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4(3H)-QUINAZOLINONES CONTAINING HETEROCYCLIC GROUP IN POSITION 3

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The corresponding 2,3-substituted 4(3H)-quinazolinones were obtained in the reactions of 2-methyl- and 2-phenyl-4-oxo-3,1-benzoxazines with 1-amino-1,2,4-triazole, 4-amino-2,3-dimethyl-1-phenyl-5-pyrazolone, 2-amino-5-ethyl-1,3,4-thiadiazole, 3-amino-6,6-dimethyl-4-oxo-4,5,6,7-tetrahydroindazole, 1-amino-3-cyano-4,6-dimethyl-2-pyridone, and 1-amino-3-cyano-6-phenyl-4-trifluoromethyl-2-pyridone. The formation of N-benzoylanthranilamides in the reactions of 2-phenyl-4-oxo-3,1-benzoxazine with 2-amino-5-ethyl-1,3,4-thiadiazole and 1-amino-3-cyano-6-phenyl-4-trifluoromethyl-2-pyridones was exceptional. The structures of two of the products have been confirmed by X-ray crystallography.

Keywords: 2-methyl- and 2-phenyl-3R-4(3H)-quinazolinones, 1,2,4-triazol-4-yl, 2,3-dimethyl-1-phenyl-5-pyrazolinon-4-yl, 1,3,4-thiadiazol-2-yl, 3-cyano-6-phenyl-4-trifluoromethyl-2-pyridon-1-yl, 6,6-dimethyl-4-oxo-4,5,6,7-tetrahydro-3-indazolyl.

There are not many examples with heterocyclic group at position 3 among the enormous number of 2,3-substituted 4(3H)-quinazolinones, but they possess a wide range of biological activities [1-7], a number of theoretical problems have been solved on their basis [8-12], and many quinazoline alkaloids are of this type [13].

Reactions of 2-methyl-4-oxo-3,1-benzoxazine **1a** with 1-amino-1,2,4-triazole (**2a**), 4-amino-2,3-dimethyl-1-phenyl-5-pyrazolinone (**2b**), 2-amino-5-ethyl-1,3,4-thiadiazole (**2c**), 3-amino-6,6-dimethyl-4-oxo-4,5,6,7-tetrahydroindazole (**2d**) [13], and 4,6-disubstituted 3-cyano-2-pyridones (**2e,f**) gave the corresponding 2-methyl-4(3H)-quinazolinones **3** in all cases.

Reactions of 2-phenyl-4-oxo-3,1-benzoxazine (**1b**) with 2-amino-5-ethyl-1,3,4-thiadiazole (**2c**) and with 1-amino-3-cyano-6-phenyl-4-trifluoromethyl-2-pyridone (**2f**) led to the corresponding N-benzoylanthranilamides **4a,b**; in all the remaining cases the corresponding 2-phenyl-4(3H)-quinazolinones **3b,d,g,i.** N-Benzoylanthranilamide **4c** was obtained in the reaction of 2,6-diaminopyridine with oxazine **1b**. The corresponding 4(3H)-quinazoline has been described in the literature [14].

The conditions for the reactions of the oxazines **1** with the amines **2** were not varied. All the reactions were carried out by melting an equimolar mixture of the oxazine **1** and the N-nucleophile **2** in a flask with a short reflux condenser on an oil bath at 160-175°C for 1-2 h.

The structures of the quinazoline derivatives **3** were confirmed by IR and ^{1}H NMR spectroscopy. In compound **3f**, in distinction from **3g**, the signals of the protons of the $C(6)–CH_3$ group of the indazole fragment appear as two separate singlets at 1.05 and 1.11 ppm, while the signals of the NH protons are characterized by chemical shifts of 13.67 (**3f**) and 13.35 (**3g**) ppm. Two carbonyl frequencies are observed in the IR spectra (**3f** 1702 and 1668 cm^{-1}, **3g** 1681 and 1668 cm^{-1}) and also NH stretching frequencies (**3f** 3170 cm^{-1}, **3g** 3240 cm^{-1}).

