An Efficient Microwave-Assisted Synthesis of 6,8-Dihydroimidazo[1,2-*a*] [1,3,5] Triazine Derivatives

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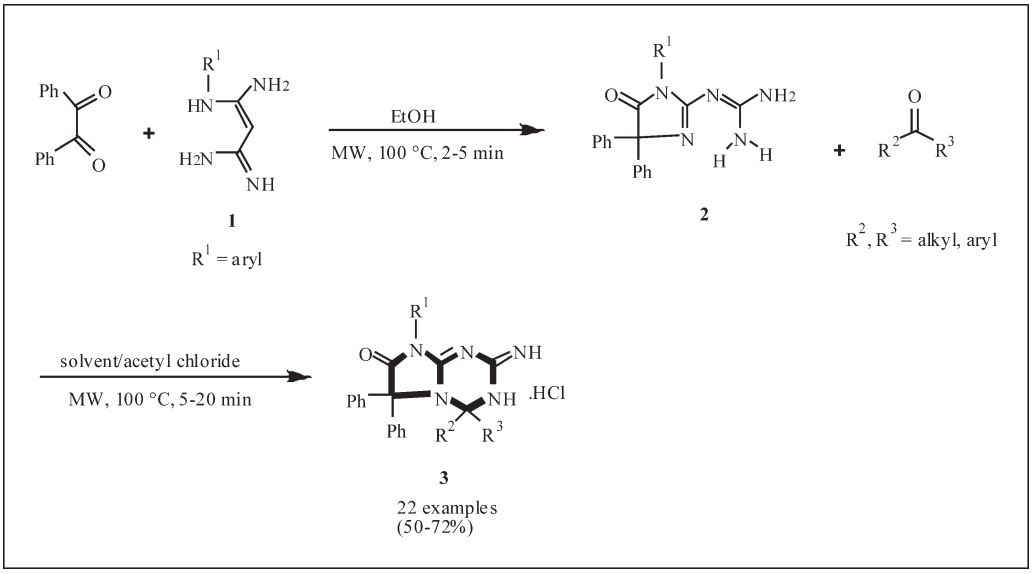

A simple, efficient, and general method has been developed for the synthesis of various 4-substituted 2-amino-6,6-diphenyl-8-aryl-6,8-dihydroimidazo[1,2-*a*] [1,3,5] triazine-7(4-*H*)ones **3a**–**3v**. This involved condensation of 1-(5-oxo-4,4-diphenyl-1-aryl-4,5-dihydro-1*H*-imidazol-2-yl)guanidines 2a and 2b, themselves obtained from the reaction of aryl biguanides 1a/b with benzil, with the requisite carbonyl compounds. Both steps were performed using microwave heating in sealed vessels.

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INTRODUCTION

Microwave-assisted organic synthesis (MAOS) has emerged over the past decade as a valuable technology for synthetic organic and medicinal chemistry. Replacing the conventional oil bath as a heat source by a microwave reactor results in a marked reduction in reaction time and an increase in reaction yield for many important transformations [1,2]. In particular, the need for rapid construction and modification of biologically active heterocyclic compounds, a major concern in drug development, has stimulated intense development of microwave synthesis technology. This is reflected in the exponential increase in the number of scientific papers, books, and reviews related to the use of this technology [3,4].

