Russian Journal of Organic Chemistry, Vol. 40, No. 11, 2004, pp. 1638–1643. Translated from Zhurnal Organicheskoi Khimii, Vol. 40, No. 11, 2004, pp. 1686–1691.
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Heterocyclization of Functionalized Heterocumulenes with C,N- and C,O-Binucleophiles: V.* Synthesis of Imidazo[1,5-*a*]imidazole Derivatives by Cyclocondensation of 1-Chloroalkyl Isocyanates with Imidazoles and Benzimidazole

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Received July 15, 2003

Abstract—1-Chloroalkyl isocyanates react with imidazole, 4(5)-phenylimidazole, and 4,5-dimethyl(phenyl)-imidazoles to give 5-aryl-5-trifluoromethyl-5,6-dihydro-7*H*-imidazo[1,5-*a*]imidazole-7-ones, and with benzimidazole affording 1-aryl-1-trifluoromethyl-1,2-dihydro-3*H*-imidazo-[1,5-*a*]benzimidazole-3-ones.

The reactions of imidazoles with aryl and alkyl isocyanates are nowadays sufficiently documented. The phenyl isocyanate is known to react with imidazole and 4,5-diphenylimidazole [2, 3] at heating in a boiling benzene to furnish N-carbamoyl derivatives. In reactions of isocyanates with imidazoles at higher temperature, for instance, at boiling in nitrobenzene, 4-nitrotoluene or in diphenyl ether products of carbamoylation of the heterocycle in position *2* were isolated [4–6]. It was established that the latter formed as a result of a rearrangement of the primary products of N-carbamoylation [5]. In some cases, in particular, in the reaction of 2-phenylcarbamoylimidazole with two equiv of phenyl isocyanate a cyclic product was isolated: 6-phenylimidazo[1,5-*a*]imidazole-5,7-dione [5]. 4(5)-Methyl- and 4(5)-cyanoimidazoles react with methyl and aryl isocyanates affording the corresponding 1-carbamoyl-4-methyl(cyano)-imidazoles [7]. The heating of 1-carbamoyl-4-methylimidazoles in nitrobenzene yielded 2-carbamoyl-4-methylimidazoles whereas with 4-cyano-substituted analogs no migration of carbamoyl group was observed.

Isocyanates containing alongside the heterocumulene group an additional electrophilic center were not brought into reactions with imidazoles. Therefore we believed it to be useful to investigate reactions between 1-chloroalkyl isocyanates **Ia–c**, highly reactive systems with pronounced alkylating and acylating ability[8], and imidazoles **IIa–d** and benzimidazole (**IIe**). This target is fairly significant for imidazole chemistry as show the recently developed procedures for effective function-alization of the imidazole ring with electrophilic reagents, in particular, with isocyanates [9, 10].

As a result of experiments we isolated 5-aryl-5-trifluoromethyl-5,6-dihydro-7*H*-imidazo[1,5-*a*]imidazole-7-ones (**IIIa–i**) and 1-aryl-1-trifluoromethyl-1,2-dihydro-3*H*-imidazo[1,5-*a*]-benzimidazole-3-ones (**IIIj–l**), little-studied fused imidazoimidazoles [5, 11]. It was established that the reaction conditions and the yields of the target products depended mainly on the structure of the imidazole used. For instance, isocyanates **Ia–c** react with unsubstituted imidazole **IIa** and 4(5)-phenylimidazole **IIb** when heated in benzene for 4 h in the presence of triethylamine affording in a 55–81% yield compounds **IIIa–f.** The benzimidazole requires a heating in toluene for 6 h, and 4,5-disubstituted imidazoles **IIc, d** undergo cyclization into compounds **IIIg–i** in 8–37% yields only at prolonged boiling in *p*-xylene.

Compounds **IIIa–l** are colorless crystalline substances whose structure is reliably established by combined application of physicochemical methods: mass spectrometry, IR and NMR (^{1}H, ^{19}F, and ^{13}C) spectroscopy, and

For Communication IV see [1].