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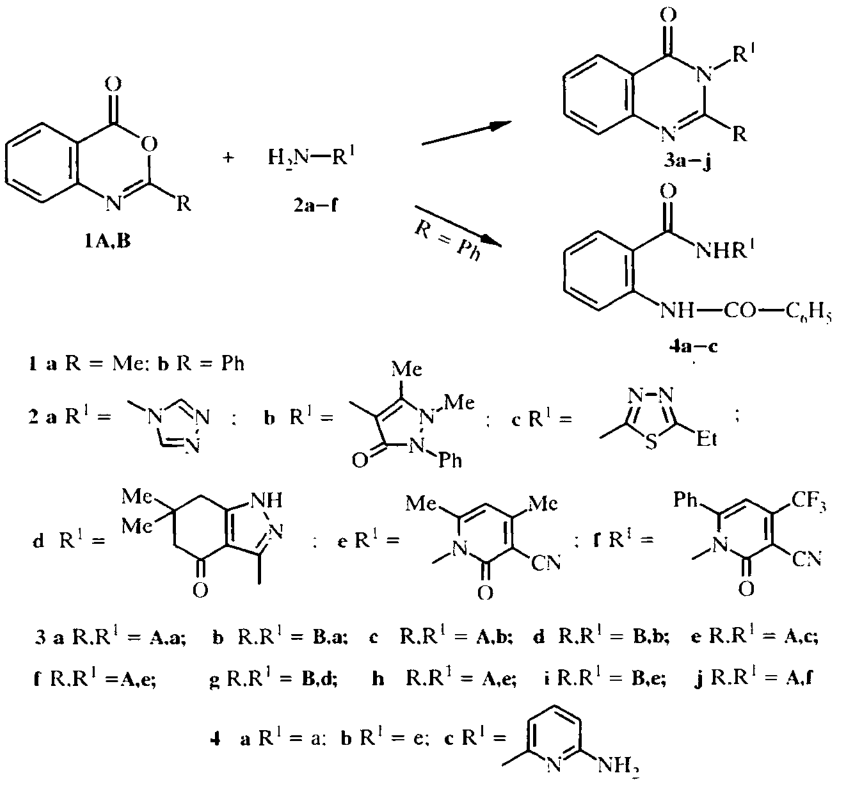
Two carbonyl stretching frequencies in the 1714-1670 cm^{-1} were also observed in the IR spectra of quinazolinones **3h,i,j**. Characteristic frequencies of the cyano group in these compounds appeared at 2220-2230 cm^{-1}. Two signals for the NH protons at 10-13 ppm were clearly observed in the ^1H NMR spectra of the diamides **4**. These signals were absent for the cyclic structures **3**.



3 a R.R^1 = A.a; b R.R^1 = B.a; c R.R^1 = A.b; d R.R^1 = B.b; e R.R^1 = A.c;
f R.R^1 = A.e; g R.R^1 = B.d; h R.R^1 = A.e; i R.R^1 = B.e; j R.R^1 = A.f

4 a R^1 = a; b R^1 = e; c R^1 =

The structures of quinazolinones **3f** and **3j** were confirmed by X-ray crystallography.

A space model of the molecule of **3j** is shown in Fig. 1 and the principal geometric parameters are given in Tables 1 and 2. The pyridone ring is planar within experimental limits and it has a geometry characteristic of 2-pyridones [16, 17]. In contrast to the previously studied 3-cyano-6-phenyl-4-trifluoromethyl-2-pyridone [16], there is a bulky substituent at position 1 of the pyridine system in the molecule of **3j** which impedes conjugation of the system of the two six-membered rings. The interfacial angle between the mean planes of the pyridone and phenyl rings in **3j** is 55.1(1)° which is close to the value (53.1°) in the structure of 1-amino-3-cyano-6-phenyl-4-trifluoromethyl-2-pyridone [18]. In its turn, the interfacial angle between the mean planes of the quinazoline and pyridone units in **3j** is 79.4(1)°. Atoms N(1) and N(2) are pyramidalized to some extent which causes destruction of the strict planarity of the corresponding rings. The height of the pyramid (displacement from the plane of the three neighboring atoms) for N(1) and N(2) is 0.070(3) and 0.104(3) Å respectively. The N(1)–N(2) single bond length is 1.403(4) Å, which coincides with the standard value (1.401 Å) [19]. The shortened C–F bond in structure **1** (mean value 1.293 Å, standard value 1.322 Å [19]) is connected with strong thermal motion of the fluorine atoms [20].

In the asymmetric part of the unit cell of compound **3f** there are two independent molecules (α and β) which are linked by a center of pseudosymmetry and which differ in the conformation of the cyclohexane unit. The shape of molecules α and β in the crystal are shown in Fig. 2. The conformation of the cyclohexane unit (torsion angles are given in Table 4) is close chair form in molecule α, whereas in molecule β it has the C_2 intermediate form [21].

TABLE 1. Coordinates of Non-hydrogen Atoms ($\times 10^4$) in the Molecule of **3j** and Equivalent Isotropic Temperature Factors

Atom	*x*	*y*	*z*	*U*(eq)
F(1)	2146(1)	6649(4)	4564(3)	136(2)
F(2)	2640(1)	5165(3)	4763(2)	98(1)
F(3)	2441(1)	6501(4)	3494(2)	130(2)
O(1)	1453(1)	1185(3)	4065(2)	56(1)
O(2)	663(1)	3040(4)	2134(2)	70(1)
N(1)	1448(1)	2316(3)	2588(2)	39(1)
N(2)	1142(1)	1246(3)	2105(2)	40(1)
N(3)	996(1)	-1348(4)	1724(3)	59(1)
N(4)	2189(1)	3107(5)	6055(3)	68(1)
C(2)	1584(1)	2194(4)	3645(3)	41(1)
C(3)	1890(1)	3339(4)	4136(3)	38(1)
C(4)	2003(1)	4468(4)	3591(3)	39(1)
C(5)	1830(1)	4542(4)	2549(3)	45(1)
C(6)	1543(1)	3487(4)	2040(3)	38(1)
C(7)	1346(1)	3607(4)	940(3)	40(1)
C(8)	1166(1)	4992(5)	562(3)	53(1)
C(9)	998(1)	5204(5)	-469(3)	60(1)
C(10)	1017(1)	4038(6)	-1111(3)	63(1)
C(11)	1196(1)	2666(6)	-742(3)	58(1)
C(12)	1359(1)	2428(5)	278(3)	48(1)
C(13)	2054(1)	3217(4)	5208(3)	47(1)
C(14)	2309(1)	5681(4)	4110(3)	45(1)
C(15)	730(1)	1720(5)	1955(3)	49(1)
C(16)	438(1)	489(6)	1590(3)	55(1)
C(17)	13(1)	780(7)	1348(3)	75(2)
C(18)	-261(2)	-411(10)	1035(4)	100(2)
C(19)	-120(2)	-1865(10)	965(4)	106(2)
C(20)	292(2)	-2190(7)	1193(4)	87(2)
C(21)	581(1)	-989(6)	1506(3)	59(1)
C(22)	1262(1)	-265(4)	2020(3)	47(1)
C(23)	1716(1)	-593(5)	2287(4)	65(1)

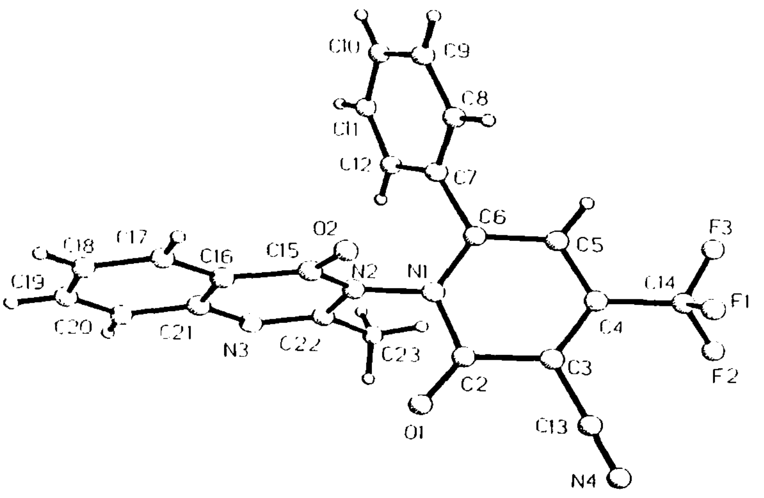


Fig. 1. Three-dimensional model of the molecule of 3-(3-cyano-6-phenyl-4-trifluoromethyl-2-pyridon-1-yl)-2-methyl-4(3H)-quinazolinone (**3j**).

TABLE 2. Bond Lengths (*l*) in Structure **3j**

Bond	*l*, Å	Bond	*l*, Å
F(1)–C(14)	1.283(5)	C(3)–C(4)	1.373(5)
F(2)–C(14)	1.290(4)	C(3)–C(13)	1.434(6)
F(3)–C(14)	1.305(5)	C(4)–C(5)	1.395(5)
O(1)–C(2)	1.217(4)	C(4)–C(14)	1.499(5)
O(2)–C(15)	1.211(5)	C(5)–C(6)	1.366(5)
N(1)–C(6)	1.374(4)	C(6)–C(7)	1.482(5)
N(1)–N(2)	1.403(4)	C(15)–C(16)	1.441(6)
N(1)–C(2)	1.413(5)	C(16)–C(21)	1.391(6)
N(2)–C(22)	1.391(5)	C(16)–C(17)	1.402(6)
N(2)–C(15)	1.412(5)	C(17)–C(18)	1.370(8)
N(3)–C(22)	1.280(5)	C(18)–C(19)	1.365(9)
N(3)–C(21)	1.387(6)	C(19)–C(20)	1.368(8)
N(4)–C(13)	1.137(5)	C(20)–C(21)	1.408(6)
C(2)–C(3)	1.449(5)	C(22)–C(23)	1.500(6)

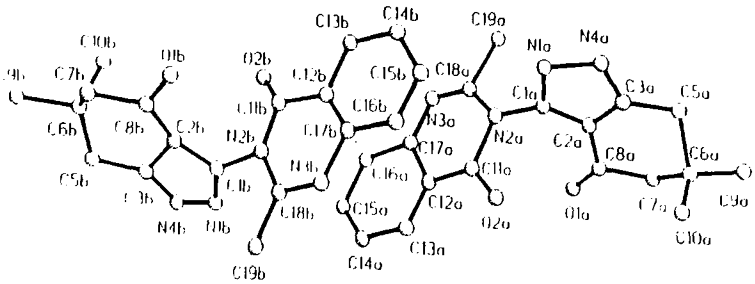


Fig. 2. Three-dimensional model and forms of the molecules in the crystal of 3-(6,6-dimethyl-4-oxo-4,5,6,7-tetrahydroindazolyl)-2-methyl-4(3H)-quinazolinone (**3f**).

TABLE 3. Bond Angles (ω) in Structure **3j**

Angle	ω, deg.	Angle	ω, deg.
C(6)–N(1)–C(2)	125.9(3)	F(1)–C(14)–F(2)	107.0(4)
C(6)–N(1)–N(2)	119.4(3)	N(4)–C(13)–C(3)	178.9(4)
N(2)–N(1)–C(2)	114.0(3)	F(1)–C(14)–F(3)	105.3(4)
C(22)–N(2)–N(1)	118.2(3)	F(2)–C(14)–F(3)	104.7(4)
C(22)–N(2)–C(15)	124.6(3)	F(1)–C(14)–C(4)	111.1(3)
N(1)–N(2)–C(15)	115.6(3)	F(2)–C(14)–C(4)	114.9(3)
C(22)–N(3)–C(21)	118.4(4)	F(3)–C(14)–C(4)	113.2(3)
O(1)–C(2)–N(1)	120.9(3)	O(2)–C(15)–N(2)	119.3(4)
O(1)–C(2)–C(3)	125.6(3)	O(2)–C(15)–C(16)	128.4(4)
N(1)–C(2)–C(3)	113.4(3)	N(2)–C(15)–C(16)	112.3(4)
C(4)–C(3)–C(13)	123.5(3)	C(21)–C(16)–C(17)	120.5(4)
C(4)–C(3)–C(2)	120.8(3)	C(21)–C(16)–C(15)	119.6(4)
C(13)–C(3)–C(2)	115.7(3)	C(17)–C(16)–C(15)	119.9(5)
C(3)–C(4)–C(5)	121.1(3)	N(3)–C(21)–C(16)	123.3(4)
C(3)–C(4)–C(14)	120.3(3)	N(3)–C(21)–C(20)	127.9(5)
C(5)–C(4)–C(14)	118.5(3)	C(16)–C(21)–C(20)	118.8(5)
C(6)–C(5)–C(4)	121.0(3)	N(3)–C(22)–N(2)	121.6(4)
C(5)–C(6)–N(1)	117.3(3)	N(3)–C(22)–C(23)	120.6(4)
C(5)–C(6)–C(7)	121.0(3)	N(2)–C(22)–C(23)	117.8(3)
N(1)–C(6)–C(7)	121.7(3)		

TABLE 4. Torsion Angles (τ) in Structure **3f**

Angle	τ, deg.	
	Molecule α	Molecule β
C(2)–C(3)–C(5)–C(6)	-40(3)	10(4)
C(3)–C(5)–C(6)–C(7)	55(2)	-47(3)
C(5)–C(6)–C(7)–C(8)	-58(3)	55(3)
C(6)–C(7)–C(8)–C(2)	37(3)	-20(4)
C(7)–C(8)–C(2)–C(3)	-10(3)	-12(4)
C(8)–C(2)–C(3)–C(5)	14(3)	19(4)

TABLE 5. Coordinates of the Non-hydrogen Atoms (× 10^4) in **3f**

Atom	Molecule α			Molecule β		
	x	*y*	*z*	*x*	*y*	*z*
N(1)	2442(9)	1310(2)	2815(9)	6025(13)	3630(4)	-810(2)
N(2)	2335(13)	2180(2)	1325(13)	6035(13)	2580(3)	733(14)
N(3)	2555(11)	810(3)	81(13)	5838(14)	4290(3)	1984(13)
O(1)	416(16)	4640(3)	446(18)	7831(10)	140(2)	1530(11)
O(2)	2797(11)	5190(3)	1732(14)	5517(10)	-280(2)	158(10)
C(1)	1954(13)	2260(3)	2003(16)	6389(18)	2750(4)	-10(2)
C(2)	1118(11)	3010(2)	1933(12)	7064(14)	1650(3)	-2(15)
C(3)	1127(13)	2670(3)	2760(14)	7103(16)	2290(4)	-898(17)
N(4)	1831(13)	1520(3)	3319(15)	6393(14)	3310(3)	-1357(15)
C(5)	379(15)	3210(3)	3025(17)	7764(13)	1540(3)	-1271(15)
C(6)	7(13)	5240(3)	2605(17)	8199(17)	-90(4)	-660(2)
C(7)	-234(19)	4910(4)	1500(2)	8571(17)	10(4)	420(2)
C(8)	506(12)	4270(3)	1248(14)	7840(2)	670(6)	730(3)
C(9)	-884(17)	5350(4)	2690(2)	9065(13)	-700(3)	-876(17)
C(10)	660(2)	6680(5)	3090(2)	7556(12)	-1860(3)	-1027(14)
C(11)	2826(12)	3940(3)	1273(13)	5712(13)	980(3)	829(14)
C(12)	3004(12)	3960(3)	376(15)	5241(12)	1090(3)	1416(14)
C(13)	3475(17)	5520(4)	370(2)	4878(14)	-570(4)	1670(17)
C(14)	3785(15)	5530(4)	-335(19)	4515(15)	-470(4)	2335(18)
C(15)	3703(14)	4130(3)	-914(17)	4551(14)	1230(3)	2807(16)
C(16)	3259(17)	2510(4)	-810(2)	4968(13)	2750(3)	2682(15)
C(17)	2904(16)	2300(3)	-109(17)	5303(14)	2610(3)	1977(15)
C(18)	2274(16)	860(4)	689(19)	6130(13)	4250(3)	1288(15)
C(19)	1663(14)	-920(3)	757(17)	6507(14)	5910(3)	1112(18)

The interfacial angles between the mean planes of the two bicyclic parts in molecules α and β are 73.2(5) and 70.6(5)° respectively. The mutual slope of the planes of the quinazoline fragments of molecules α and β is 5.9(5)°. The low precision of the determination of the structure is a result of the small size of the crystal studied which did not permit a satisfactory analysis of the geometry of the molecule.

