

## Synthesis of N-quinonyltaurines

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**Summary.** Both 1,4-benzoquinones and 1,4-naphthoquinones were attached to the non-proteinogenic amino acid taurine to form N-quinonyl taurine derivatives. The products were formed via the direct Michael-like addition or by substitution of a good leaving group. An attempt to bridge the two moieties via an ureido spacer resulted in the formation of a bis-quinonylamino isocyanurate derivative. Preliminary MO calculations provided internal ground-state geometries and orbital coefficients of the HOMO levels in two representing taurine conjugates.

**Keywords:** Amino acids – Taurine – Quinones – Isocyanates – Isocyanurate

### Introduction

Taurine ( $\beta$ -aminoethanesulphonic acid) is a widespread naturally occurring non-proteinogenic amino acid, biosynthesized from methionine and cysteine, in conjunction with vitamin B6 (Hayes and Sturman, 1981). It is abundantly distributed in the human body in its free form and can be found in high concentrations in the brain, in the heart, in skeletal muscles and also in the central nervous system. Taurine plays a vital role in many physiological events, such as osmoregulation, anti-oxidation, detoxification (Huxtable, 1992), membrane stabilization (Gaul and Rassin, 1979), neuromodulation (Barbeau et al., 1975; Kuriyama, 1980), retinal and cardiac functions (Wright et al., 1986) and brain development (Sturman et al., 1977). Taurine has also been implicated in the immune and inflammatory responses through its antioxidant ability as well as through its capacity to modulate myeloperoxidase activity and antimicrobial function in leucocytes (Gordon et al., 1986; Masuda et al., 1986; McLoughlin et al., 1991; Watson et al., 1994).

Taurine has various pharmacological properties. For example, taurine is an inhibitory neurotransmitter, and it may be used as a mild sedative in the treatment of epilepsy and other excitable brain states (Hajek et al., 1997; Anyanwu and Harding, 1993). Taurine was also suggested as an immune suppressor, by sparing L-cysteine, in visual problems and eye disease (Imaki and Sturman, 1995), in cases of cirrhosis and liver failure (Invernizzi et al., 1999), depression (Scheller et al., 2000), in cases of male infertility due to low sperm motility (Hamamah et al., 1999), and as a supplement for newborns and new mothers (Shambaugh, 1998). Taurine plays also a very important role in maintaining the correct composition of bile and solubility of cholesterol (Hayes and Trautwein, 1989; Ryan, 1989). It has been found to have an effect on blood sugar levels similar to that of insulin (Silaeva et al., 1976), and its supplements have been shown to lower blood pressure (Azuma et al., 1992).

As part of a program to synthesize and study N-quinonyl amino acids and N-quinonyl peptides, we have prepared a library of novel quinonic compounds in the last few years. Thus, 1,4-naphthoquinone, 2-chloro-1,4-naphthoquinone, 2-bromo-1,4-naphthoquinone, 3-methyl-1,4-naphthoquinone and 2-phenylthio-1,4-benzoquinone were linked to a variety of proteinic as well as non-proteinic amino acids (Bade Shrestha-Dawadi et al., 1996; Gorohovsky and Bittner, 2001; Alnabary and Bittner, 2000; Bittner et al., 2001; Bittner et al., 2002) have been synthesized. Their electrochemical and EPR properties were also studied (Rahimipour et al., 1996; 1998; Bittner et al., 2000a; Bittner et al., 2001). In this context, and because p-quinones are capable of binding covalently

to a variety of biologically active molecules leading to immobilization of systems and to generation of reactive oxygen species (ROS) (Powis, 1989), it can be expected that new quinone-aurine conjugates would have significant biological behaviour e.g. anti-cancer and anti-malarial activities.

In this paper, the synthesis of the novel N-quinonyl taurines, their spectral analysis, as well as ground state geometries calculations of few representatives, are presented. The redox properties and semiquinone anion-radical formation by the naphthoquinonyl derivatives of taurine, studied by EPR techniques, were previously described by us (Bittner et al., 2000a).

