Alkylation of 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide*

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Alkylation of 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide **1** and its silver salt **10** with different alkylating agents (diazomethane, diazoacetone, bromoacetone, α-bromoacetophenone, methyl iodide, methyl vinyl ketone) was studied. Alkylation of compound **1** with diazo compounds and salt **10** with halocompounds results predominantly in *O*-alkylation products, 1-alkoxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxides. The Michael reaction of compound **1** with methyl vinyl ketone involves the triazole nitrogen atom to give 1-(3-oxobutyl)-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 3,4,6-trioxide. The structures of the compounds synthesized were established by ^{1}H, ^{13}C, ^{14}N NMR spectroscopy and mass spectrometry.

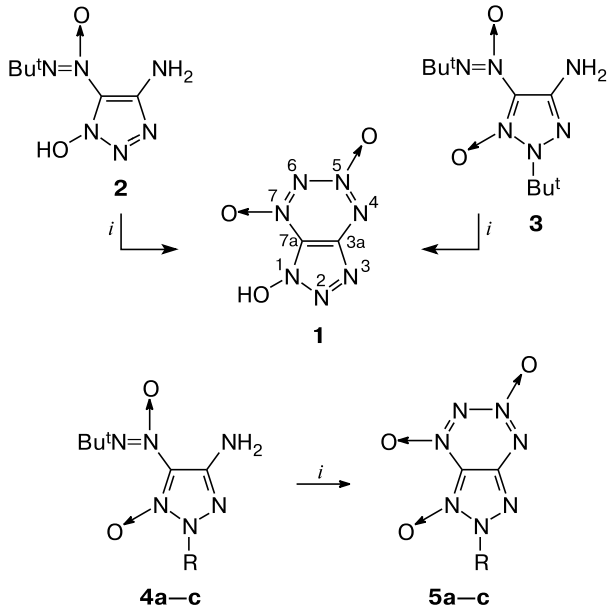
Key words: 1,2,3-triazole 1-oxides, 1,2,3,4-tetrazine 1,3-dioxides, alkylation, ^{1}H, ^{13}C, ^{14}N NMR spectroscopy.

Recently, we developed synthetic procedure to access 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (**1**) by the reaction of aminotriazoles **2** and **3** with HNO_3—H_2SO_4—Ac_2O.[1] This procedure was also applied to transform aminotriazoles **4a**—**c** into triazolotetrazines **5a**—**c** (Scheme 1).[1]

These compounds represent novel heterocyclic system comprising annulated 1,2,3,4-tetrazine 1,3-dioxide and triazole *N*-oxide cycles. The closest known analog bearing the 1,2,3,4-tetrazine and triazole cycles is 2-phenyl-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine,[2] which is unstable even at room temperature. Increased thermal stability of 1,2,3,4-tetrazine 1,3-dioxide as compared with 1,2,3,4-tetrazine is due to the stabilizing effect of two oxygen atoms. It is of note that 1,2,3,4-tetrazine 1,3-dioxides annulated to various heterocycles exhibit different thermal stability. Thus, [1,2,5]oxadiazolo[3,4-*e*][1,2,3,4]tetrazine 4,6-dioxide (furazanotetrazine dioxide, FTDO) melts with decomposition at 112 °C.[3] As compared to FTDO, recently synthesized triazolotetrazines **5a**—**c** (see Scheme 1) are more stable and melt with decomposition at ~210—230 °C. Compound **1** is also quite stable (m.p. 180—185 °C with decomp.).[1]

The aims of the present work are to study the alkylation direction of the heterocyclic system **1**, synthesize triazolotetrazines differing from the known analogs **5** by the position of the alkyl groups, and reveal the dependence of the thermal stability of triazolotetrazines on the position of the alkyl substituents.