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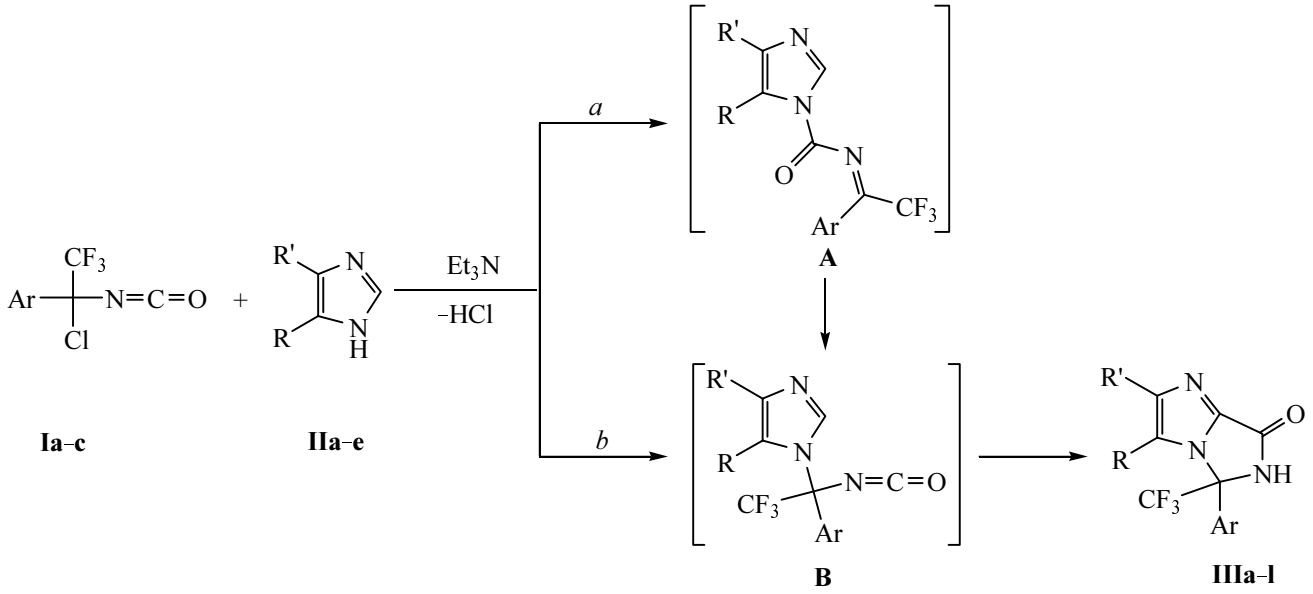


I, Ar = Ph (**a**), 4-MeC_6H_4 (**b**), 4-$MeOC_6H_4$ (**c**); II, R, R' = H (**a**); R = H, R' = Ph (**b**); R = R' = Me (**c**); R = R' = Ph (**d**); R, R' = benzo (**e**); **III**, R = R' = H, Ar = Ph (**a**), 4-MeC_6H_4 (**b**), 4-$MeOC_6H_4$ (**c**); R = H, R' = Ph, Ar = Ph (**d**), 4-MeC_6H_4 (**e**), 4-$MeOC_6H_4$ (**f**); R = R' = Me, Ar = Ph (**g**), 4-MeC_6H_4 (**h**); R = R' = Ar = Ph (**i**); R, R' = benzo, Ar = Ph (**j**), 4-MeC_6H_4 (**k**), 4-$MeOC_6H_4$ (**l**).

