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DERIVATIVES OF ARBORINE [1-METHYL-2-(PHENYLMETHYL)-4(1H)-QUINAZOLINONE]

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A method has been developed for the reaction of 2-cyanomethylbenzoic acid with N-methylanthranilic acid to give 2-[(1-methyl-4-oxo-1,4-dihydro-2-quinazolin-2-yl)methyl]benzoic acid, its esters were synthesized. The spectroscopic chracteristics of the isomeric compounds have been studied and compared in solution and in the solid state.

Keywords: 2-methylaminobenzoic acid, 2-cyanomethylbenzoic acid, 2-[(1-methyl-4-oxo-1,3-dihydro-quinazolin-2-yl)methyl]benzoic acid, X-ray structural analysis.

The alkaloid arborine was separated in 1951 from the plant *Glycosmis arborea* growing in India and its structure as 1-methyl-2-(phenylmethyl)-4(1H)-quinazolinone was established in 1961 [1]. The *Glycosmis arborea* preparations are used in the ayurvedic system of medicine as antipyretic and anthelmintic agents. Many arborine derivatives substituted at position 1 show high biological activity [2, 3].

We have previously proposed a method [4] for the synthesis of 2-[(4-oxo-3,4-dihydroquinazolin-2-yl)methyl]benzoic acid (**1a**) as a structural analog of the alkaloid glycosminine resulting from the condensation of 2-cyanomethylbenzoic (**2**) and anthranilic acids.

Continuing our work in this area we have studied the condensation of acid **2** with N-methylanthranilic acid (**3**). The reaction occurs upon heating equimolar amounts of the components in dioxane over 6 h to give 2-(4-oxo-1-methyl-1,4-dihydro-2-quinazolinylmethyl)benzoic acid (**4a**) in good yield. The structure of its ester **4c** has been shown using X-ray structural analysis (Figure 1). An interesting feature of this compound is the marked nonplanarity of the pyrimidine ring and this is likely due to crystal packing effects (shortened intermolecular contacts $C_{(1)}\cdots H_{(10b')}$ (0.5-*x*, -0.5+*y*, *z*) 2.69 and $C_{(9)}\cdots C_{(15')}$ (0.5-*x*, 0.5+*y*, *z*) 3.39 Å where the sums of the van der Waal radii are 2.87 and 3.42 Å respectively [5]). The maximal values of the endocyclic torsional angles are $C_{(2)}$–$C_{(1)}$–$N_{(1)}$–$C_{(8)}$ -6.3(5) and $N_{(1)}$–$C_{(8)}$–$N_{(2)}$–$C_{(7)}$ 6.3(5)º.

Such a disturbance to the heterocycle planarity is evidence of high conformational flexibility in similar dihydroaromatic rings [6, 7] and this allows the molecule to change its geometry sufficiently easy when steric strain arises.

The benzene ring $C_{(11)}\cdots C_{(16)}$ is orientated almost perpendicularly to the mean plane of the quinazoline fragment (torsional angle $C_{(8)}$–$C_{(10)}$–$C_{(11)}$–$C_{(16)}$ -79.2(4)º). The ester substituent lies in the plane of the benzene