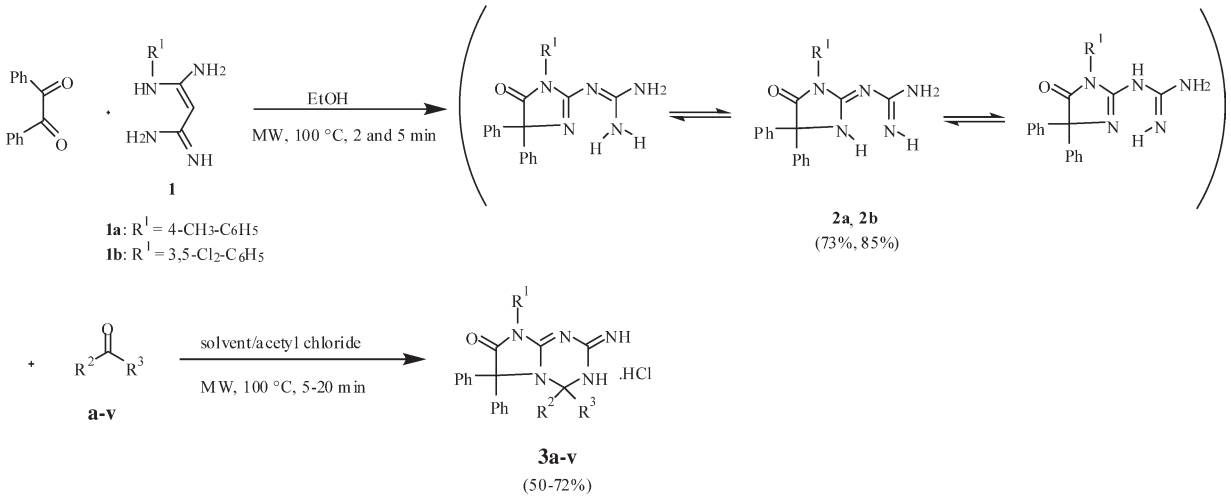
In this work, we report a simple and convenient method for the synthesis of 6,8-dihydroimidazo[1,2-a] [1,3,5] triazines under microwave irradiation conditions. The 6,8-dihydroimidazo[1,2-a] [1,3,5] triazine system is a core structure element in a number of molecules with potential application as antitumor, antibacterial, and antiparasitic agents, and as herbicide antagonists [5–21].

RESULTS AND DISCUSSION

Imidazoltriazines with structure **3** have been obtained by a two-step procedure (Scheme 1) involving the heating of 1-substitued biguanides with benzil to give 1-(5-oxo-4,4-diphenyl-1-aryl-4,5-dihydro-1H-imidazol-2-yl)guanidine intermediates **2** as a mixture of tautomers, and subsequent ring closure of these mixtures to the target compounds on further heating [5,22–25].

Transposing this process to microwave conditions, it was found that the reaction of benzil (1 equiv) with the 1-substituted biguanides **1a** and **1b** (1 equiv) in ethanol in a sealed tube (pressure-rated reaction vial) at 100°C in a self-tuning single-mode microwave cavity (5CEM Discovery apparatus) was complete after only 2–5 min. On cooling, the precipitated material was isolated by simple filtration, washing with cold ethanol, and

Scheme 1



recrystallization to give the known 1-(5-oxo-4,4-diphenyl-1-aryl-4,5-dihydro-1H-imidazol-2-yl)guanidines **2a** and **2b** (73% and 85%, respectively) [22]. These intermediates were, in turn, reacted with a series of aldehydes and ketones using microwave irradiation to construct a 22 member library containing the novel 6,8-dihydroimidazo[1,2-a] [1,3,5] triazines **3a**–**3v** (Table 1). In the experiment, compounds **2a** or **2b** in acetone containing a catalytic amount of acetyl chloride (see Experimental) were place in a sealed vessel and reacted in the microwave cavity at 100°C. The reaction time was varied from 5 to 20 min in increments of 5 min. However, in general, the reactions were complete after heating for 10 min, as judged by TLC. When a temperature above 100°C was used a complex reaction mixture was obtained from which the product was obtained in lower yield. The mass, IR, and NMR spectra unambiguously confirmed the structures **3a–3w**.

Table 1

Microwave-assisted synthesis of 6,8-dihydroimidazo [1,2-a] [1,3,5] triazines **3a–3v**.