also by X-ray diffraction analysis. In the mass spectra of compounds synthesized appeared molecular ion peaks of medium intensity. IR spectra contain strong absorption bands of the stretching vibrations of the C=O groups in the region 1720–1750 cm^{-1} characteristic of polycyclic γ-lactones [12], and also wide absorption bands of the stretching vibrations of NH groups (3190–3210 cm^{-1}) suggesting the presence of intermolecular hydrogen bonds between amide fragments of the molecules in the solid state. In the ^1H NMR spectra of compounds **IIIa–c** registered in DMSO-d_6 the protons H^2 and H^3 appeared as singlets. However in $CDCl_3$ and $(CD_3)_2CO$ the latter were observed as doublets with a small coupling constant (J 1.0 Hz). The singlet from the proton H^3 in compounds **IIId–f** is located at 8.6 ppm due to the influence of the ring currents of a phenyl substituent in position *2* that most likely is coplanar with the imidazole ring. On the other hand, it should be indicated that the H^8 proton in compounds **IIIj–l** experienced no appreciable shielding by the ring current of an aryl substituent in position *1*. In the ^{19}F NMR spectra the signals from CF_3 groups of compounds belonging to type **III** appeared at –74...–80 ppm revealing that these substituents were attached to sp^3-hybridized carbon atoms [13]. Therewith the dependence of the chemical shift value of ^{19}F on the bulk of the substituent on position *3* is very clearly pronounced: With the growing volume of the substituent the signals shift downfield. In the ^{13}C NMR spectra of compounds **IIIa** and **IIIj** quartets from carbons located in the position *5* (*1*) of bicyclic structure appear at 77 ppm ($^2J_{C-F}$ 33.0 and 32.0 Hz respectively), the CF_3 groups give rise to quartets at 127 ppm ($^1J_{C-F}$ 286.0 and 288.0 Hz respectively) and singlets from C=O groups are seen at 157.8 and 157.6 ppm respectively suggesting that both compounds belong to the same structural type.

The structure of compound **IIIk*** was unambiguously proved by X-ray diffraction analysis. It was established that in the crystal two symmetrically independent molecules **A** and **B** of compound **IIIk**. The principal bond lengths and bond angles are given in a table, the general view of molecule **IIIk** are located, **A** is presented on Fig.1. The tricyclic system $N^1N^2N^3C^{1-9}$ is approxim-ately planar: The deviation of atoms from the mean-square plane in molecule **A** do not exceed 0.033 Å, in molecule **B** 0.114 Å. The dihedral angle between the 5-membered rings $N^1N^2C^{1-3}$ and $N^2N^3C^{3-5}$ in molecules **A** and **B** is only 3.6 and 7.3 deg, between the ring $N^2N^3C^{3-5}$ and the benzene ring C^{4-9} 1.5 and 0.6 deg respectively. The benzene ring C^{11-16} is turned with respect to the $N^1N^2N^3C^{1-9}$ moiety by 58.1 deg in molecule **A** and by 52.5 deg in molecule **B**. In the crystal of compound **IIIk** the tricyclic structures $N^1N^2N^3C^{1-9}$ of molecules **A** and **B** form a dihedral angle of 147.2 deg. By hydrogen bonds N^1–$H^1\cdots O^1$ [$N^1\cdots O^1$ 2.763(2), $H^1\cdots O^1$ 1.89(2), N^1–H^1 0.88(2) A, $N^1H^1O^1$ 172(1)°], and N^4–$H^4\cdots O^2$ [$N^4\cdots O^2$

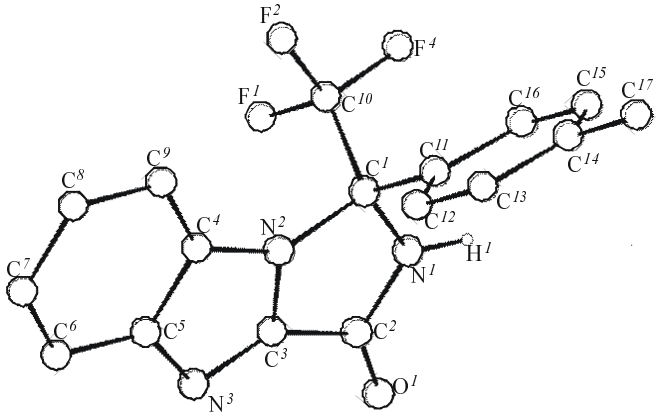
* Numeration of atoms is different from that used in describing NMR spectra.