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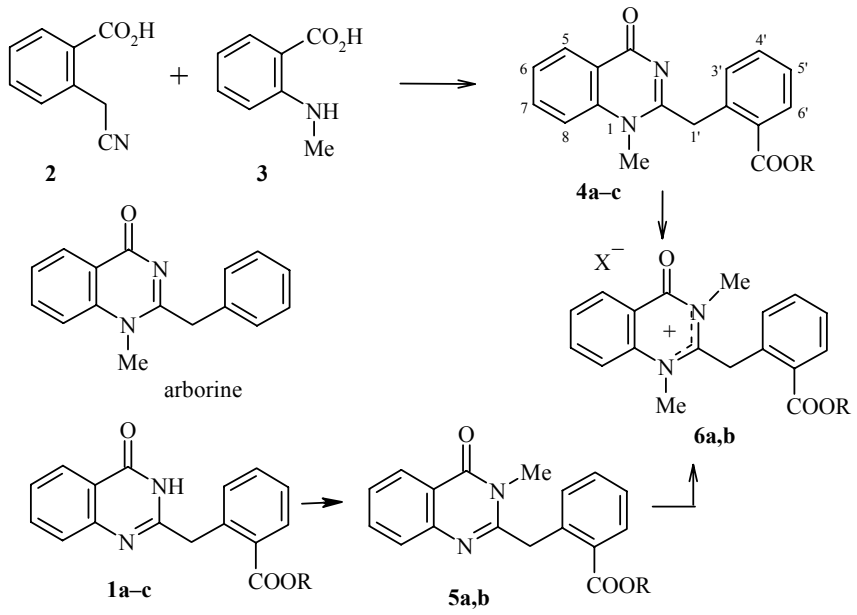
ring (torsional angles $C_{(15)}$–$C_{(16)}$–$C_{(17)}$–$O_{(3)}$ 1.5(4) and $C_{(17)}$–$O_{(3)}$–$C_{(18)}$–$C_{(19)}$ 178.8(3)º). This substituent orientation is also stabilized by the formation of attractive intramolecular shortened contacts $O_{(2)}\cdots H_{10a)}$ 2.29 and $O_{(3)}\cdots H_{(15)}$ 2.31 Å (sum of van der Waal radii 2.45 Å).

A feature of the IR spectrum of acid **4a** is the lowered carbonyl group stretching frequency for the COOH group at 1685 cm^{-1}, due to the intramolecular hydrogen bond involving the nitrogen atom of the quinazolone ring. For the same reason an even lower frequency (1670 cm^{-1}) was seen by us in acid **1a**. Compound **4a** behaves as a conventional amino acid and shows amphoteric properties, being soluble in 2N HCl and in 2N alkali solution. The acids **4a** and **1a** we have obtained can be esterified without difficulty. Both classical (alcohol and a stream of dry hydrogen chloride) and recent (DMSO + alkyl halide + triethylamine) methods of esterification give a high yield of the corresponding esters **4b,c** and **1b,c**.



1, 4 **a** R = H, **b** R = Me, **c** R = Et; **5** **a** R = Me, **b** R = Et;
6 **a** R = Me, X = $MeOSO_3$, **b** R = Et, X = ClO_4

On the basis of the general understanding of quinazolones we assign a 4(3H)-quinazolinone structure to the acid **1a**. Linked with the method developed for preparing acid **4a** and its esters **4b,c** it became possible in this study to determine the position of the quinazolone ring NH proton in acid **1a** and its esters **1b,c**. For this purpose we additionally prepared the methyl ester of the acid **1b** and both esters **1b,c** were alkylated using methyl iodide in DMSO in the presence of potassium carbonate. The alkylation of quinazolin-4-ones has been quite well studied and there are reports in the chemical literature of the introduction of an alkyl group not only at atom $N_{(1)}$ [8] and $N_{(3)}$ [9] but also possible alkylation involving the carbonyl oxygen atom [10].

An important feature in connecting the structure of the methyl esters **1b,c** with structures **5a,b** is the presence in the IR spectra of "quinazolone" type absorption bands [11], in addition the esters obtained differ in melting point and spectroscopic parameters from the esters of 2-[(1-methyl-4-oxo-1,4-dihydro-2-quinazolinyl)methyl]benzoic acid (**4b,c**). On the basis of analysing their IR spectra an O-methylated structure for **5a,b** was declined by us and in our hands they proved to be the two pairs of isomeric esters **4b,c** and **5a,b**. The melting points of the esters obtained from the 3-methyl-(4H)-quinazol-4-one **5a** proved to be lower than the corresponding 1-methyl-(4H)-quinazol-4-ones **4b,c**. At the same time, the chemical shifts of the proton-containing groups in the NMR spectra of the isomeric esters proved very similar. The greatest difference