Scheme 1



Ambident anion of tetrazolotetrazine **6** could be represented as resonance structures **6a**—**d**. Methylation of an-

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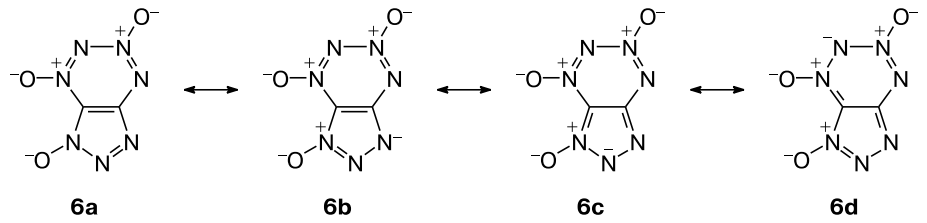
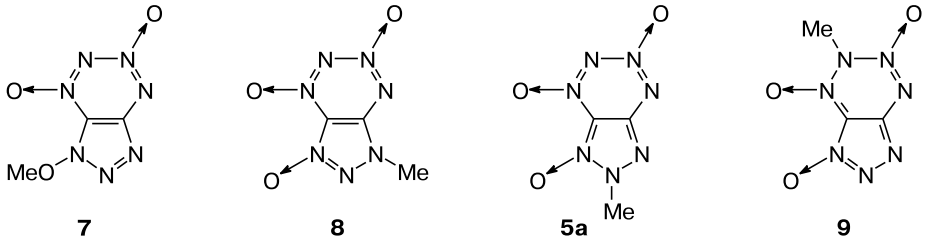


6a **6b** **6c** **6d**



7 **8** **5a** **9**

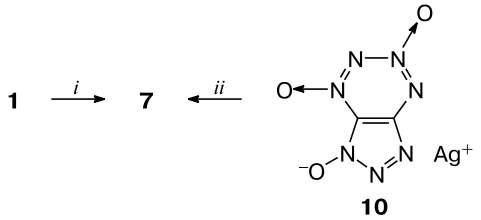
Compound	**5a**	**7**	**8**	**9**
ΔE_0/kcal mol^{-1}	1	14	0	15

ion **6** or its *H*-form **1** could result in the corresponding methyl derivatives **5a** and **7**—**9**.

The DFT calculations at B3LYP/6-311+G(d,2p) level of theory* of the total energies of methylated isomers **5a**, **7**—**9** in gas phase[4] predict *N*(3)-methylated structure **8** to be the most thermodynamically stable.

Nevertheless, methylation of triazolotetrazine **1** with diazomethane results in *O*-methylated derivative **7** (71%). Compound **7** is also the major product (85%) of the methylation of salt **10** with methyl iodide in anhydrous MeCN (Scheme 2). These results can be explained by the fact that the reaction proceeds under kinetic control.

Scheme 2

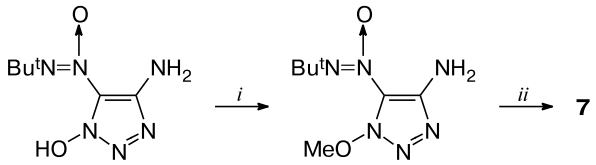


i. CH_2N_2, EtOAc. *ii*. MeI, MeCN.

The position of the methyl group of triazolotetrazine **7** is confirmed by NMR data. $^1H—^{13}C$ HMBC spectrum shows no spin-spin coupling between the methyl group protons and the ^{13}C atoms of the triazole cycle. This allows us to eliminate structure **8**. Structure **5a** is excluded by a comparison of the present spectrum with the NMR spectrum of the product obtained previously.[1]

The structure of compound **7** is also confirmed by the counter synthesis (Scheme 3). Methylation of 4-amino-5-(*tert*-butylazoxy)-1*H*-1,2,3-triazol-1-ol **2** leads predominantly to *O*-isomer **11** (position of the methyl group is confirmed by $^1H—^{13}C$ HMBC spectrum).[5] The reaction of compound **11** with a $HNO_3—H_2SO_4—Ac_2O$ mixture results in triazolotetrazine **7** in 62% yield.

Scheme 3



i. CH_2N_2, Et_2O, MeCN, yield of isomer **11** is 85%; *ii*. $HNO_3—H_2SO_4$ (1 : 2), Ac_2O, yield of triazolotetrazine **7** is 62%.

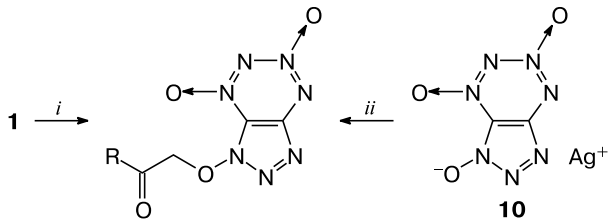
Compound **1** reacts with diazoacetone in anhydrous MeCN in the presence of $BF_3 \cdot Et_2O$ at the oxygen atom of the 1,2,3-triazole 1-oxide cycle to give product **12** (75%). Note that in the absence of $BF_3 \cdot Et_2O$ no reaction occurs (*cf.* Refs 6, 7). Bromoacetone and α-bromoacetophenone react with salt **10** similarly affording *O*-derivatives **12** and **13** in the yields of 83% and 60%, respectively (Scheme 4).