## Materials and methods

IR spectra were recorded on a Nicolet 5ZDX FT-IR spectrophotometer for KBr pellets. UV-Vis spectra were measured on a UV-Vis Jasco V-560 spectrophotometer  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  spectra were recorded on a Bruker WP 200 or 500 SY spectrometer for solutions in  $\text{d}_6\text{-DMSO}$  and against TMS as internal standard. Mass spectra (CI in methane) were obtained on a Finnigan 4020 quadrupole spectrometer. The correct elemental composition was proved by high resolution mass spectrometry (HRMS), which was performed on High Resolution Magnetic Sector Mass Spectrometer VG Fison's AutoSpec. For some taurine derivatives, only MS-FAB experiment was performed. Melting points were determined using a Thomas-Hoover capillary apparatus and are uncorrected. All starting materials, reagents and solvents were of commercial quality and used as received. 2-Phenylthio-1,4-benzoquinone was synthesized according to the procedure of Dimroth (Dimroth et al., 1940). Most compounds were purified by gravity column chromatography on silica gel (70–230 mesh). Density functional calculations were carried out with the MacSPARTAN PRO Semi-Empirical Program, while standard RHF/AM1 basis set was chosen. During geometry optimization, no symmetry constraints were applied.

### Synthesis

#### 2-(1,4-Dioxo-1,4-dihydro-naphthalen-2-ylamino)-ethanesulfonic acid (**1**)

A solution of taurine (0.6 g, 5 mmol) in water (20 ml) was added dropwise to a heated solution of 1,4-naphthoquinone (1.5 g, 10 mmol) in EtOH (100 ml, 95%). The reaction mixture was refluxed for 3 h, cooled to room temperature and the solvent removed under reduced pressure. The orange product was purified by silica gel column chromatography using  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (9:1) as eluent to yield 0.56 g (40%) melting at 285–287°C.

$^1\text{H-NMR}$  ( $\text{d}_6\text{-DMSO}$ )  $\delta$  (ppm) (J (Hz)): 7.95 (d, 1H, 7.6), 7.92 (d, 1H, 7.6), 7.81 (t, 1H, 7.4), 7.71 (t, 1H, 7.5), 7.74 (t, NH, 5.3), 5.62 (s, 1H), 3.36–3.39 (m, 2H), 2.74 (t, 2H, 6.6).

IR (KBr)  $\nu$  ( $\text{cm}^{-1}$ ): 3455, 3355, 1696, 1635.

UV-Vis (MeOH)  $\lambda_{\text{max}}$  (nm), (log  $\epsilon$ ): 222 (3.77), 270 (3.84), 332 (2.94), 446 (3.04).

HRMS (DCI/ $\text{CH}_4$ ) (m/z): 281.033394 ([M] $^+$ , calcd. 281.035794 for  $\text{C}_{12}\text{H}_{11}\text{NO}_5\text{S}$ ), 200, 174.

#### 2-(3-Chloro-1,4-dioxo-1,4-dihydro-naphthalen-2-ylamino)-ethanesulfonic acid (**2**)

A solution of taurine (3.75 g, 30 mmol) in 1N solution of KOH (30 ml) was added dropwise to a suspension of 2,3-dichloro-1,4-naphthoquinone (2.27 g, 10 mmol) in methanol (150 ml). The mixture was stirred at room temperature for 24 h, then acidified with 10% HCl to pH = 1.5. The solvents were evaporated under reduced pressure and the red crude product was purified using silica gel column chromatography and eluted with a mixture of  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (1:1). Yield: 2.96 g (94%). M.p. = 268–270°C.

$^1\text{H-NMR}$  ( $\text{d}_6\text{-DMSO}$ )  $\delta$  (ppm) (J (Hz)): 7.95 (dd, 2H, 6.9, 1.6), 7.89 (br s, NH), 7.69–7.86 (m, 2H), 4.01–4.09 (m, 2H), 2.78 (t, 2H, 6.3).