Compound	Carbonyl Compound	R^1	R^2	R^3	Time (min)	Yield (%)
3a[a]	Acetone	4-CH_3-C_6H_5	CH_3	CH_3	10	65
3b[a]	2-Butanone	4-CH_3-C_6H_5	CH_3	CH_3CH_2	15	68
3c[a]	Cyclopentanone	4-CH_3-C_6H_5	$R^2 = R^3 = C_5H_8$		20	50
3d[b]	Anizaldehyde	4-CH_3-C_6H_5	H	4-OCH_3-C_6H_5	10	72
3e[b]	2-Chlorobenzaldehyde	4-CH_3-C_6H_5	H	2-Cl-C_6H_5	15	67
3f[b]	2,4-Dichlorobenzaldehyde	4-CH_3-C_6H_5	H	2,4-Cl_2-C_6H_5	5	72
3g[b]	*o*-Tolyl aldehyde	4-CH_3-C_6H_5	H	2-CH_3-C_6H_5	15	65
3h[b]	*m*-Tolyl aldehyde	4-CH_3-C_6H_5	H	3-CH_3-C_6H_5	10	68
3i[b]	4-Biphenylaldehyde	4-CH_3-C_6H_5	H	C_6H_5-C_6H_4	20	69
3j[b]	3-Nitrobenzaldehyde	4-CH_3-C_6H_5	H	3-NO_2-C_6H_5	15	71
3k[b]	3-(2-Nitrophenyl) propenal	4-CH_3-C_6H_5	H	2-NO_2-C_6H_5CHCH	5	68
3l[b]	4-Chlorobenzaldehyde	4-CH_3-C_6H_5	H	2-Cl-C_6H_5	20	54
3m[a]	Acetone	3,5-Cl_2-C_6H_5	CH_3	CH_3	15	66
3n[a]	2-Pentanone	3,5-Cl_2-C_6H_5	CH_3	$CH_3CH_2CH_2$	20	71
3o[a]	2-Butanone	3,5-Cl_2-C_6H_5	CH_3	CH_3CH_2	15	67
3p[a]	Cyclopentanone	3,5-Cl_2-C_6H_5	$R^2 = R^3 = C_5H_8$		20	52
3q[b]	*o*-Tolyl aldehyde	3,5-Cl_2-C6H5	H	2-CH_3-C_6H_5	10	63
3r[b]	*m*-Totyl aldehyde	3,5-Cl_2-C_6H_5	H	3-CH_3-C_6H_5	10	58
3s[b]	2-Chlorobenzaldehyde	3,5-Cl_2-C_6H_5	H	2-Cl-C_6H_5	10	61
3t[b]	2,4-Dichlorobenzaldehyde	3,5-Cl_2-C_6H_5	H	2,4-Cl_2-C_6H_5	10	64
3u[b]	3-Nitrobenzaldehyde	3,5-Cl_2-C_6H_5	H	3-NO_2-C_6H_5	10	63
3v[b]	3-(Nitrophenyl) propenal	3,5-Cl_2-C_6H_5	H	2-NO_2-C_6H_5CHCH	10	65

[a] Method A in the Experimental section.
[b] Method B in the Experimental section.

CONCLUSIONS

An efficient, rapid, and clean method for the preparation of a 22-membered library of 6,8-dihydroimidazo[1,2-a] [1,3,5] triazines has been developed using microwave-assisted synthesis.

EXPERIMENTAL

Materials. All commercially available reagents were used without further purification. Commercial solvents were distilled from an appropriate drying agent before use according to standard procedures.

Analysis. TLC analysis was performed on aluminum-precoated silica gel 60 plates. ^{1}H NMR spectra were recorded on a Varian Unity Inova 400 MHz spectrometer using DMSO-d_6 as a solvent. Chemical shifts (δ) are expressed in ppm downfield from TMS as internal standard. The letters s, d, t, q, and m are used to indicate singlet, doublet, triplet, quadruplet, and multiplet, respectively. IR spectra were taken on a Perkin-Elmer FT-IR 2000 spectrometer. Low-resolution mass spectra were obtained in the atmospheric pressure chemical ionization (positive or negative APCI) mode. All melting points (uncorrected) were recorded on a SMP2 apparatus.

Equipment. Microwave syntheses were carried out on a CEM Corp. Discover laboratory microwave with Explorer unit. Reaction times refer to hold times at the temperatures indicated and not to total irradiation time.

General procedure for synthesis of 1-(5-Oxo-4,4-diphenyl-1-aryl-4,5-dihydro-1H-imidazol-2-yl)guanidines 2a and 2b. Arylbiguanide hydrochloride (**1a** and correspondingly **1b**, 5 mmol) was added to the solution of sodium (0.11 g, 5 mmol) in absolute ethanol (25 mL). Precipitated sodium chloride is filtered off and benzil (1.05 g, 5 mmol) dissolved in absolute ethanol (6 mL) was added to the filtrate in a 30 mL microwave vial equipped with a pressure and temperature sensor, as well as a magnetic stirrer. The sealed tube was placed in a homogeneous microwave synthesis system. After irradiation at 100°C, measured by an internal fiber-optic temperature sensor immersed in the reaction mixture, for 2 (**2a**) and 5 (**2b**) min, respectively, the reaction mixture was cooled, and the precipitate was collected, washed with cold ethanol, and recrystallized from ethanol to give highly pure title.

