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Paper

Cobalt (II) catalyzed C(sp)-H bond functionalization of alkynes with phenyl hydrazines: A facile access to diaryl 1,2-diketones†‡

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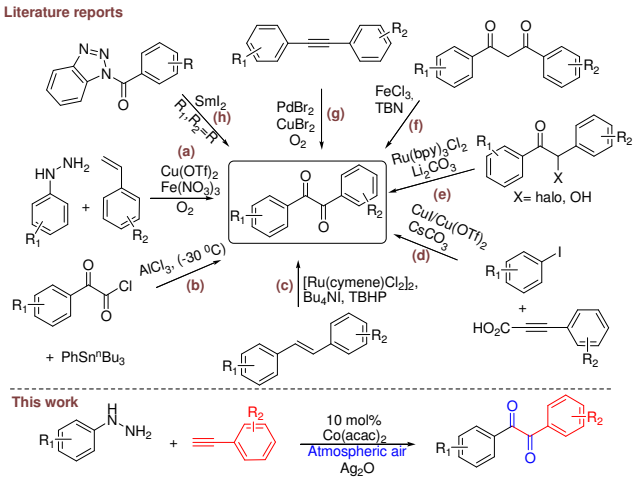
A cobalt acetylacetonate catalyzed oxidative diketonation of alkynes via C(sp)-H bond functionalization has been described. The reaction involves a free-radical mechanism, wherein the phenyl radical formed from phenyl hydrazine couples with Co(II) activated alkyne to produce 1,2-diketones. The reaction proceeds at room temperature in DMF with the use of Ag_2O/air as oxidizing system. The utility of the protocol for synthesis of a series of imidazoles including a potent platelet aggregation inhibitor trifenagrel has been demonstrated.

Introduction[1]

Diaryl 1,2-diketones are privileged building blocks for the synthesis of biologically active heterocycles including imidazoles, quinoxalines and indolone-*N*-oxides.[1-4] 1,2-Diketones are also precursors for the synthesis of *N*-heterocyclic carbenes which are used as ligands in organometallic chemistry and catalysis.[5] Because of their importance in medicinal and organometallic chemistry, 1,2-diketones are attractive chemotypes to synthetic chemists.[6] Numerous methods are available for their synthesis (Scheme 1) including (a) radical coupling of phenyl hydrazine with styrene in the presence of copper triflate/ ferric nitrate,[7] (b) $AlCl_3$-catalyzed cross-coupling of α-oxo acid chloride with organostannane compound at –30 °C),[8] (c) