarbonyl)ethyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]propionate (1e). Yield 50%, m.p. 288—290 °C. ^{1}H NMR, δ: 2.43—2.62 (m, 4 H, CH_2); 2.88—3.00 (m, 2 H, CH_2); 3.35—3.51 (m, 2 H, CH_2); 3.54 (s, 6 H, OMe); 6.76—7.48 (m, 10 H, Ph); 8.35 (s, 2 H, NH). ^{13}C NMR, δ: 33.25, 36.41 (CH_2); 51.46 (OMe); 83.87 (C<u>C</u>Ph); 127.34, 127.99, 128.53 (Ph); 135.39 (C(Ph)); 158.87 (CO); 171.47 (COO). Found (%): C, 61.83; H, 5.60; N, 12.03. $C_{24}H_{26}N_4O_6$. Calculated (%): C, 61.79; H, 5.62; N, 12.01.

Methyl 3-[8-(2-methoxycarbonyl)ethyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]propionate (2e). Yield 15%, m.p. 187—190 °C. ^{1}H NMR, δ: 2.76 (t, 4 H, CH_2, J = 7.6 Hz); 3.13—3.27 (m, 2 H, CH_2); 3.33—3.49 (m, 2 H, CH_2); 3.57 (s, 6 H, OMe); 6.73—6.84 (m, 2 H, Ph); 6.94—7.02 m, 2 H, Ph); 7.03—7.16 (m, 6 H, Ph); 8.21 (s, 2 H, NH). ^{13}C NMR, δ: 33.68, 38.20 (CH_2); 51.39 (OMe); 79.33, 89.84 (C<u>C</u>Ph); 127.11, 127.42, 127.74, 128.13, 128.25, 128.58 (Ph); 133.25, 137.19 (C(Ph)); 159.68 (CO); 171.23 (COO). Found (%): C, 61.80; H, 5.58; N, 12.05. $C_{24}H_{26}N_4O_6$. Calculated (%): C, 61.79; H, 5.62; N, 12.01.

Methyl 4-[6-(3-methoxycarbonyl)propyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]butanoate (1f). Yield 35%, m.p. 276—278 °C. ^{1}H NMR, δ: 1.69—1.81 (m, 4 H, CH_2); 2.26 (t, 4 H, CH_2, J = 7.7 Hz); 2.56—2.73 (m, 2 H, CH_2); 3.20—3.47 (m, 2 H, CH_2); 3.56 (s, 6 H, OMe); 6.88—7.02 (m, 4 H, Ph); 7.03—7.14 (m, 6 H, Ph); 8.21 (s, 2 H, NH). ^{13}C NMR, δ: 24.34, 30.87, 39.67 (CH_2); 51.17 (OMe); 83.94 (C<u>C</u>Ph); 127.14, 127.75, 128.25, 129.47, 129.54 (Ph); 135.41, 135.49 (C(Ph)); 158.98 (CO); 172.91 (COO). Found (%): C, 63.12; H, 6.13; N, 11.30. $C_{26}H_{30}N_4O_6$. Calculated (%): C, 63.15; H, 6.11; N, 11.33.

Methyl 4-[8-(3-methoxycarbonyl)propyl-1,5-diphenyl-3,7-dioxo-2,4,6,8-tetraazabicyclo[3.3.0]octan-2-yl]butanoate (2f). Yield 8%, m.p. 165—167 °C. ^{1}H NMR, δ: 1.82—2.06 (m, 4 H, CH_2); 2.32 (t, 4 H, CH_2, J = 7.3 Hz); 2.87—3.02 (m, 2 H, CH_2); 3.10—3.24 (m, 2 H, CH_2); 3.55 (s, 6 H, OMe); 6.70—6.80 (m, 2 H, Ph); 6.80—7.02 (m, 2 H, Ph); 7.03—7.16 (m, 6 H, Ph);

8.08 (s, 2 H, NH). ^{13}C NMR, δ: 24.65, 30.77, 41.56 (CH_2); 51.17 (OMe); 79.16, 89.97 (CPh); 127.06, 127.41, 127.73, 128.06, 128.44 (Ph); 133.59, 137.35 (C(Ph)); 159.93 (CO); 172.80 (COO). Found (%): C, 63.16; H, 6.10; N, 11.35. $C_{26}H_{30}N_4O_6$. Calculated (%): C, 63.15; H, 6.11; N, 11.33.

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