Principal bond lengths (d, Å) and bond angles (ω, deg) β in two symmetrically independent molecules **A** and **B** of compound **IIIk**

Bond	d		Angle	ω	
	A	**B**		**A**	**B**
N^1–C^1	1.459(2)	1.456(2)	$C^1N^1C^2$	114.7(1)	115.0(1)
N^1–C^2	1.356(2)	1.357(2)	$C^1N^2C^3$	112.4(1)	112.0(1)
N^2–C^1	1.459(2)	1.461(2)	$C^3N^2C^4$	106.7(1)	106.5(1)
N^2–C^3	1.369(2)	1.372(2)	$C^3N^3C^5$	102.7(1)	102.9(1)
N^2–C^4	1.384(2)	1.387(2)	$N^1C^1N^2$	100.3(1)	100.4(1)
N^3–C^3	1.304(2)	1.304(2)	$N^1C^2C^3$	105.0(1)	104.7(1)
N^3–C^5	1.398(2)	1.395(2)	$N^2C^3N^3$	115.2(1)	115.1(1)
C^2–C^3	1.476(2)	1.478(2)	$N^2C^3C^2$	107.6(1)	107.6(1)
C^4–C^5	1.414(2)	1.412(2)	$N^2C^4C^5$	103.6(1)	103.7(1)
			$N^3C^5C^4$	111.7(1)	111.7(1)

2.816(2), $H^4\cdots O^2$ 1.94(2), N^4–H^4 0.88(2) A, $N^4H^4O^2$ 173(1)°] the molecules of compound **IIIk** are joined into centrosymmetrical dimers **AA** and **BB**.

The cyclocondensation of compounds **Ia** and **IIa** was monitored by taking ^{19}F NMR spectra of the reaction mixture first at room temperature and then at heating for 0.5, 1, 2, and 4 h. Thus we were able to observe in 1–1.5 h after mixing the reagents the formation of intermediate products **A** (–67 ppm) [14] and **B** (–75 ppm) [15] in a ratio about 1:0.7 and also of the target compound **IIIa** (–80 ppm). At heating in benzene the signals belinging the intermediates **A** and **B** gradually disappeared. This allowed us to presume that the reaction probably proceeded through primary formation both of N-acylated (**A**) and N-alkylated (**B**) compounds. *N*-(*N*-Alkylidenecarbamoyl)imidazoles **A** because of insufficient electrophilic quality of the azomethine bond are not prone to cyclocondensation and undergo an intramolecular anionotropic shift of the imidazolyl group in the triad –C=N–C= resulting in more electrophilic 1-(*N*-imidazolyl)alkyl isocyanates **B**. The latter are capable to undergo cyclization into fused imidazo[1,5-*a*]imidazoles partially even at room temperature totally in contrast to the reactions of unsubstituted isocyanates that add to the position *2* of imidazole at a temperature higher than 200°C presumably via intermolecular mechanism [6]. The migration in the azaallyl triad involving halogen atoms [8], dithiophosphato [16], isocyanatO [17], azido [18], imino [19], aroxy(thioaroxy) [20], and alkoxy groups [21] was formerly observed by spectral and synthetic methods. It should be also pointed out that in some instances the generation of isocyanate-type systems from the isomeric respective N-alkylidene derivatives, e.g., 1-phenoxyalkyl isocyanates from N-alkylideneuretanes underlies the cyclization of the latter [22].