2-[1-(4-Methylphenyl)-5-oxo-4,4-diphenyl-2-imidazolline-2-yl]-guanidines (2a). ^{1}H NMR (400 MHz, DMSO) δ 2.34 (s, 3H), 7.53–7.90 (m, 14H); IR (KBr) υ_{max}/cm^{-1}: 3115, 3166, 3061, 1593, 1537; UV–vis (MeOH) λ_{max}/nm 204 (0.406).

2-[1-(3,5-Dichlorophenyl)-5-oxo-4,4-diphenyl-2-imidazolline-2-yl]-guanidines (2b). ^{1}H NMR (400 MHz, DMSO) δ 7.21–7.98 (m, 13H); IR (KBr) υ_{max}/cm^{-1}: 3430, 3176, 3084, 1709, 1640, 1611, 1597, 1536, 798, 747, 697; UV–vis (MeOH) λ_{max}/nm 206 (0.688).

Method A: General procedure for synthesis of 6,8-dihydroimidazo[1,2-a] [1,3,5] triazines (3a–3c and 3m–3p) (carbonyl compounds with low boiling point). To a suspension of 1 equiv arylbiguanide (**2a** or **2b**) (0.1 mmol, 38.3 mg or 43.8 mg) in 3 mL of ketone or aldehyde in a microwave vial, 5 equiv acetyl chloride (0.5 mmol, 57.5 mg) was added. The vial was sealed and irradiated in a microwave reactor at 100°C for 10–20 min. The precipitates were collected by filtration and recrystallized from ethanol to give corresponding compound **3**.

Method B: General procedure for synthesis of 6,8-dihydroimidazo[1,2-a] [1,3,5] triazines (3d–3l and 3q–3v) (carbonyl compounds with high boiling point). To a suspension of 1 equiv arylbiguanide (**2a** or **2b**) (0.1 mmol, 38.3 mg or 43.8 mg) and 5 equiv of the ketone or aldehyde (0.5 mmol) in ethanol (3mL) in a microwave vial, 5 equiv acetyl chloride (0.5 mmol, 57.5 mg) was added. The vial was sealed and irradiated in a microwave reactor at 100°C for 10–20 min. The precipitates were collected by filtration and recrystallized from ethanol to give corresponding compound **3**.

2-Imino-4,4-dimethyl-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3a). mp: 255–257°C; ^{1}H NMR (400 MHz, DMSO) δ 1.10 (s, 6H), 2.36 (s, 3H), 7.33–7.64 (m, 14H), 7.98 (s, 1H), 8.85 (s, 1H), 9.74 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3467, 3273, 3091, 2797, 1772, 1658, 1630, 1576, 1534, 1495, 1452, 1192, 967, 698; MS (positive APCI, *m*/*z*): 424 [35, (M + 1)], 423 (100, M); UV–vis (MeOH) λ_{max}/nm 207 (0.510).

2-Imino-4-methyl-4-ethyl-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3b). mp: 255–257°C; ^{1}H NMR (400 MHz, DMSO) δ 0.66 (t, J = 7.2 Hz, 3H), 0.78–0.84 (m, 1H), 1.04–1.11 (m, 1H), 1.37 (s, 3H), 2.35 (s, 3H), 7.32–7.66 (m, 14H), 8.21 (s, 1H), 8.89 (s, 1H), 10.29 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3374, 3073, 2970, 2726, 1766, 1678, 1611, 1569, 1513, 1491, 724; MS (positive APCI, *m*/*z*): 438 [23, (M + 1)], 437 (100, M); UV–vis (MeOH) λ_{max}/nm 259 (0.179), 249 (0.159), 204 (0.603).