IR (KBr)  $\nu$  ( $\text{cm}^{-1}$ ): 3353, 3220, 1683, 1637.

UV-Vis (MeOH)  $\lambda_{\text{max}}$  (nm), (log  $\epsilon$ ): 238 (4.21), 274 (4.46), 468 (3.63).

HRMS (DCI/ $\text{CH}_4$ ) (m/z): 315.996918 ([MH] $^+$ , calcd. 316.004647 for  $\text{C}_{12}\text{H}_{11}\text{NO}_5\text{SCl}$ ), 280, 268, 230.

#### 2-(5-Phenylthio-1,4-dioxo-1,4-dihydro-benzene-2-ylamino)-ethanesulfonic acid (**3**)

This compound has been synthesized previously (Bittner et al., 2000). Some of its spectroscopic properties are shown below:

$^1\text{H-NMR}$  ( $\text{d}_6\text{-DMSO}$ )  $\delta$  (ppm) (J (Hz)): 7.78 (t, NH, 5.4), 7.57 (s, 5H), 5.43 (s, 1H), 5.42 (s, 1H), 3.30–3.32 (m, 2H), 2.68 (t, 2H, 6.6).

IR (KBr)  $\nu$  ( $\text{cm}^{-1}$ ): 3442, 3368, 1660, 1631, 1603.

UV-Vis (MeOH)  $\lambda_{\text{max}}$  (nm), (log  $\epsilon$ ): 222 (4.24), 360 (3.98), 516 (2.71).

MS (FAB) (m/z): 337.99 [M-H] $^-$ , 190.

#### 2-(3-Chloro-6,7-dicyano-1,4-dioxo-1,4-dihydro-benzene-2-ylamino)-ethanesulfonic acid (**4**)

A solution of taurine (3.75 g, 30 mmol) in 1N KOH (30 ml) was added to a suspension of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (2.27 g, 10 mmol) in methanol (50 ml). The mixture was stirred at room temperature for 24 h, then acidified with 10% HCl to pH = 1.5. The precipitated deep red crude product was purified using silica gel column chromatography with MeOH as eluent. Yield: 3.04 g (96%). M.p. = 245–247°C.

$^1\text{H-NMR}$  ( $\text{D}_2\text{O}$ )  $\delta$  (ppm) (J (Hz)): 3.29 (m, 2H), 3.06 (t, 6.5).

$^{13}\text{C-NMR}$  ( $\text{D}_2\text{O}$ )  $\delta$  (ppm): 180.0 (C=O), 170.4 (C=O), 167.9, 154.5, 117.4 (CN), 110.1 (CN), 103.2, 47.3, 35.3.

IR (KBr)  $\nu$  ( $\text{cm}^{-1}$ ): 3462, 3220, 2230 (CN), 2213 (CN), 1629.

UV-Vis ( $\text{H}_2\text{O}$ )  $\lambda_{\text{max}}$  (nm), (log  $\epsilon$ ): 212 (3.54), 266 (3.37), 338 (3.69), 516 (2.58).

MS (FAB $^-$ ) (m/z): 315.18 [M] $^-$ , 275, 241.

#### 2-(3-Bromo-1,4-dioxo-1,4-dihydro-naphthalen-2-ylamino)-ethanesulfonic acid (**5**)

A solution of taurine (3.75 g, 30 mmol) in 1N KOH (30 ml) was added dropwise to a suspension of 2,3-dibromo-1,4-naphthoquinone (3.15 g, 10 mmol) in methanol (150 ml). The mixture was stirred at room temperature for 24 h, then acidified with 10% HCl to pH = 1.5. The solvents were evaporated under reduced pressure and the red crude product was purified on silica gel column eluting with a mixture of  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (1:1). Recrystallization from  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  gave the pure product as red needles. 2.70 g (75%). M.p. > 240°C (decomp.).