occurred in the resonance for the N-methyl group protons of compounds **4b,c** and **5a,b**. The signals for this group assigned to the 3-methyl-(4H)-quinazol-4-one series were to higher field by 0.2 ppm. In the IR spectra of the isomeric esters **4b,c** and **5a,b** the stretching vibrations assigned to the ester carbonyl group were seen at the same frequency of 1695 cm^{-1} which points to the disappearance of the intramolecular hydrogen bond in the methylated products. For all four compounds **4b,c** and **5a,b** the ester C–O stretching vibrations appear as strong, single bands in the range 1070-1080 cm^{-1}. As regards the carbonyl group absorption of the quinazolone ring there clearly arises a difference among the isomeric esters. In esters **4b,c** the carbonyl group absorbs at 1630 cm^{-1} and in the esters **5a,b** at 1655-1660 cm^{-1}. It should be noted that such a remarkably low frequency for $\nu_{C=O}$, particularly for esters **4b,c**, is in agreement with tabulated $\nu_{C=O}$ frequencies for other isomeric quinazol-4-ones [12].

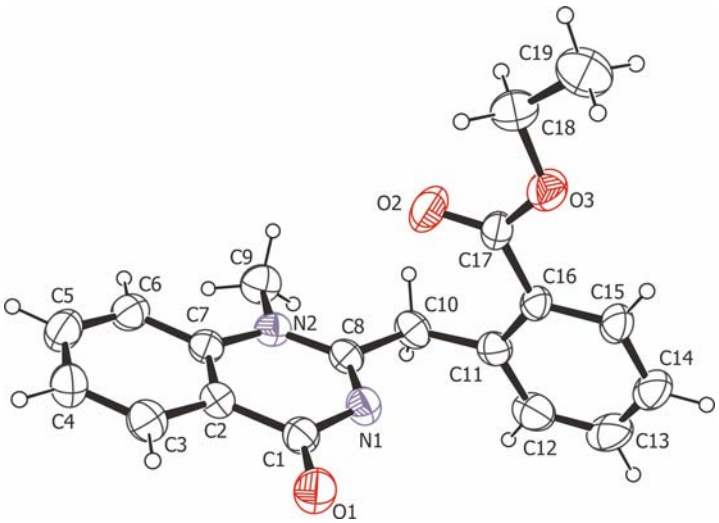


Fig. 1. Molecular structure of ethyl 2-[(1-methyl-4-oxo-1,4-dihydro-2-quinazolinyl)methyl]benzoate (**4c**). Thermal ellipsoids for the non-hydrogen atoms are shown at the 30% probability level.

The electronic transitions for the esters **4c** and **5b** are observed in three regions: 1) at lowest wavelength (less than 250 nm) single bands with a uniform structure and close intensities; 2) in the medium region (260-285 nm) two local maxima, in ester **5b** being close in intensity and in compound **4c** the long wavelength being more intense; 3) at longer wavelength (295-320 nm) two localized maxima in each of the spectra but in both compounds the first being more intense than the second.

The differences in the electronic spectra of esters **4c** and **5b** consist of differences in the absorption band intensities in the medium and long wavelength regions. In compound **5** the intensity of the medium band is greater ($\Delta\varepsilon \sim 2000$) and the long wavelength band lower ($\Delta\varepsilon \sim 4000$) than the intensities of the corresponding bands in ester **4c**. Comparison of the electronic spectra of the ester **1c** with the spectra of the model compounds **4c** and **5b** shows a similarity in the features of the spectra of esters **5b** and **1c** and a difference of the latter from the electronic spectrum of ester **4c**. This leads us to conclude that the ester **1c** has a 4(3H)-quinazolinone structure. Although less thorough, the same conclusion can be reached by comparison of the IR spectra of the esters **4c, 5b** and **1c**.

The esters **4a-c** and **5a,b** show marked basic properties. They readily form simple salts with mineral acids and are quaternized by alkylating agents. Moreover, the different starting esters (e.g. the pairs **4b** and **5a** or **4c** and **5b**) give identical quaternary salts (e.g. **6a** and **6b** respectively). In these salts the $N_{(1)}$-methyl group proton resonances are seen at higher field than the $N_{(3)}$-methyl protons ($\Delta\delta \sim 0.3$-0.4 ppm). The assignment of signals was made in this case on the basis of NOE experiments.