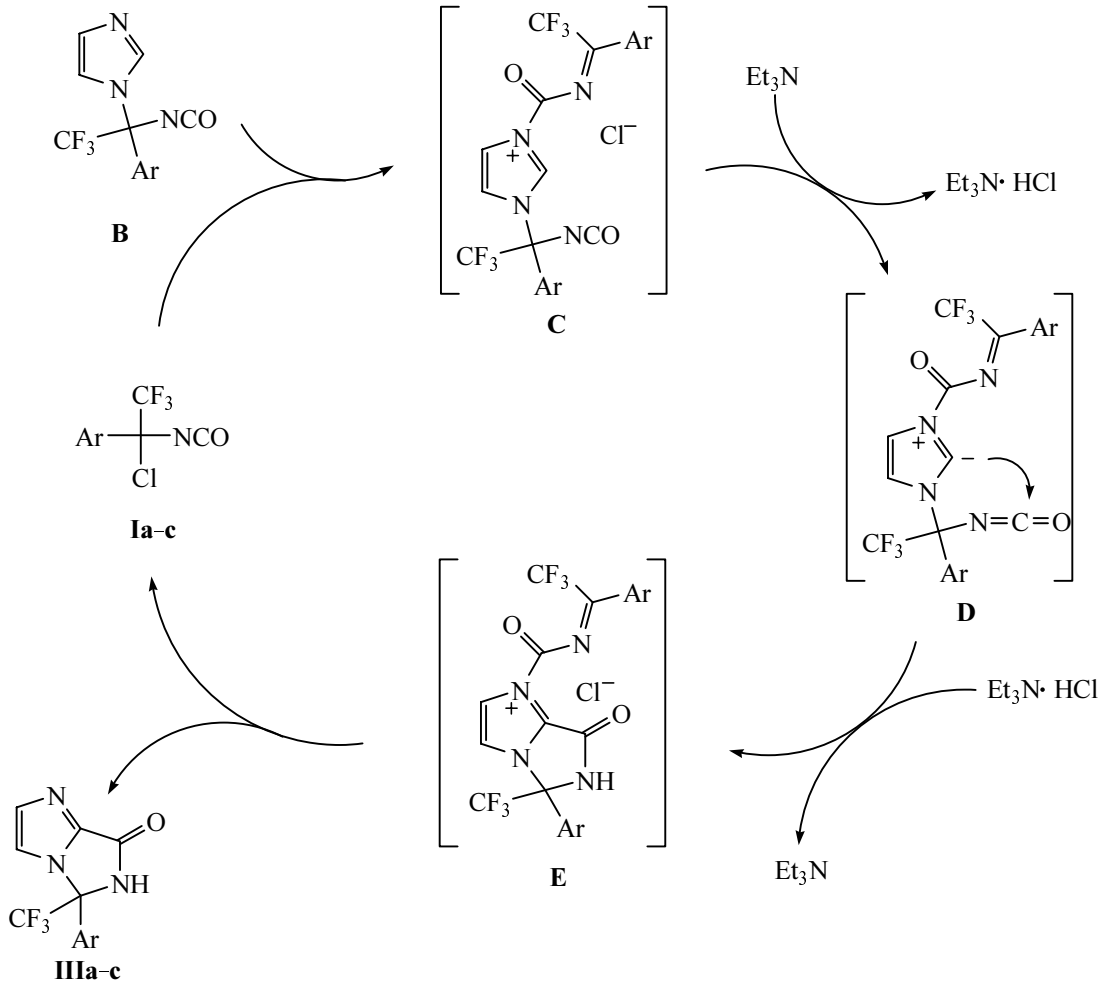


General view of **A** molecule 1-(4-tolyl)-1-trifluoromethyl-1,2-dihydro-3*H*-imidazo[1,5-*a*]benzimidazoles-3-one (**IIIk**).

We suggested a scheme of cyclization of the **B** type intermediate compounds based on the concept of an "ylide" mechanism [23]. The trace amounts of 1-chloroalkyl isocyanate **I** present in the reaction mixture are capable to acylate 1-(*N*-imidazolyl)alkyl isocyanate **B** furnishing imidazolium salt **C** that under the action of triethylamine eliminates a proton and converts into ylide **D**. Further the intramolecular carbamoylation of ylide carbon atom occurs by the action of isocyanate group followed by protonation with triethylammonium hydrochloride of the arising imidazole ring. Salt **E** due to the low basicity of the "pyridine" nitrogen of the fused imidazo[1,5-*a*]imidazole system decomposes into the target reaction product **III** and the initial 1-chloroalkyl isocyanate (**I**) that again enters into the catalytic cycle.