$^1\text{H-NMR}$  ( $\text{d}_6\text{-DMSO}$ )  $\delta$  (ppm) (J (Hz)): 7.90–7.95 (m, 2H), 7.67–7.84 (m, 2H of the aromatic ring and the amidic H), 4.04 (m, 2H), 2.79 (t, 2H, 6.1).

IR (KBr)  $\nu$  ( $\text{cm}^{-1}$ ): 3516, 3301, 1689, 1655.

UV-Vis (MeOH)  $\lambda_{\max}$  (nm), (log  $\epsilon$ ): 236 (4.15), 274 (4.39), 334 (3.30), 466 (3.57).

HRMS (DCI/CH<sub>4</sub>) (m/z): 381.219790 ([M + H]<sup>+</sup>·H<sub>2</sub>O, (some sulfonic acid derivatives has the tendency to form as the monohydrate) calcd. 381.220640 for C<sub>12</sub>H<sub>15</sub>NO<sub>6</sub>SBr), 338, 320, 292, 224.

2-((3-[1,4-Dioxo-3-(2-sulfoethylamino)-1,4-dihydronaphthalen-2-yl]-2,4,6-trioxo-1,3,5-triazinan-1-yl)-1,4-dioxo-1,4-dihydronaphthalen-2-ylamino)ethanesulfonic acid (**6**)

2,3-Dichloro-1,4-naphthoquinone (2.27 g, 10 mmol) was added to a suspension of sodium isocyanate (1.2 g, 15 mmol) in dry (CaH<sub>2</sub>) dimethylformamide (40 ml). The mixture was purged with dry N<sub>2</sub> and stirred at room temperature for 24 h under a slow stream of nitrogen. To the solution, taurine (2.5 g, 20 mmol) in dimethylformamide (10 ml) was added and the mixture was further stirred at room temperature for 48 h. The solvent was evaporated under reduced pressure and an excess of water (100 ml) was added. Undissolved material was filtered off and the filtrate was evaporated under reduced pressure. The crude was purified using silica gel column chromatography and CH<sub>2</sub>Cl<sub>2</sub>/MeOH (9:1) as eluent. Yield: 1.18 g, (34%). M.p. > 270°C (decomp.).

<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO)  $\delta$  (ppm) (J (Hz)): 8.25 (br s, 2H), 8.01 (t, 4H, 8.0), 7.88 (td, 2H, 7.30, 1.40), 7.77 (td, 2H, 7.4, 1.7), 3.44–3.55 (m, 4H), 2.73 (t, 4H, 5.8). The imidic hydrogen and the two sulfonic-acids hydrogens were not observed.

IR (KBr)  $\nu$  (cm<sup>-1</sup>): 3451, 3281, 1731, 1702, 1687.

UV-Vis (MeOH)  $\lambda_{\max}$  (nm), (log  $\epsilon$ ): 222 (3.85), 266 (3.95), 328 (3.03), 432 (3.14).

MS (FAB<sup>-</sup>) (m/z): [M-H]<sup>-</sup>: 686.18, 578, 343, 322, 305, 255, 213.

## Results and discussion

### a. Synthesis of N-quinonyltaurines

Several modified quinones were prepared, bearing each a  $\beta$ -aminoethane sulphonic acid (taurine) attached directly via its amino group (see Figure 1). The various quinones used differ in their reduction potentials. The phenylthio-benzoquinone (**3**) is a relatively low oxidizer, the naphthoquinone (**1**) has an average potential, while the chloro or bromo-derivatives (**2** and **5**) are stronger and the chlorodicyano derivative (**4**) is the strongest oxidizing quinone.