EXPERIMENTAL

IR spectra for the compounds in CsI tablets were recorded on a Pye-Unicam SP3-300 instrument. ^{1}H NMR spectra were measured on a Varian Mercury 400 (400 MHz) spectrometer using DMSO-d_6 solvent and TMS as internal standard. UV spectra were recorded on a Specord M-40 spectrophotometer in methanol solvent at 5×10^{-5} M concentration.

X-ray Structural Analysis. Crystals of **4c** are rhombic (ethanol), $C_{19}H_{18}N_2O_3$, at 298 K: a = 15.694(1), b = 10.6785(6), c = 19.539(1) Å, V = 3274.5(4) Å^3, M_r = 322.35, Z = 8, space group *Pbca*, d_{calc} = 1.308 g/cm^3, μ(MoKα) = 0.09 mm^{-1}, F(000) = 1360. The unit cell parameters and intensities of 9448 reflections (3024 independent with R_{int} = 0.053) were measured on an Xcalibur 3 automatic, four circle diffractometer (MoKα, graphite monochromator, CCD detector, ω-scanning, $2\theta_{max}$ = 51º). The structure was solved by a direct method using the SHELXTL program package [13]. The positions of the atoms were calculated geometrically and refined using the "riding" model with U_{iso}(H) = nU_{eq} (C) (n = 1.5 for methyl groups and n = 1.2 for other hydrogen atoms). The structure was refined in F^2 full matrix least squares analysis for non-hydrogen atoms to wR_2 = 0.182 for 3024 reflections (R_1 = 0.074 for 1721 reflections with $F > 4\sigma(F)$, S = 1.13). The crystallographic data (excluding the structural factors) has been placed in the Cambridge structural data base (reference CCDC 608867).

2-Cyanomethylbenzoic Acid (2) was prepared according to method [14].

2-[(4-Oxo-3,4-dihydro-2-quinazolinyl)methyl]benzoic acid (1a) was prepared according to method [4]. ^{1}H NMR spectrum, δ, ppm (J, Hz): 12.7 (1H, s, COOH); 12.1 (1H, s, NH); 8.05 (1H, d, J = 8.0, H-5); 7.91 (1H, d, J = 7.2, H-6'); 7.65 (1H, t, J = 7.6, H-7); 7.47 (1H, t, J = 7.8, H-4'); 7.42 (1H, d, J = 8.4, H-8); 7.37 (1H, t, J = 8.0, H-6); 7.36 (1H, t, J = 8.0, H-5'); 7.32 (1H, d, J = 8.0, H-3'); 4.35 (2H, s, 1'-CH_2).

Methyl 2-[(4-Oxo-3,4-dihydro-2-quinazolinyl)methyl]benzoate (1b). A. Triethylamine (0.3 ml, 2 mmol) and methyl iodide (0.13 ml, 2 mmol) were added dropwise to a solution of acid **1a** (0.56 g, 2 mmol) in DMSO (5 ml). The reaction mixture was stirred and held at room temperature for 48 h and then diluted with water. The colorless precipitate was washed with water and alcohol. Yield 0.56 g (90%); mp 188ºC (acetic acid).

B. A suspension of acid **1a** (1.12 g, 4 mmol) in dry methanol (50 ml) was saturated with dry hydrogen chloride for 30 min until the precipitate dissolved. The reaction mixture was refluxed for 3 h, solvent removed under reduced pressure, and the residue was treated with saturated sodium bicarbonate solution. The precipitate was filtered off and washed with water and alcohol. Yield 1 g (81%).

The substance obtained by method A was spectroscopically identical to the compound prepared by method B and the melting point of a mixed sample was not depressed. IR spectrum, ν, cm^{-1}: 3190 (N–H), 1710 (ester C=O), 1670 (quinazolone C=O), 1610 (C=N), 1480, 1450, 1430, 1270. ^{1}H NMR spectrum, δ, ppm (J, Hz): 12.2 (1H, s, NH); 8.05 (1H, d, J = 7.6, H-5); 7.89 (1H, d, J = 8, H-6'); 7.65 (1H, t, J = 7.8, H-7); 7.50 (1H, t, J = 7.8, H-4'); 7.39 (1H, t, J = 8.0, H-5'); 7.39 (1H, t, J = 8.0, H-6); 7.36 (1H, d, J = 7.2, H-3'); 7.36 (1H, d, J = 7.2, H-8); 4.31 (2H, s, 1'-CH_2); 3.77 (3H, s, –OCH_3). Found, %: C 70.23; H 4.69; N 9.33. $C_{17}H_{14}N_2O_3$. Calculated, %: C 70.38; H 4.79; N 9.52.

Ethyl 2-[(4-Oxo-3,4-dihydro-2-quinazolinyl)methyl]benzoate (1c) with mp 176ºC (acetic acid) was prepared by the method in [4]. IR spectrum, ν, cm^{-1}: 3200 (N–H), 1710 (ester C=O), 1670 (quinazolone C=O), 1600 (C=N), 1250. UV spectrum, λ_{max}, nm (log ε): 313 (3.59), 301 (3.67), 269 (3.92), 263 (3.94). ^{1}H NMR spectrum, δ, ppm (J, Hz): 12.22 (1H, s, NH); 8.07 (1H, d, J = 8.0, H-5); 7.88 (1H, d, J = 6.8, H-6'); 7.70 (1H, t, J = 6.8, H-7); 7.44 (1H, t, J = 6.8, H-4'); 7.44 (1H, t, J = 6.8, H-5'); 7.44 (1H, t, J = 6.8, H-6); 7.39 (1H, d, J = 8.4, H-3'); 7.39 (1H, d, J = 8.4, H-8); 4.31 (2H, s, 1'-CH_2); 4.19 (2H, q, J = 7.2, OCH_2); 1.24 (3H, t, J = 7.2, OCH_2CH_3).

2-(1-Methyl-4-oxo-1,4-dihydro-2-quinazolinylmethyl)benzoic Acid (4a). A mixture of 2-cyanomethylbenzoic acid (**2**, 0.81 g, 5 mmol) and N-methylanthranilic acid (**3**, 0.76 g, 5 mmol) was dissolved in dry dioxane (30 ml) and the mixture was refluxed for 6 h. The precipitate was filtered, washed with 2-propanol, and

recrystallized from DMF to give the colorless compound. Yield 1.25 g (88%); mp 259ºC (DMF). IR spectrum, ν, cm^{-1}: 2660-2960 (N–H), 1690 (carboxyl C=O), 1680 (4-quinazolone C=O), 1580 (C=N), 1530 (C–N), 1450, 1430, 1250 (C–O). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 12.7 (1H, s, CO_2H); 8.04 (1H, d, J_o = 7.6, J_m = 2.0, H-5); 7.99 (1H, d, *J* = 7.6, H-6'); 7.75 (1H, t, J_o = 7.6, J_m = 1.2, H-7); 7.66 (1H, d, *J* = 8.8, H-8); 7.49 (1H, t, *J* = 7.2, H-4'); 7.42 (1H, t, *J* = 7.6, H-6); 7.37 (1H, t, *J* = 7.4, H-5'); 7.27 (1H, d, *J* = 6.8, H-3'); 4.60 (2H, s, 1'-CH_2); 3.79 (3H, s, –NCH_3). Found, %: C 68.98; H 4.83; N 9.64. $C_{17}H_{14}N_2O_3$. Calculated, %: C 69.38; H 4.79; N 9.52.

Methyl 2-[(1-Methyl-4-oxo-1,4-dihydro-2-quinazolinyl)methyl]benzoate (4b) was prepared from acid **4a** using the preparative method B for compound **1b**. Yield 80%; mp 202ºC (2-propanol). IR spectrum, ν, cm^{-1}: 1710 (ester C=O), 1630 (quinazolone C=O), 1580 (C=N), 1530, 1470, 1450, 1290, 1250. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.03 (1H, d, *J* = 8.0, H-5); 7.99 (1H, d, *J* = 8.0, H-6'); 7.78 (1H, t, *J* = 7.6, H-7); 7.71 (1H, d, *J* = 8.0, H-8); 7.56 (1H, t, *J* = 7.4, H-4'); 7.44 (1H, t, *J* = 8.0, H-6); 7,42 (1H, t, *J* = 8.0, H-5'); 7.33 (1H, d, *J* = 7.6, H-3'); 4.59 (2H, s, 1'-CH_2); 3.81 (3H, s, NCH_3); 3.72 (3H, s, OCH_3). Found, %: C 70.26; H 5.30; N 9.17. $C_{18}H_{16}N_2O_3$. Calculated, %: C 70.12; H 5.23; N 9.09.