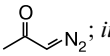
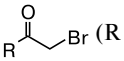
It is recently found[1] that triazolotetrazine **1** reacts with *tert*-butanol in a $CF_3CO_2H—H_2SO_4$ mixture to yield more thermodynamically stable isomer **14** (Scheme 5). This is due apparently to the reversibility of *tert*-butylation under the reaction conditions used.

Compound **1** reacts with methyl vinyl ketone in MeCN to give *N*(3)-substituted compound **15**; however, at room temperature the reaction is very slow. The reactions of this type involving *N*-heterocycles are often carried out in the presence of the strong bases (for example, Et_3N),[8,9] but

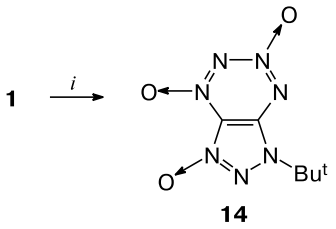
* Calculations were performed in the Computation Center of the Institute of Organic Chemistry RAS.

Scheme 4



i. $BF_3 \cdot Et_2O$,  ; *ii*.  (R = Me, Ph).

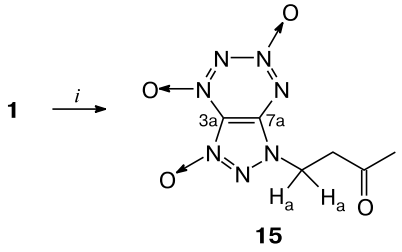
Scheme 5



i. Bu^tOH, CF_3CO_2H, H_2SO_4.

triazolotetrazine **15** does not form under these conditions. Though, it is found that addition of $BF_3 \cdot Et_2O$ noticeably accelerates the reaction (optimum amount is 0.5 equiv.), and the reaction completes within 1 h at room temperature affording compound **15** in a moderate yield (36%) (Scheme 6).

Scheme 6



i.  , $BF_3 \cdot Et_2O$, MeCN.

Position of a substituent in triazolotetrazine **15** is established by $^1H—^{13}C$ HMBC spectrum exhibiting spin-spin couplings between the H_a protons of the substituent and the C(7a) atom of the bicycle.

NMR spectra of the compounds synthesized. All signals in the ^1H and ^{13}C NMR spectra of the compounds synthesized are attributed (Table 1). The assignment is performed taking into account the significant broadening of the signal of the C atom directly bonded to the *N*-oxide fragment of the 1,2,3,4-tetrazine 1,3-dioxide cycle resulting from the spin-spin coupling of the ^{13}C and ^{14}N nuclei.

^{14}N NMR spectra (acetone-d_6) of compounds **7**, **12**—**15** (Table 2) exhibit the signals of the N(5) and N(7) of 1,2,3,4-tetrazine 1,3-dioxide in the range of δ −(40—60) ($\Delta\nu_{1/2}$ = 20—120 Hz). In the case of salt **10**, these signals (DMSO-d_6, δ −(40—60), $\Delta\nu_{1/2}$ = 155—325 Hz) are significantly broadened. In Tables 1 and 2, the NMR spectra of potassium salt **16** are given for a comparison.[1] It is worthy to note that the difference between chemical shifts

Table 1. ^1H and ^{13}C NMR spectra of compounds **1**, **7**, **10**, and **12**—**16** (δ, *J*/Hz)[a]