The N-naphthoquinonyltaurine (**1**) and the N-phenylthiobenzoquinonyltaurine (**3**) have been synthesized via a direct reductive 1,4-Michael-type addition of the  $\beta$ -amino group to the appropriate quinone. In the first stage, the reduced product (the hydroquinonic form) is obtained. However, a spontaneous redox process occurs using a second equivalent of the starting quinone and yielding the end product, namely the N-quinonyltaurine (Bittner et al., 2000a; 2001). This process is feasible due to the higher oxidation potential of the starting quinone as compared to its amino derivative. Other organic or

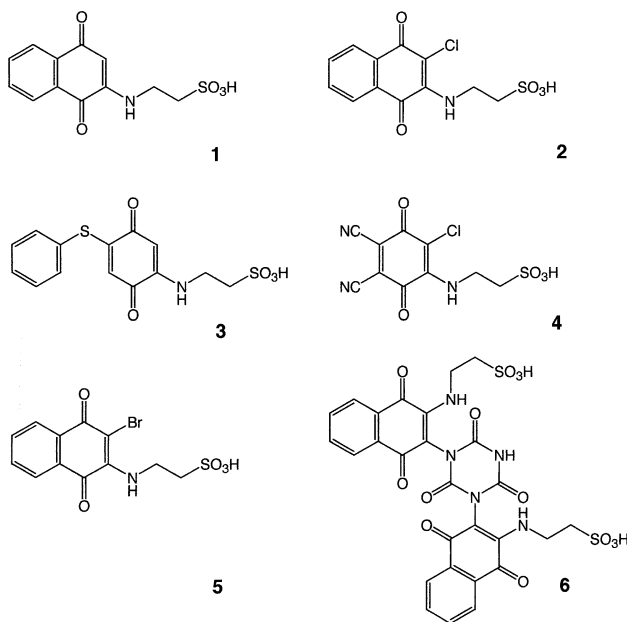
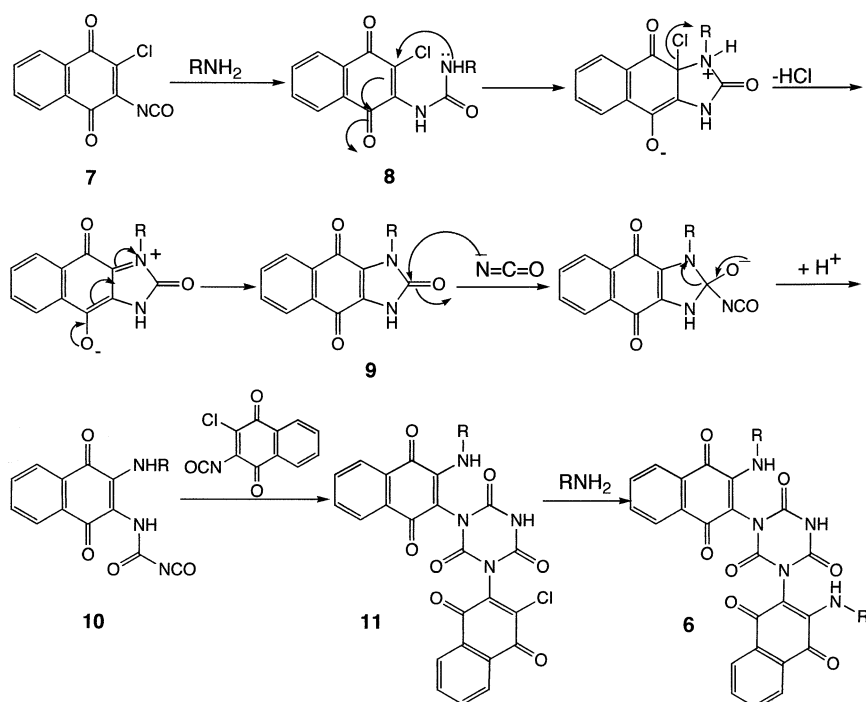


Fig. 1. N-Quinonyltaurines

inorganic oxidizing agents as well as oxygen itself can also transfer the reduced form to the quinonic end products. In the present case, low to average yields (25–45%) were obtained as compared to reactions with haloquinones and also as compared to analogous reactions with  $\beta$ -aminocarboxylic acid e.g. with  $\beta$ -alanine (Bittner et al., 2001). It is well documented that the basicity of  $\beta$ -alanine ( $pK_{a2}$  = 10.19) is higher than the basicity of taurine ( $pK_{a2}$  = 8.74). The lower basicity of taurine is reflected by its nucleophilic nature and in comparable conditions, its reaction with the quinone is retarded.

A somewhat different route led to the preparation of the halogenated N-quinonyltaurines (**2**, **4** and **5**) (see Fig. 1). In these cases, the taurine reacts with 2,3-dichloro-1,4-naphthoquinone, 2,3-dibromo-1,4-naphthoquinone or 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ). Schematically, the reaction resembles a substitution process, displacing one of the halogen atoms and eliminating HCl or HBr. In these cases hydroquinones are not formed, thus no redox follow-up is required, and only one equivalent of the starting dihaloquinone is needed. Contrary to the reaction with the “naked” quinones, the process with dihaloquinones gave high yields, up to 96% in the reaction with DDQ. It seems that substituting the quinonic ring with halogens enhances its electrophilicity and facilitates the reaction (even with the weak nucleophilic  $\beta$ -amino group of taurine).



**Scheme 1.** Synthesis of bis-(2,2'-taurino-1,1',4,4'-naphthoquinon-3,3'-diyl)isocyanurate

In a former paper, we showed that reactive quinonyl isocyanates can be successfully used as intermediates in the preparation of quinonyl-carbamates, quinonyl-ureas and quinonyl-isocyanurates (Bittner et al., 2000a,b). This methodology seemed to open a route to facile construction of new quinonyl-taurines where the two moieties are bridged via a ureido spacer. Reaction of 2,3-dichloronaphthoquinone with sodium or potassium isocyanate proceeded smoothly, probably via Michael-type addition and yielded the quinonyl-isocyanate **7** (see Scheme 1). The following reaction with taurine, was accomplished in the same pot, without prior isolation of the quinonyl-isocyanate. Work-up of the reaction mixture gave, as the main product (33%), compound **6**, a cyanurate spacing between two naphthoquinonyl moieties, both bearing a taurine residue attached via an amino group.

It seems that the quinonylisocyanate reacted as expected with the primary amino group of taurine, yielding the ureido derivative **8**. However, under the reaction conditions, compound **8** spontaneously reacted further. The substituted ureidic nitrogen proved nucleophilic enough to substitute the second chlorine on the quinonic ring to form the five-membered heterocyclic structure **9**. The presence of an excess of isocyanate anions in the solution induces the attack of the ureidic carbonyl, followed by

reopening of the ring and formation of the N-acylisocyanate **10**. The subsequent reaction of **10** with the starting isocyanate **7** provided the bis-quinonyl isocyanurate **11**, to which a second taurine residue was further linked to yield the end product **6**.

#### *b. Calculated optimum geometry of 1 and 6*

The determination of possible conformations of promising pharmaceutical candidates is of vital importance in the analysis of drugs as well as in interpretation of their mode of action. In order to provide a preliminary picture of the geometry and electronic configuration of N-quinonyl-taurines, we calculated the internal ground-state geometry and the orbital coefficients of the HOMO levels for N-(1,4-naphthoquinone-2-yl)taurine (**1**) and for bis-(2,2'-taurino-1,1',4,4'-naphthoquinon-3,3'-diyl)isocyanurate (**6**). The MO calculations were made using McSpartan PRO semi-empirical program.