Ethyl 2-[(1-Methyl-4-oxo-1,4-dihydro-2-quinazolinyl)methyl]benzoate (4c) was prepared similarly to compound **4b** by esterification of acid **4a** using absolute ethanol. Yield 85%; mp 200ºC (2-propanol). IR spectrum, ν, cm^{-1}: 1700 (ester C=O), 1630 (quinazolone C=O), 1580 (C=N), 1530,1470, 1450, 1290, 1250. UV spectrum, λ_{max}, nm (log ε): 317 (3.84), 305 (3.97), 275 (3.85), 266 (3.80). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.03 (1H, d, *J* = 7.6, H-5); 7.98 (1H, d, *J* = 7.2, H-6'); 7.77 (1H, t, *J* = 7.6, H-4'); 7.71 (1H, d, *J* = 8.4, H-3'); 7.54 (1H, t, *J* = 7.8, H-7); 7,43 (1H, t, *J* = 7.6, H-6); 7.40 (1H, t, *J* = 7.6, H-5'); 7.32 (1H, d, *J* = 8.0, H-8); 4.59 (2H, s, 1'-CH_2); 4.15 (2H, q, *J* = 7.2, OCH_2); 3.81 (3H, s, NCH_3); 1.2 (3H, t, *J* = 7.2, OCH_2CH_3). Found, %: C 71.06; H 5.70; N 8.81. $C_{19}H_{18}N_2O_3$. Calculated, %: C 70.79; H 5.63; N 8.69.

Methyl 2-[3-Methyl-4-oxo-3,4-dihydro-2-quinazolinyl)methyl]benzoate (5a). Potassium carbonate (0.6 g) was added to a solution of the ester **1b** (0.56 g, 2 mmol) in DMSO (5 ml). Methyl iodide (0.25 ml, 4 mmol) was then introduced dropwise with stirring and the reaction mixture was held for 48 h at room temperature. It was diluted with water and the colorless precipitate was filtered off and washed with water and alcohol. Yield 0.5 g (85%); mp 155ºC (acetic acid). IR spectrum, ν, cm^{-1}: 1700 (ester C=O), 1670 (quinazolone C=O), 1580 (C=N), 1480, 1460, 1430, 1250. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.10 (1H, d, *J* = 7.6, H-5); 7.96 (1H, d, *J* = 7.6, H-5'); 7.66 (1H, t, *J* = 7.6, H-7); 7.53 (1H, t, *J* = 7.6, H-4'); 7.41 (1H, t, *J* = 7.6, H-6); 7.41 (1H, t, *J* = 7.6, H-5'); 7.34 (1H, d, *J* = 8.4, H-8); 7.31 (1H, d, *J* = 7.6, H-3'); 4.60 (2H, s, 1'-CH_2); 3.72 (2H, s, –OCH_3); 3.62 (3H, s, 3-CH_3). Found, %: C 70.21; H 5.28; N 9.14. $C_{18}H_{16}N_2O_3$. Calculated, %: C 70.12; H 5.23; N 9.09

Ethyl 2-[(3-Methyl-4-oxo-3,4-dihydro-2-quinazolinyl)methyl]benzoate (5b) was prepared from ester **1c**, potassium carbonate, and methyl iodide in DMSO by the method reported for ester **5a**. Yield 87%; mp 121ºC (acetic acid). IR spectrum, ν, cm^{-1}: 1700 (ester C=O), 1670 (quinazolone C=O), 1580 (C=N), 1470, 1250. UV spectrum, λ_{max}, nm (log ε): 313 (3.59), 305 (3.68), 273 (3.96), 263 (3.96). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.09 (1H, d, *J* = 7.6, H-5); 7.95 (1H, d, *J* = 8.0, H-6'); 7.64 (1H, t, *J* = 7.6, H-7); 7.52 (1H, t, *J* = 7.2, H-4'); 7.39 (1H, t, *J* = 7.6, H-6); 7.39 (1H, t, *J* = 7.6, H-5'); 7.33 (1H, d, *J* = 8.4, H-3'); 7.30 (1H, d, *J* = 6.8, H-8); 4.57 (2H, s, 1'-CH_2); 3.60 (3H, s, 3-CH_3); 4.14 (2H, q, *J* = 7.2, OCH_2CH_3); 1.16 (3H, t, *J* = 7.2, OCH_2CH_3). Found, %: C 70.96; H 5.55; N 8.78. $C_{19}H_{18}N_2O_3$. Calculated, %: C 70.79; H 5.63; N 8.69.