EXPERIMENTAL

X-ray diffraction analysis on a single crystal of compound **IIIk** of the size 0.14×0.20×0.22 mm was carried out at 120 K on automatic CCD diffractometer Smart-6K (MoK_α radiation, λ 0.71073 Å, θ_{max} 27 deg). From collected total 13664 reflections 6541 were independent (R_{int} 0.031). Crystals of compound **IIIk** triclinic, a 9.632(1), b 10.499(1), c 16.004(1) Å, α 73.29(1), β 80.80(1), γ 83.23(1)°, V 1525.7(2) Å^3, M 331.3, Z 4 (two independent molecules), d_{calc} 1.44 g/cm^3, μ 1.18 cm^{-1}, F(000) 680.2, space group P 1Ï (N 2). The structure



was solved by the direct method and refined by the least-mean-square method in a full-matrix anisotropic approximation applying software package CRYSTALS [24]. In refining 6541 reflections were used with $I > 3(I)$ (529 refined parameters, 12.4 reflections per parameter). All hydrogen atoms were revealed from the difference synthesis of the electron density and refined in isotropic approximation. Chebyshev weight scheme was used in refining [25] with five parameters: 0.49, 0.32, 0.20, 0.05, and –0.07. Final values of divergence factors were R 0.048 and R_W 0.046, GOF 1.083. The residual electron density from the difference Fourier series was 0.29 and –0.22 e/ Å^3. A complete set of the X-ray structural data for compound IIIk was deposited into the Cambridge Structural Database (no. CCDC 212602).

IR spectra were recorded on spectrophotometer UR-20 from samples prepared as KBr pellets. ^{1}H, ^{13}C, and ^{19}F NMR spectra were registered in $(CD_3)_2SO$–CCl_4, 2:1, on spectrometer Varian-Gemini (at 299.95, 75.4, and 282.2 MHz respectively), internal references TMC (^{1}H, ^{13}C) and F (^{19}F). Mass spectra were measured on MKh-1321 instrument at direct sample admission into the ion source, accelerating voltage for ionizing electrons 70 V, temperature in the ionizing chamber 150°C.

1-Chloroalkyl isocyanates **Ia–c** were prepared as described in [26].

5-Aryl-5-trifluoromethyl-5,6-dihydro-7*H*-imidazo[1,5-*a*]imidazole-7-ones (IIIa–i), 1-aryl-1-trifluoromethyl-1,2-dihydro-3*H*-imidazo[1,5-*a*]-imidazole-3-ones (IIIj–l). To a suspension of 4 mmol of compound **IIa, b** in 20 ml of benzene, or compound **IIc, d** in 20 ml of *p*-xylene, or compound **IIe** in 20 ml of toluene was added at stirring a solution of 4 mmol of isocyanate **Ia–c** and 0.4 g (4 mmol) of triethylamine in 10 ml of the same solvent. The reaction mixture was stirred for 4 h at room temperature, left standing for 12 h, and then the precipitate of triethylamine hydrochloride was filtered off. The filtrate was heated at reflux for 4 h (with imidazoles **IIa, b**), 10 h (with imidazoles **IIc, d**), or 6 h (with benzimidazole **IIe**), then the solvent

was evaporated, and the residue was crystallized from a mixture ethyl acetate–hexane, 5:1.

Compound IIIa. Yield 81%, mp 210–211°C. IR spectrum, cm^{-1}: 1740 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 7.43 s (1H, H^2), 7.43–7.50 m (3H arom), 7.70–7.74 m (2H arom), 8.07 s (1H, H^3), 11.17 s (1H, NH). ^{13}C NMR spectrum, δ, ppm: 77.20 q (C^5, $^2J_{C-F}$ 33.0 Hz) , 119.36 (C^2), 123.07 q (CF_3, $^1J_{C-F}$ 286.6 Hz), 127.09 ($C^{3',5'}$), 129.00 ($C^{2',6'}$), 131.03 ($C^{1'}$), 131.63 (C^4), 137.53 (C^3), 143.14 (C^{7a}), 157.75 (C=O). ^{19}F NMR spectrum, δ, ppm: –79.85. Mass spectrum, *m/z*: 267 M^+. Found, %: C 54.17; H 3.05; N 15.54. $C_{12}H_8F_3N_3O$. Calculated, %: C 53.93; H 3.00; N 15.73.