Compound	^{13}C			^1H (*J*/Hz)
	C(3a)	C(7a)[b]	R	
1[c]	149.8	119.9	—	—
7	153.2	121.6	71.1 (Me)	4.46 (Me)
10	149.3	120.3	—	—
12	153.6	122.3	26.7 ($CH_2C(O)\underline{Me}$) 84.6 ($H_2C(O)Me$) 200.5($CH_2\underline{C}(O)Me$)	2.15 (s, 3 H, Me) 5.48 (s, 2 H, CH_2)
13	153.6	122.4	83.3 ($\underline{C}H_2C(O)Ph$) 128.4, 129.5, 133.9, 135.0 ($CH_2C(O)\underline{Ph}$) 191.4 ($CH_2\underline{C}(O)Ph$)	6.33 (s, 2 H, CH_2) 7.55—7.62 (m, 3 H, Ph) 7.93—7.97 (m, 2 H, Ph)
14[c]	144.5	123.5	28.0 ($C\underline{Me}_3$) 65.6 ($\underline{C}Me_3$)	1.72 (s, 9 H, $C\underline{Me}_3$)
15	144.9	123.0	29.7 ($CH_2CH_2C(O)\underline{Me}$) 40.1($CH_2\underline{C}H_2C(O)Me$) 43.2($\underline{C}H_2CH_2C(O)Me$) 204.8($CH_2CH_2\underline{C}(O)Me$)	2.15 (s, 3 H, Me) 3.15 (t, 2 H, $CH_2C\underline{H}_2Ac$, *J* = 6.10) 4.52 (t, 2 H, $C\underline{H}_2CH_2Ac$, *J* = 6.10)
16[c]	148.9	119.9	—	—

[a] ^1H and ^{13}C NMR spectra of triazolotetrazines **1**, **10**, and **12**—**16** were recorded in DMSO-d_6, NMR spectra of triazolotetrazine **7** were obtained in acetone-d_6.

[b] The signals of the bridgehead C(7a) atom are broadened.

[c] See Ref. 1

of the N(5) and N(7) atoms for *O*- and *N*(3)-substituted triazolotetrazines is 18—20 ppm, while for *N*(2)-substituted compounds this difference is 12—13 ppm.[1] For *N*-substituted triazolotetrazines **14** and **15**, the signals of N(O) atoms of the 1,2,3-triazole 1-oxide cycle appear at about δ −80 ($\Delta\nu_{1/2} \approx 130$ Hz, acetone-d_6). In $^1H-^{15}N$ HSQC spectra, the N(1) atoms of the triazole cycle of the *O*-substituted derivatives **7** and **13** resonate in the range of δ −(115—120).

Thermal stability of triazolotetrazines is evaluated by the thermal behavior of the compounds upon heating on a Kofler melting point apparatus (Table 3). This method is not precise but allows drawing several preliminary conclusions.

It should be underlined that thermal stability of *H*-form **1** is similar to that of salts **10** and **16**. Apparently, temperature ~180—200 °C characterizes the stability of anionic heterocyclic system **6**, wherein the acidic proton of *H*-form **1** does not reduce the stability. *N*(2)-Alkylated derivatives **5a—c** also exhibit similar thermal stability (210—230 °C).[1]

Meanwhile, triazolotetrazines substituted at the O and N(3) atoms of the hydroxytriazole are less stable. Probably, the first step of the thermal decomposition of these compounds proceeds *via* cyclic intermediates involving the H atoms of the alkyl substituent (*cf.* Ref. 10) or involves the cleavage of the N—OR bond in the compounds **7**, **12**, and **13**, but not the destruction/decomposition of the tetrazine 1,3-dioxide cycle itself.

Table 2. ^{14}N ($\Delta\nu_{1/2}$/Hz) and ^{15}N (δ) NMR spectra of compounds **1**, **7**, **10**, and **12—16**[a]

Compound	^{14}N ($\Delta\nu_{1/2}$/Hz) (^{15}N (δ))		
	N(1)	N(5)	N(7)
1[b]	—	−42 (340)	−60 (130)
7	−117[c,d]	−41 (65)	−61 (35)
10	—	−45 (325)	−58 (155)
12	—	−41 (85)	−60 (30)
13	−120[c,e,f]	−41 (120)	−60 (40)
14[b]	−81 (130)	−40 (55)	−58 (20)
		−41 (185)[e]	−58 (90)[e]
15	−80 (130)	−37 (50)	−56 (25)
		−39 (300)[c]	−58 (120)[c]
16[b]	—	−43 (180)	−59 (45)

[a] If not stated otherwise, ^{14}N and ^{15}N NMR spectra of triazolotetrazines **1**, **7**, **12—15** were recorded in acetone-d_6. NMR spectra of compounds **10**, **16** were run in DMSO-d_6. The N(2) and N(3) atoms of compounds **14** and **15** resonate at δ −48 and −183, −204, respectively (assignment by $^1H-^{15}N$ HSQC NMR technique).
[b] See Ref. 1.
[c] The $^1H-^{15}N$ HSQC NMR data.
[d] The INEPT experiment data are following δ −116.4, $^3J_{N(1),Me} = 3.77$ Hz.
[e] In DMSO-d_6.
[f] The INEPT experiment data are following δ −119.6, $^3J_{N(1),CH_2} = 3.77$ Hz.