2-Imino-8-(4-methylpheyl)-6,6-diphenyl-4-spirocyclopentanon-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3c). mp: 270–272°C (dec.); ^{1}H NMR (400 MHz, DMSO) δ 1.02–1.86 (m, 8H), 2.10 (s, 3H), 7.34–7.58 (m, 14H), 8.03 (s, 1H), 8.94 (s, 1H), 10.06 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3359, 3036, 2962, 2739, 1767, 1681, 1610, 1567, 1490, 1450, 1193, 727, 703; MS (positive APCI, *m*/*z*): 450 [25, (M + 1)], 449 (100, M); UV–vis (MeOH) λ_{max}/nm 205 (0.610).

2-Imino-4-(4-methoxyphenyl)-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3d). mp: 274–276°C; ^{1}H NMR (400 MHz, DMSO) δ 0.66 (t, J = 7.2 Hz, 3H), 1.08 (m, 2H), 1.37 (s, 3H), 7.54–7.86 (m, 13H), 8.23 (s, 1H), 8.95 (s, 1H), 10.01 (s, 1H), IR (KBr) υ_{max}/cm^{-1}: 3353, 3053, 2795, 1777, 1674, 1611, 1588, 1487, 728, 712; MS (positive APCI, *m*/*z*): 502 [37, (M + 1)], 501 (100, M); UV–vis (MeOH) λ_{max}/nm 207 (0.554).

2-Imino-4-(2-chlorophenyl)-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3e). mp: 277–279°C; ^{1}H NMR (400 MHz, DMSO) δ 238 (s, 3H), 6.52 (s, 1H), 7.05–7.64 (m, 18H), 8.33 (s, 1H), 9.03 (s, 1H), 10.18 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3366, 3000, 2670, 1770, 1677, 1616, 1573, 1488, 1195, 760, 728; MS (positive APCI, *m*/*z*): 507 [40, (M + 2)], 506 [47, (M + 1)], 505 (100, M); UV–vis (MeOH) λ_{max}/nm 205 (0.569).

2-Imino-4-(2,4-dichlorophenyl)-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3f). mp: 278–280°C; ^{1}H NMR (400 MHz, DMSO) δ 2.38 (s, 3H), 6.55 (s, 1H), 7.11–7.63 (m, 17H), 8.23 (s, 1H), 9.04 (s, 1H), 10.21 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3356, 3036, 2623, 1766, 1679, 1616, 1579, 1492, 1191, 762, 733, 693; MS (positive APCI, *m*/*z*): 541 [70, (M + 2)], 539 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.531).

2-Imino-4-(2-methylpheyl)-8-(4-methylpheyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3g). mp: 278–280°C; ^{1}H NMR (400 MHz, DMSO) δ 2.15 (s, 3H), 2.39 (s, 3H), 6.38 (s, 1H), 6.85–7.60 (m, 18H), 8.23 (s, 1H), 8.95 (s, 1H), 10.15 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3360, 3021, 2702, 1769, 1677, 1616, 1573, 1486, 1192, 725; MS (positive APCI, *m*/*z*): 486 [27, (M + 1)], 485 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.720).

2-Imino-4-(3-methylpheyl)-8-(4-methylpheyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3h). mp: 220–222°C; ^{1}H NMR (400 MHz, DMSO) δ 2.28 (s, 3H), 2.39 (s,3H), 6.33 (s,1H), 6.66–7.61 (m, 18H), 8.16 (s, 1H), 8.98 (s, 1H), 10.07 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3423, 3108, 2951, 1767, 1650, 1610, 1581, 1498, 1180, 696, 486; MS (positive APCI, *m*/*z*): 486 [25, (M + 1)], 485 (100, M); UV–vis (MeOH) λ_{max}/nm 207 (0.529).

2-Imino-4-(biphenyl-4-yl)-8-(4-methylpheyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3i). mp: 257–259°C; ^{1}H NMR (400 MHz, DMSO) δ 2.39 (s, 3H), 6.48 (s, 1H), 7.04–7.62 (m, 23H), 8.54 (s, 1H), 9.03 (s, 1H), 10.17 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3352, 3060, 2747, 1768, 1665, 1615, 1579, 1495, 1193, 764, 732, 697; MS (positive APCI, *m*/*z*): 548 [47, (M + 1)], 547 (100, M); UV–vis (MeOH) λ_{max}/nm 260 (0.179), 243 (0.155), 205 (0.433).