The calculated structures are shown in Figure 2 and 3. It can be seen that, in compound **1**, the HOMO orbitals are distributed along the quinonic side to which the NH group is attached. This NH group presents a vinylogous amide character, resulting in a high degree of conjugation between the lone pair of the nitrogen atom (N1) and the quinonic  $\alpha,\beta$ -

unsaturated system (C2—C3—C4—O2). A different distribution was obtained for compound **6**. In the later case, the calculated HOMO shows a relatively high electron density along the region of the taurinic NH groups (N1 and N5), but the cyanuric nitrogens (N2

and N4) participate in the total  $\pi$ -delocalization as well. Having an imidic character, the contributions of the cyanuric nitrogens are relatively smaller.

In Table 1, the calculated bond lengths of 2-aurino-1,4-naphthoquinone are compared with the crystallographic data of 2-amino-1,4-naphthoquinone (Gaultier and Hauw, 1969). It can be seen that the conjugated C=O bond C4—O2 are longer (1.224 Å, and 1.238 Å) in both molecules, as compared with the nonconjugated C=O bonds C1—O1 (1.208 Å and 1.226 Å). The C2—N1 bond in the taurine derivative is somewhat longer (1.387 Å) than in the amino-substituted naphthoquinone (1.360 Å), which is reasonably due to the substitution effect. The other bond lengths differ only slightly from that measured in other amino-substituted naphthoquinones (e.g.  $\beta$ -alanyl derivative), which implies that the sulfonic group has only minor effect. The calculated distance N1—H...O1=C1 was found to be 2.77 Å, which indicates a strong intramolecular hydrogen bond between the carbonyl and amino groups.

The calculated bond lengths of bis-(2,2'-taurino-1,1',4,4'-naphthoquinon-3,3'-yl)isocyanurate (**6**) are given in Table 2. All the quinonic carbonyls have almost the same calculated bond lengths (about 1.235 Å) which proves that they participate in  $\pi$ -delocalization with a lone nitrogen. The isocyanurate carbonyls, having an imidic character, are longer (around 1.242 Å). It seems that structural constraints in this complex molecule inhibits formation of hydrogen bonds between the taurinic NH and the quinonic carbonyl. However, weak hydrogen bonds can be noticed between N5—H (see Fig. 3) and the isocyanurate C14=O7 bond (the N5...O7 distance is 2.90 Å) and also between N5—H and the S2=O12 (N5...O12 = 2.98 Å).

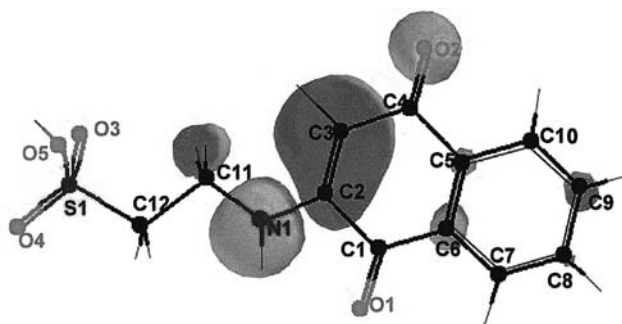


Fig. 2. Highest occupied molecular orbital for N-(1,4-naphthoquinon-2-yl)taurine

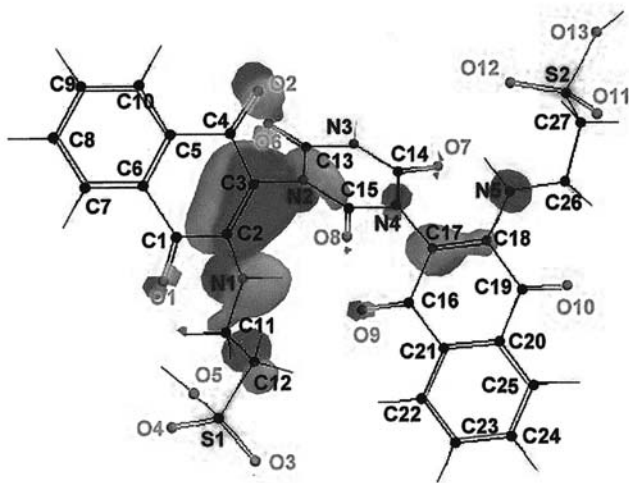


Fig. 3. Highest occupied molecular orbital for bis-(2,2'-taurino-1,1',4,4'-naphthoquinon-3,3'-diyl)isocyanurate

Table 1. Bond lengths (Å) of 2-amino-1,4-naphthoquinone and N-(1,4-naphthoquinon-2-yl)taurine

2-Amino-1,4-naphthoquinone		N-(1,4-naphthoquinon-2-yl)taurine	
C1—C2	1.487	C1—C2	1.509
C2—C3	1.349	C2—C3	1.361
C3—C4	1.448	C3—C4	1.461
C4—C5	1.485	C4—C5	1.482
C5—C6	1.385	C5—C6	1.405
C6—C1	1.486	C6—C1	1.473
C1—O1	1.208	C1—O1	1.226
C4—O2	1.224	C4—O2	1.238
C2—N1	1.360	C2—N1	1.387
		N1—C11	1.441
		C11—C12	1.525
		C12—S1	1.695
		S1—O3	1.373
		S1—O4	1.368
		S1—O5	1.652

**Table 2.** Bond lengths (Å) of bis-(2,2'-taurino-1,1',4,4'-naphthoquinon-3,3'-diyl)isocyanurate

<b>C1—C2</b>	1.510	<b>C11—C12</b>	1.528	<b>N4—C14</b>	1.423	<b>C21—C16</b>	1.482
<b>C2—C3</b>	1.388	<b>C12—S1</b>	1.694	<b>N4—C15</b>	1.427	<b>C16—O9</b>	1.241
<b>C3—C4</b>	1.484	<b>S1—O3</b>	1.375	<b>C13—O6</b>	1.241	<b>C19—O10</b>	1.234
<b>C4—C5</b>	1.480	<b>S1—O4</b>	1.374	<b>C14—O7</b>	1.246	<b>C18—N5</b>	1.375
<b>C5—C6</b>	1.403	<b>S1—O5</b>	1.644	<b>C15—O8</b>	1.241	<b>N5—C26</b>	1.449
<b>C6—C1</b>	1.471	<b>C3—N2</b>	1.423	<b>N4—C17</b>	1.467	<b>C26—C27</b>	1.525
<b>C1—O1</b>	1.235	<b>N2—C13</b>	1.410	<b>C17—C18</b>	1.388	<b>C27—S2</b>	1.696
<b>C4—O2</b>	1.234	<b>C15—N2</b>	1.421	<b>C18—C19</b>	1.512	<b>S2—O11</b>	1.369
<b>C2—N1</b>	1.378	<b>N3—C13</b>	1.403	<b>C19—C20</b>	1.471	<b>S2—O12</b>	1.372
<b>N1—C11</b>	1.439	<b>C14—N3</b>	1.400	<b>C20—C21</b>	1.402	<b>S2—O10</b>	1.654

## Conclusions

Six conjugates of  $\beta$ -aminoethane sulphonic acid (taurine) with different types of p-quinones were synthesized. With the most reactive 2,3-dichloro-1,4-naphthoquinone, 2,3-dibromo-1,4-naphthoquinone and DDQ, only one equivalent of the quinone was required to obtain high yields of conjugates. With the less reactive 1,4-naphthoquinone and 2-phenylthio-1,4-benzoquinone, two equivalents of the quinone were needed and only low to average yields were obtained. An attempt to build new quinonyltaurines where the two moieties are bridged via a ureido spacer, resulted in the formation of a cyanurate spacing between two naphthoquinonyl moieties (each quinone bearing a taurine residue linked to its amino group). Preliminary, MO calculations provided internal ground-state geometries and orbital coefficients of the HOMO levels in two representing conjugates. It is expected that this novel taurines related to redox active molecules will exhibit interesting biological and pharmacological properties.

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