Table 3. Thermal stability of triazolotetrazines

Compound	R	M.p. (decomp.)
1	H	180—185
7	Me	155—159
10	Ag	197—198[a]
12	$CH_2C(O)Me$	136—138
13	$CH_2C(O)Ph$	133—139
14	Bu^t	176—178[b]
15	$CH_2CH_2C(O)Me$	158—164
16	K	192—193[a,b]

[a] Temperature of the beginning of decomposition without melting.
[b] See Ref. 1.

In summary, in the present work the alkylation of 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (**1**) is studied. It is found that the reactions of tetrazolotetrazine **1** with diazo compounds and Ag salt **10** with alkylhalides result predominantly in *O*-alkylation products, while triazolotetrazine **1** reacts with methyl vinyl ketone following the Michael-type reaction to give *N*(3)-substituted product.

Experimental

Caution! All compounds synthesized are sensitive to impact and friction and have to be handled as explosives.

^1H, ^{13}C, ^{14}N and ^{15}N NMR spectra were run on a Bruker DRX-500 spectrometer at working frequencies of 500.1, 125.8, 36.1, and 50.7 MHz, respectively. The chemical shifts are given relative to $SiMe_4$ (^1H, ^{13}C) or $MeNO_2$ (^{14}N, ^{15}N, external standard, high field chemical shifts are negative). Mass spectra (EI, 70 eV) were recorded on a Kratos MS-300 instrument. High resolution mass spectra (ESI) were obtained on a Bruker micrOTOF II mass spectrometer. The course of the reaction was monitored by TLC on Merck 60 F_{254} plates. Silica gel Merck 40—63 was used for the column chromatography. The melting points are given uncorrected. Solutions of diazomethane[11] and diazoacetone[12] in Et_2O were obtained as earlier described.

1-Hydroxy[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide silver salt (10). To a vigorously stirred solution of triazolotetrazine **1** (176 mg, 1.03 mmol) in H_2O (5 mL), $(NH_4)_2CO_3$ (49 mg, 0.515 mmol) was added at 25 °C. After 5 min stirring, a solution of $AgNO_3$ (352 mg, 2.06 mmol) in water (1 mL) was added by portions and the mixture was stirred for 5 min. The precipitate was collected using porous metal filter, washed with water (2×5 mL), and dried in desiccator over P_2O_5. Silver salt **10** was obtained in the yield of 210 mg (73%), red crystals. Compound **10** can also be obtained by direct addition of $AgNO_3$ to an aqueous solution of triazolotetrazine **1**; however, in this case, the yield does not exceed 50—55%. Found (%): C, 8.54; Ag, 38.80; N, 35.22. $C_2AgN_7O_3$. Calculated (%): C, 8.64; Ag, 38.81; N, 35.28.

1-Methoxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (7). *Caution! This compound is especially sensitive to impact and friction and has to be handled as primary explosive.* ***A.*** To a suspension of salt **10** (80 mg, 0.29 mmol) in anhydrous MeCN (1.5 mL), methyl iodide (205 mg, 1.44 mmol) was added and the reaction mixture was vigorously stirred for 1.5 h at 25 °C. The

precipitate was collected, washed with MeCN (2 mL), the solvent was removed *in vacuo*. Chromatography of the residue (elution with petroleum ether—AcOEt (3 : 1)) afforded *O*-methyl derivative **7** in the yield of 46 mg (85%), bright yellow crystals.

B. To a suspension of triazolotetrazine **1** (85 mg, 0.497 mmol) in EtOAc (8 mL), a solution of CH_2N_2 in Et_2O was added by portions until complete consumption of the starting compound **1** (TLC monitoring). The solvent was removed *in vacuo*. Purification of the residue by chromatography (silica gel, elution with petroleum ether—AcOEt (3 : 1)) afforded *O*-methyl derivative **7** in the yield of 65 mg (71%).

C. To a solution of 1-methoxy-1,2,3-triazole **11** (84 mg, 0.4 mmol) in Ac_2O (3 mL), a solution of HNO_3 (25 mg, 0.4 mmol, $d = 1.5$ g cm^{-3}) in Ac_2O (0.5 mL) and a solution of 93% H_2SO_4 (84 mg, 0.8 mmol, $d = 1.83$ g cm^{-3}) in Ac_2O (0.5 mL) were added at 10 °C. The reaction mixture was stirred for 1 h at 25 °C, poured into ice-water (15 g), and additionally stirred for 30 min. The mixture was extracted with $CHCl_3$ (5×15 mL), the organic layer was dried with $MgSO_4$, the solvent was removed *in vacuo*. Purification of the residue by chromatography (silica gel, elution with petroleum ether—AcOEt (3 : 1)) afforded *O*-methyl derivative **7** in the yield of 45 mg (62%). MS (ESI): found *m/z* 208.0186 $[M + Na]^+$; $C_6H_7N_7O_4$; calculated *m/z* 208.0190 $[M + Na]^+$.

1-[(5,7-Dioxido-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazin-1-yl)oxy]acetone (12). ***A.*** To a solution of triazolotetrazine **1** (610 mg, 3.57 mmol) in anhydrous MeCN (20 mL), a solution of diazoacetone (~two-fold excess) was added at 25 °C. Then, $BF_3 \cdot Et_2O$ (329 mg, 2.32 mmol) was added dropwise with stirring until the complete consumption of the starting triazolotetrazine **1** (TLC monitoring) and changing the color of the reaction mixture from red to yellow. After 10 min stirring, ~70% of the solvent was removed *in vacuo*, silica gel was added, and the solvent was removed to dryness. Chromatography (silica gel, successive elution with petroleum ether—AcOEt, 3 : 1, 2 : 1, 1 : 1) afforded compound **12** in the yield of 610 mg (75%), yellow crystals.

B. To a stirred suspension of salt **10** (210 mg, 0.760 mmol) in MeCN (5 mL), bromoacetone (0.318 mL, 520 mg, 3.80 mmol) was added at 25 °C. After 5 h stirring, AgBr was filtered off and washed with MeCN (3×5 mL). To the filtrate, slica gel was added and the solvent was removed *in vacuo*. Purification of the residue by chromatography (silica gel, successive elution with petroleum ether—AcOEt 3 : 1, 2 : 1, 1 : 1) afforded compound **12** in the yield of 143 mg (83%). MS (ESI): found *m/z* 250.0285 $[M + Na]^+$; $C_5H_5N_7O_4$; calculated *m/z* 250.0295 $[M + Na]^+$.

1-[(5,7-Dioxido-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazin-1-yl)oxy]-1-phenylethanone (13). To a stirred suspension of salt **10** (241 mg, 0.87 mmol) in MeCN (5 mL), α-bromoacetophenone (429 mg, 2.17 mmol) was added at 25 °C. After 5 h stirring, AgBr was filtered off and washed with MeCN (3×5 mL). Silica gel was added to the filtrate and the solvent was removed *in vacuo*. The product was isolated by silica gel column chromatography. First, excess of ketone was eluted with petroleum ether—AcOEt (10 : 1, 120 mL); then, the product **13** was isolated by successive elution with petroleum ether—AcOEt, 3 : 1, 2 : 1, 1 : 1. Compound **13** was obtained in the yield of 150 mg (60%), yellow crystals. MS (ESI): found *m/z* 312.0454 $[M + Na]^+$; $C_{10}H_7N_7O_4$; calculated *m/z* 312.0452 $[M + Na]^+$.

4-(3,4,6-Trioxido-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazin-1-yl)butan-2-one (15). To a vigorously stirred solution of triazolotetrazine **1** (200 mg, 1.17 mmol) in anhydrous MeCN (4 mL), methyl vinyl ketone (410 mg, 4.88 mmol) was added at 25 °C followed by dropwise addition of $BF_3 \cdot Et_2O$ (83 mg, 0.585 mmol). After 1 h stirring, silica gel was added and the solvent was removed *in vacuo*. Purification of the residue by column chromatography (silica gel, elution with petroleum ether—AcOEt, 1 : 1) afforded compound **15** in the yield of 95 mg (34%), orange crystals. MS (ESI): found *m/z* 264.0452 $[M + Na]^+$; $C_6H_7N_7O_4$; calculated *m/z* 264.0452 $[M + Na]^+$.

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