2-Imino-4-(3-nitrophenyl)-8-(4-methylpheyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3j). mp: 276–279°C; ^{1}H NMR (400 MHz, DMSO) δ 2.39 (s, 3H), 6.69–7.99 (m, 18H), 8.46 (s, 1H), 9.10 (s, 1H), 10.27 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3187, 3096, 2960, 1771, 1675, 1650, 1606, 1493, 1193, 690; MS (positive APCI, *m*/*z*): 518 [17, (M + 2)], 516 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.606).

2-Imino-4-(2-nitrostyryl)-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3k). mp: 279–281°C (dec.); ^{1}H NMR (400 MHz, DMSO) δ 2.36 (s, 3H), 5.95 (d, J = 8.4 Hz, 1H), 6.11 (dd, J_1 = 15.6 Hz, J_2 = 8.4 Hz, 1H) 6.49 (d, J = 14.2 Hz, 1H), 7.07–7.86 (m, 16H), 7.85 (d, J = 7.8 Hz, 1H), 8.26 (s, 1H), 9.00 (s, 1H), 9.71 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3424, 3115, 2363, 1773, 1675, 1660, 1612, 1518, 1198, 768, 695; MS (positive APCI, *m*/*z*): 543 [37, (M + 1)], 542 (100, M); UV–vis (MeOH) λ_{max}/nm 205 (0.466).

2-Imino-4-(4-chlorophenyl)-8-(4-methylpheyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3l). mp: 283–285°C; ^{1}H NMR (400 MHz, DMSO) δ 2.38 (s, 3H), 6.47 (s, 1H), 7.08–7.61 (m, 18H), 8.43 (s, 1H), 9.02 (s, 1H), 10.13 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3368, 3086, 2682, 1779, 1672, 1613, 1578, 1494, 1192, 728, 697; MS (positive APCI, *m*/*z*): 506 [55, (M + 1)], 505 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.456).

2-Imino-4,4-dimethyl-8-(3,5-dichlorophenyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3m). mp: 271–273°C; ^{1}H NMR (400 MHz, DMSO) δ 1.10 (s, 6H), 7.55–7.86 (m, 13H), 8.04 (s, 1H), 8.92 (s, 1H), 9.80 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3361, 3022, 2755, 1780, 1678, 1614, 1588, 1491, 1454, 1427, 1174, 1029, 728; MS (positive APCI, *m*/*z*): 479 [95, (M + 2)], 478 [35, (M + 1)], 477 (100, M); UV–vis (MeOH) λ_{max}/nm 208 (0.469).

2-Imino-4-methyl-4-propyl-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3n). mp: 248–252°C; ^{1}H NMR (400 MHz, DMSO) δ 0.50–0.53 (t, J = 7.2 Hz, 3H), 0.66–0.75 (m, 2H), 1.03–1.19 (m, 1H), 1.19–1.23 (M, 1H), 1.43 (s, 3H), 7.34–7.87 (m, 17H), 8.03 (s, 1H), 8.88 (s, 1H), 9.76 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3360, 3026, 2778, 1777, 1675, 1613, 1589, 1492, 1197, 759, 727; MS (positive APCI, *m*/*z*): 507 [50, (M + 2)], 506 [27, (M + 1)], 505 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.887).

2-Imino-4-methyl-4-ethyl-8-(3,5-dichlorophenyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3o). mp: 265–267°C; ^{1}H NMR (400 MHz, DMSO) δ 0.66 (t, J = 7.2 Hz, 3H), 1.08 (m, 2H), 1.37 (s, 3H), 7.54–7.86 (m, 13H), 8.23 (s, 1H), 8.95 (s, 1H), 10.01 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3353, 3053, 2795, 1777, 1674, 1611, 1588, 1487, 728, 712; MS (positive APCI, *m*/*z*): 492 [60, (M + 1)], 491 (85, M), 437 [80, (M-54)]; UV–vis (MeOH) λ_{max}/nm 207 (0.554).

2-Imino-8-(3,5-dichlorophenyl)-6,6-diphenyl-4-spirocyclopentanon-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3p). mp: 267–269°C (dec.); ^{1}H NMR (400 MHz, DMSO) δ 1.01–2.06 (m, 8H), 7.54–7.89 (m, 13H), 8.07 (s, 1H), 9.00 (s, 1H), 10.08 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3360, 3021, 2800, 1778, 1676, 1611, 1588, 1486, 1186, 727, 710; MS (positive APCI, *m*/*z*): 505 [75, (M + 2)], 504 [35, (M + 1)], 503 (100, M); UV–vis (MeOH) λ_{max}/nm 207 (0.452).