EXPERIMENTAL

IR spectra of nujol (1800-1500 cm^{-1}) and hexachlorobutadiene mulls (3600-2000 cm^{-1}) were recorded with a Specord IR-75 spectrometer. C–H Vibration frequencies in the 3050-2000 cm^{-1} region are not reported. ^1H NMR spectra of DMSO-d_6 solutions with TMS as internal standard were recorded on a Bruker WH-90/DS (90 MHz) spectrometer.

General Procedure for the Synthesis of 4(3H)-Quinazolinones 3 and Diamides 4. A mixture of a 4-oxo-3,1-benzoxazine **1** (5 mmol), aminoheterocycle **2** (5 mmol), and a catalytic amount of *p*-toluenesulfonic acid was heated in a flask with a short reflux condenser for 1.5 h on an oil bath at 160-175°C (bath temperature). The reaction mixture was cooled and was crystallized.

2-Methyl-3-(1,2,4-triazol-4-yl)-4(3H)-quinazolinone (3a). Yield 41%; mp 227-228°C (methanol). IR spectrum: 1702, 1628, 1610, 1568, 1520, 1504; 3110 cm^{-1}. ^{1}H NMR spectrum: 2.25 (3H, s, CH_3); 7.56-8.23 (4H, m, C_6H_4); 9.38 ppm (2H, s, 2 =CH–). Found, %: C 58.33; H 4.06; N 30.66. $C_{11}H_9N_5O$. Calculated, %: C 58.15; H 3.99; N 30.82.

2-Phenyl-3-(1,2,4-triazol-4-yl)-4(3H)-quinazolinone (3b). Yield 28%; mp 301-303°C (methanol). IR spectrum: 1705, 1620, 1605, 1600, 1580, 1500; 3140, 3080 cm^{-1}. ^{1}H NMR spectrum: 7.49 (5H, m, C_6H_5); 7.60-8.39 (4H, m, C_6H_4); 8.82 ppm (2H, s, 2 =CH–). Found, %: C 66.66; H 3.69; N 24.13. $C_{16}H_{11}N_5O$. Calculated, %: C 66.43; H 3.83; N 24.21.

3-(2,3-Dimethyl-1-phenyl-5-pyrazolinon-4-yl)-2-methyl-4(3H)-quinazolinone (3c). Yield 55%; mp 228-229°C (dioxane). IR spectrum: 1690-1678, 1630, 1602, 1570 cm^{-1}. ^{1}H NMR spectrum: 2.18 (3H, s, CH_3); 2.43 (3H, s, CH_3); 3.28 (3H, s, CH_3); 7.36-8.18 ppm (9H, m, C_6H_5, C_6H_4). Found, %: C 68.04; H 5.40; N 16.60. $C_{19}H_{18}N_4O_2$. Calculated, %: C 68.25; H 5.43; N 16.76.

3-(2,3-Dimethyl-1-phenyl-5-pyrazolinon-4-yl)-2-phenyl-4(3H)-quinazolinone (3d). Yield 82%; mp 85-87°C (7:3 ethyl acetate–toluene, R_f 0.13, silica gel Aeros, 35-70μm, pore diameter 6 nm). IR spectrum: 1693-1673, 1610, 1595, 1563, 1500 cm^{-1}. ^{1}H NMR spectrum: 2.07 (3H, s, CH_3); 3.05 (3H, s, CH_3); 7.12-8.25 ppm (14H, m, $2C_6H_5$, C_6H_4). Found, %: C 73.30; H 4.80; N 13.88. $C_{25}H_{20}N_4O_2$. Calculated, %: C 73.51; H 4.94; N 13.72.

3-(5-Ethyl-1,3,4-thiadiazol-2-yl)-2-methyl-4(3H)-quinazolinone (3e). Yield 38%; mp 136-137°C (dioxane). IR spectrum: 1692, 1610, 1582, 1560, 1500 cm^{-1}. ^{1}H NMR spectrum: 1.27 (3H, t, 3J = 7 Hz, CH_3); 2.31 (3H, s, CH_3); 2.98 (2H, q, ^3J = 7 Hz, CH_2); 7.34-8.16 ppm (4H, m, C_6H_4). Found, %: C 57.11; H 4.40; N 20.41; S 11.60. $C_{13}H_{12}N_4OS$. Calculated, %: C 57.34; H 4.44; N 20.57; S 11.77.