2-[2-(Ethoxycarbonyl)phenyl]methyl-1,3-dimethyl-4-oxo-1,4-dihydroquinazolin-3-ium Methylmethosulfate (6a). A. A mixture of compound **5a** (0.62 g, 2 mmol) and dimethylsulfate (0.4 ml, 2.2 mmol) was fused on an oil bath at 120-140ºC for 1 h. The solid residue was triturated with acetone and filtered. Yield 0.53 g (61%); mp 158ºC (alcohol).

B. Prepared from the methyl ester **4b** and dimethylsulfate by the method given for **6a.**

The substance obtained by method A was spectroscopically identical to that prepared by method B and the melting point of a mixed sample was not depressed. IR spectrum, ν, cm^{-1}: 1710 (ester C=O), 1615 (quinazolone C=O), 1555 (C=N), 1490, 1270, 1250, 1225. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.43 (1H, d,

J = 7.6, H-5); 8.20-8.12 (3H, m, H-7,4',6'); 7.87 (1H, t, *J* = 7.6, H-6); 7.58-7.51 (2H, m, H-3',5'); 7.39 (1H, d, *J* = 8.0, H-8); 5.28 (2H, s, 1'-CH_2); 4.05 (3H, s, 3-CH_3); 3.70 (3H, s, 1-CH_3); 3.94 (3H, s, –$COOCH_3$); 3.45 (3H, s, –$COCH_3$). Found, %: C 55.18; H 5.19; N 6.57; S 7.51. $C_{20}H_{22}N_2O_7S$. Calculated, %: C 55.29; H 5.10; N 6.45; S 7.38.

2-[2-(Ethoxycarbonyl)phenyl]methyl-1,3-dimethyl-4-oxo-1,4-dihydroquinazolin-3-ium Perchlorate (6b). A. A mixture of compound **4c** (0.65 g, 2 mmol) and methyl tosylate (0.4 g, 2.1 mmol) was fused on an oil bath at 140ºC for 1 h. The melt was cooled, dissolved in ethanol (10 ml), and treated with a saturated alcohol solution of $NaClO_4$. The colorless precipitate was filtered off and washed with water. Yield 0.54 g (62%); mp 158ºC (alcohol).

B. Prepared from the ethyl ester **5b** and methyl tosylate using method A in the synthesis of compound **6b**.

The substance obtained by method A was spectroscopically identical to that obtained by method B and the melting point of a mixed sample was not depressed. IR spectrum, ν, cm^{-1}: 1720 (ester C=O), 1615 (quinazolone C=O), 1555 (C=N), 1490, 1270, 1250. UV spectrum, λ_{max}, nm (log ε): 347 (3.52), 290 (3.51), 284 (3.56). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 8.39 (1H, d, *J* = 7.6, H-5); 8.18–8.11 (3H, м, H-7,4',6'); 7.87 (1H, t, *J* = 7.0, H-6); 7.56-7.50 (2H, m, H-3',5'); 7.40 (1H, d, *J* = 8.0, H-8); 5.22 (2H, s, 1'-CH_2); 4.07 (3H, s, 3-CH_3); 3.65 (3H, s, 1-CH_3); 4.39 (2H, q, *J* = 7.2, –OCH_2CH_3); 1.42 (3H, t, *J* = 7.2, –OCH_2CH_3). Found, %: C 55.23; H 4.96; Cl 8.22; N 6.53. $C_{20}H_{21}ClN_2O_7$. Calculated, %: C 54.99; H 4.85; Cl 8.12; N 6.41.

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