Compound IIIb. Yield 78%, mp 194–195°C. IR spectrum, cm^{-1}: 1750 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 2.38 s (3H, CH_3), 7.33 d (2H, $H^{3',5'}$, *J* 8.0 Hz), 7.44 s (1H, H^2), 7.64 d (2H, $H^{2',6'}$, *J* 8.0 Hz), 8.08 s (1H, H^3), 11.14 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –79.76. Mass spectrum, *m/z*: 281 M^+. Found, %: C 55.28; H 3.79; N 15.19. $C_{13}H_{10}F_3N_3O$. Calculated, %: C 55.53; H 3.56; N 14.95.

Compound IIIc. Yield 66%, mp 98–99°C. IR spectrum, cm^{-1}: 1740 (C=O), 3190 (N–H). ^1H NMR spectrum, δ, ppm: 3.81 s (3H, CH_3O), 7.02 d (2H, $H^{3',5'}$, *J* 9.0 Hz), 7.41 s (1H, H^2), 7.68 d (2H, $H^{2',6'}$, *J* 8.0 Hz), 8.01 s (1H, H^3), 11.09 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –80.13. Mass spectrum, *m/z*: 297 M^+. Found, %: C 52.20; H 3.59; N 13.81. $C_{13}H_{10}F_3N_3O_2$. Calculated, %: C 52.53; H 3.37; N 14.14.

Compound IIId. Yield 64%, mp >250°C. IR spectrum, cm^{-1}: 1745 (C=O), 3190 (N–H). ^1H NMR spectrum, δ, ppm: 7.29 t (1H, $H^{4''}$, *J* 7.1 Hz), 7.41 d.d (2H, $H^{3'',5''}$, *J* 7.0 Hz), 7.54–7.57 m (3H arom), 7.78–7.84 m (2H arom), 7.93 d (2H, $H^{2'',6''}$, *J* 7.0 Hz), 8.68 s (1H, H^3), 11.24 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –79.99. Mass spectrum, *m/z*: 343 M^+. Found, %: C 62.65; H 3.68; N 12.41. $C_{18}H_{12}F_3N_3O$. Calculated, %: C 62.97; H 3.50; N 12.24.

Compound IIIe. Yield 60%, mp >250°C. IR spectrum, cm^{-1}: 1730 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 2.39 m (3H, CH_3), 7.20–7.45 m (5H arom), 7.71 d (2H, $H^{2',6'}$, *J* 8.0 Hz), 7.91 d (2H, $H^{2'',6''}$, *J* 7.0 Hz), 8.65 s (1H, H^3), 11.19 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –79.83. Mass spectrum, *m/z*: 357 M^+. Found, %: C 64.07; H 4.07; N 11.63. $C_{19}H_{14}F_3N_3O$. Calculated, %: C 63.87; H 3.92; N 11.76.

Compound IIIf. Yield 55%, mp >250°C. IR spectrum, cm^{-1}: 1730 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 3.82 s (3H, CH_3O), 7.08 d (2H, $H^{3',5'}$, *J* 8.0 Hz), 7.29 t (1H, $H^{4''}$, *J* 7.9 Hz), 7.40 d.d (2H, $H^{3'',5''}$, *J* 8.0 Hz), 7.76 d (2H, $H^{2',6'}$, *J* 8.0 Hz), 7.91 d (2H, $H^{2'',6''}$, *J* 8.0 Hz), 8.65 s (1H, H^3), 11.17 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –79.94. Mass spectrum, *m/z*: 373 M^+. Found, %: C 61.46; H 3.59; N 11.05. $C_{19}H_{14}F_3N_3O_2$. Calculated, %: C 61.13; H 3.75; N 11.26.

Compound IIIg. Yield 37%, mp 172–173°C. IR spectrum, cm^{-1}: 1740 (C=O), 3190 (N–H). ^1H NMR spectrum, δ, ppm: 1.94 s (3H, CH_3), 2.20 s (3H, CH_3), 7.38–7.40 m (2H arom), 7.50–7.55 m (3H arom), 10.61 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –74.21. Mass spectrum, *m/z*: 295 M^+. Found, %: C 57.23; H 4.28; N 14.03. $C_{14}H_{12}F_3N_3O$. Calculated, %: C 56.95; H 4.07; N 14.23.