3-(6,6-Dimethyl-4-oxo-4,5,6,7-tetrahydro-3-indazolyl)-2-methyl-4(3H)-quinazolinone (3f). Yield 31%; mp 300-301°C (dioxane). IR spectrum: 1704, 1668, 1604, 1572, 1512; 3170, 3100 cm^{-1}. ^{1}H NMR spectrum: 1.05 (3H, s, CH_3); 1.11 (3H, s, CH_3); 2.13 (3H, s, CH_3); 2.29 (2H, s, CH_2); 2.77 (2H, s, CH_2); 7.48-8.20 (4H, m, C_6H_4); 13.67 ppm (1H, br. s, NH). Found,%: C 66.88; H 5.50; N 17.14. $C_{18}H_{18}N_4O_2$. Calculated, %: 67.07; H 5.62; N 17.32.

3-(6,6-Dimethyl-4-oxo-4,5,6,7-tetrahydro-3-indazolyl)-2-phenyl-4(3H)-quinazolinone (3g). Yield 30%; mp 222°C (dioxane). IR spectrum: 1681, 1668, 1628, 1592, 1568, 1516; 3240, cm^{-1}. ^{1}H NMR spectrum: 0.63 (3H, s, CH_3); 1.02 (3H, s, CH_3); 1.94 (1H, d, ^2J = 14 Hz, CH_2); 2.36 (1H, d, ^2J = 14 Hz, CH_2); 2.49 (1H, d, ^2J = 13 Hz, CH_2); 2.81 (1H, d, ^2J = 13 Hz, CH_2); 7.32 (5H, m, C_6H_5); 7.50-8.24 (4H, m, C_6H_4); 13.35 ppm (1H, br. s, NH). Found,%: C 71.70; H 5.30; N 14.41. $C_{23}H_{20}N_4O_2$. Calculated, %: 71.86; H 5.24; N 14.57.

3-(3-Cyano-4,6-dimethyl-2-pyridon-1-yl)-2-methyl-4(3H)-quinazolinone (3h). Yield 52%; mp 225-226°C (1:3 methanol–water). IR spectrum: 2224, 1714, 1670, 1606, 1540 cm^{-1}. ^{1}H NMR spectrum: 2.24 (3H, s, CH_3); 2.32 (3H, s, CH_3); 2.45 (3H, s, CH_3); 6.67 (1H, s, =CH–); 7.54-8.25 ppm (4H, m, C_6H_4). Found, %: C 66.40; H 4.46; N 18.02. $C_{17}H_{14}N_4O_2$. Calculated, %: C 66.65; H 4.61; N 18.29.

3-(3-Cyano-4,6-dimethyl-2-pyridon-1-yl)-2-phenyl-4(3H)-quinazolinone (3i). Yield 70%; mp 191-192°C (3:4 ethyl acetate–toluene, R_f 0.29). IR spectrum: 1708, 1676, 1592, 1562, 1536; 2220 cm^{-1}. ^{1}H NMR spectrum: 2.33 (6H, s, $2CH_3$); 6.49 (1H, s, =CH–); 7.54 (5H, s, C_6H_5); 7.21-8.36 ppm (4H, m, C_6H_4). Found, %: C 71.50; H 4.45; N 15.02. $C_{22}H_{16}N_4O_2$. Calculated, %: C 71.73; H 4.38; N 15.21.

3-(3-Cyano-6-phenyl-4-trifluoromethyl-2-pyridon-1-yl)-2-methyl-4(3H)-quinazolinone (3j). Yield 73%; mp 223-224°C (methanol). IR spectrum: 1710, 1692, 1610, 1548; 2230 cm^{-1}. ^{1}H NMR spectrum: 2.33 (3H, s, CH_3); 7.22 (1H, s, =CH–); 7.41 (5H, m, C_6H_5); 7.51-8.20 ppm (4H, m, C_6H_4). Found, %: C 62.46, H 3.06; N 13.28. $C_{22}H_{13}F_3N_4O$. Calculated, %: C 62.56; H 3.10; N 13.26.