2-Imino-4-(2-methylpheyl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2, 3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3q). mp: 273–275°C; ^{1}H NMR (400 MHz, DMSO) δ 2.19 (s, 3H), 6.38 (s, 1H), 8.00–6.38 (m, 17H), 8.47 (s, 1H), 9.04 (s, 1H), 10.24 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3368, 3046, 2695, 1773, 1675, 1617, 1590, 1482, 759, 729, 706; MS (positive APCI, *m*/*z*): 541 [70, (M + 1)], 539 (100, M); UV–vis (MeOH) λ_{max}/nm, 207 (0.425).

2-Imino-4-(3-methylpheyl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3r). mp: 269–271°C; ^{1}H NMR (400 MHz, DMSO) δ 2.49 (s, 3H), 6.30 (s, 1H), 6.67–7.96 (m, 17H), 8.39 (s, 1H), 9.00 (s, 1H), 9.98 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3358, 3059, 2696, 1776, 1677, 1659, 1619, 1575, 1490, 1187, 751, 697; MS (positive APCI, *m*/*z*): 541 [83, (M + 2)], 539 (100, M), 538 [55, (M-1)]; UV–vis (MeOH) λ_{max}/nm 207 (0.383).

2-Imino-4-(2-chlorophenyl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3s). mp: 280–282°C; ^{1}H NMR (400 MHz, DMSO) δ 6.51 (s, 1H), 7.05–7.61 (m, 17H), 8.24 (s, 1H), 9.10 (s, 1H), 10.15 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3355, 3021, 2688, 1774, 1673, 1613, 1481, 1197, 758, 706; MS (positive APCI, *m*/*z*): 561 [100, (M + 2)], 560 [40, (M + 1)], 559 (55, M); UV–vis (MeOH) λ_{max}/nm 208 (0.419).

2-Imino-4-(2,4-dichlorophenyl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one. HCl (3t). mp: 270–272°C; ^{1}H NMR (400 MHz, DMSO) δ 6.54 (s, 1H), 7.07–7.95 (m, 16H), 8.51 (s, 1H), 9.15 (s, 1H), 10.40 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3355, 3062, 2680, 1781, 1673, 1617, 1587, 1494, 1449, 1186, 752, 698; MS (positive APCI, *m*/*z*): 597 [30, (M + 1)], 595 (M, 100), 593 [60, (M-2)]; UV–vis (MeOH) λ_{max}/nm 208 (0.325).

2-Imino-4-(3-nitrophenyl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3u). mp: 274–276°C; ^{1}H NMR (400 MHz, DMSO) δ 6,70 (s, 1H), 7.00–7.98 (m, 17H), 8.51 (s, 1H), 9.11 (s, 1H), 10.31 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 3349, 3065, 2667, 1787, 1680, 1620, 1527, 1493, 1187, 753, 693, 680; MS (positive APCI, *m*/*z*): 572 [55, (M + 2)], 570 (100, M); UV–vis (MeOH) λ_{max}/nm 206 (0.497).

2-Imino-4-(2-nitrostyryl)-8-(3,5-dichlorophenyl)-6,6-diphenyl-2,3-dihydro-4H-imidazo[2,3-d]-1,3,5-triazin-7(6H)one.HCl (3v). mp: 280–282°C (dec.); ^{1}H NMR (400 MHz, DMSO) δ 5.98–6.07 (m, 2H), 6.51 (d, J = 14.2 Hz, 1H), 7.06–7.92 (m, 16H), 8.39 (s, 1H), 9.07 (s, 1H), 9.83 (s, 1H); IR (KBr) υ_{max}/cm^{-1}: 334, 3028, 2787, 1773, 1679, 1664, 1612, 1523, 1487, 1185, 734, 699; MS (positive APCI, *m/z*): 598 [97, (M + 2)], 597 [70, (M + 1)], 596 (100, M); UV–vis (MeOH) λ_{max}/nm 207 (0.614).

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