Compound IIIh. Yield 28%, mp 178–179°C. IR spectrum, cm^{-1}: 1720 (C=O), 3190 (N–H). ^1H NMR spectrum, δ, ppm: 1.95 s (3H, CH_3), 2.20 s (3H, CH_3), 2.39 s (3H, CH_3), 7.20–7.35 m (4H arom), 10.50 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –74.44. Mass spectrum, *m/z*: 309 M^+. Found, %: C 8.53; H 4.29; N 13.28. $C_{15}H_{14}F_3N_3O$. Calculated, %: C 58.25; H 4.53; N 13.59.

Compound IIIi. Yield 8%, mp >250°C. IR spectrum, cm^{-1}: 1740 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 6.68 d (2H arom), 7.14–7.61 m (13H arom), 10.85 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –73.68. Mass spectrum, *m/z*: 419 M^+. Found, %: C 68.90; H 3.71; N 10.39. $C_{24}H_{16}F_3N_3O$. Calculated, %: C 68.74; H 3.82; N 10.02.

Compound IIIj. Yield 75%, mp 188–189°C. IR spectrum, cm^{-1}: 1750 (C=O), 3210 (N–H). ^1H NMR spectrum, δ, ppm: 7.35–7.62 m (8H arom), 7.95 m (1H arom), 11.54 s (1H, NH). ^{13}C NMR spectrum, δ, ppm: 77.41 q (C^1, $^2J_{C-F}$ 32.0 Hz), 123.42 q (CF_3, $^1J_{C-F}$ 288.5 Hz), 112.43, 122.93, 124.67, 126.23 (C^5, C^6, C^7, C^8), 126.78 ($C^{3',5'}$), 129.80 ($C^{2',6'}$), 130.79 ($C^{1'}$), 131.19 (C^4), 147.29 (C^{3a}), 148.61 ($C^{4a,8a}$), 157.62 (C=O). ^{19}F NMR spectrum, δ, ppm: –76.12. Mass spectrum, *m/z*: 317 M^+. Found, %: C 60.81; H 3.12; N 12.93. $C_{16}H_{10}F_3N_3O$. Calculated, %: C 60.57; H 3.15; N 13.25.

Compound IIIk. Yield 74%, mp 199–200°C. IR spectrum, cm^{-1}: 1745 (C=O), 3190 (N–H). ^1H NMR spectrum, δ, ppm: 2.39 s (3H, CH_3), 7.29 d (2H, $H^{3',5'}$, *J* 9.0 Hz), 7.35–7.40 m (3H arom), 7.44 d (2H, $H^{2',6'}$, *J* 8.0 Hz), 7.90–7.94 m (1H arom), 11.37 C (1H, NH). ^{19}F NMR spectrum, δ, ppm: –76.60. Mass spectrum, *m/z*: 331 M^+. Found, %: C 61.97; H 3.53; N 12.61. $C_{17}H_{12}F_3N_3O$. Calculated, %: C 61.63; H 3.63; N 12.69.

Compound IIIl. Yield 30%, mp 161–162°C. IR spectrum, cm^{-1}: 1740 (C=O), 3200 (N–H). ^1H NMR spectrum, δ, ppm: 3.82 s (3H, CH_3O), 7.06 d (2H, $H^{3',5'}$, *J* 9.0 Hz), 7.30–7.45 m (3H arom), 7.50 d (2H, $H^{2',6'}$, *J* 9.0 Hz), 7.95 m (1H arom), 11.31 s (1H, NH). ^{19}F NMR spectrum, δ, ppm: –76.15. Mass spectrum, *m/z*: 347 M^+. Found, %: C 59.08; H 3.31; N 12.43. $C_{17}H_{12}F_3N_3O_2$. Calculated, %: C 58.79; H 3.46; N 12.10.

The study was carried out under financial support of the Royal Society for a Joint Project Grant and EPSRC for a Senior Research Fellowship.

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