5-Ethyl-1,3,4-thiadiazol-2-ylamide of N-Benzoylanthranilic Acid (4a). Yield 37%; mp 176-177°C (methanol). IR spectrum: 1675, 1650, 1610, 1595, 1535, 1500; 3250-3150 cm^{-1}. ^{1}H NMR spectrum: 1.32 (3H, t, ^3J = 7 Hz, CH_3); 3.02 (2H, q, ^3J = 7 Hz, CH_2); 7.22-8.33 (9H, m, C_6H_5, C_6H_4); 11.38 (1H, br. s, NH); 13.24 ppm (1H, br. s, NH). Found, %: 61.16; H 4.50; N 15.70; S 8.90. $C_{18}H_{16}N_4O_2S$. Calculated, %: C 61.35; H 4.57; N 15.89, S 9.09.

3-Cyano-6-phenyl-4-trifluoromethyl-2-pyridon-1-ylamide of N-Benzoylanthranilic Acid (4b). Yield 35%; mp 141-142°C (methanol). IR spectrum: 1689, 1650, 1645, 1608, 1588, 1542, 1500, 2220 cm^{-1}. ^{1}H NMR spectrum: 7.07 (1H, br. s, NH); 7.13 (1H, t, ^3J = 8 Hz, C_6H_4); 7.20-8.12 (13H, m, $2C_6H_5$, C_6H_4, =CH); 8.75 (1H, d, ^3J = 8 Hz, C_6H_4); 12.2 ppm (1H, br. s, NH). Found, %: C 64.33; H 3.29; N 11.11. $C_{27}H_{17}F_3N_4O_3$. Calculated, %: C 64.54; H 3.41; N 11.15.

6-Amino-2-pyridylamide of N-Benzoylanthranilic Acid (4c). Yield 69%; mp 192-193°C (3:1 ethanol–DMF). IR spectrum: 1675, 1648, 1635, 1614; 1588, 1575, 1526, 1500; 3460, 3330, 3300-3250 cm^{-1}. ^{1}H NMR spectrum: 5.82 (2H, br. s, $-NH_2$); 6.27 (1H, dd, ^3J = 8 Hz, ^4J = 1 Hz, C_5H_3N); 7.18-8.1 (10H, m, C_6H_5, C_6H_4, C_6H_5N); 8.53 (1H, dd, $3J$ = 8 Hz, ^4J = 1 Hz, C_5H_3N); 10.34 (1H, br. s, NH); 11.66 ppm (1H, br. s, NH). Found, %: C 68.47; H 4.71; N 16.62. $C_{19}H_{16}N_4O_2$. Calculated, %: C 68.66; H 4.85; N 16.86.

X-ray Diffraction Study of Quinazolinones 3f,j. Crystals of **3j**, composition $C_{22}H_{13}F_3N_4O_2$, grown from methanol, monoclinic: a 34.080(7), b 8.687(2), c 14.073(3) Å; β = 108.30(3)°; V = 3945.5(15) Å^3; d = 1.422 g/cm^3; Z = 8, $F(000)$ = 1728, space group $C2/c$. The intensities of 2153 independent reflexions were measured on a Syntex P21 automatic diffractometer (MoKα radiation, graphite monochromator), $\theta/2\theta$-scanning to $2\theta_{max}$ = 45°. The structure was solved by direct methods using SHELXS [22] and was refined using SHELXL [23] by the least squares method in the anisotropic approximation for non-hydrogen atoms to R = 0.059. Crystals of compound **3f** with the composition $C_{18}H_{18}N_4O_2$, grown from methanol, were monoclinic with the following crystallographic parameters: a 16.352(3), b 7.160(1), c 15.289(3) Å; β 116.02(3)°; V = 1608.6(5) Å^3; M 322.36; d_{calc} = 1.331 g/cm^3; Z = 4; space group Pc. The intensities of 2396 independent intensities were measured on a Syntex P21 automatic diffractometer (MoKα radiation, graphite monochromator, $\theta/2\theta$-scanning, θ_{max} = 22.5°). 1302 Independent reflexions with $I \geq 2\sigma(I)$ were used in the calculations. The structure was solved by direct methods with program [22] and refined by full matrix least squares [23] anisotropically for O and N atoms and isotropically for C atoms to a final value of R = 0.071. Coordinates of the non-hydrogen atoms are given in Table 5.

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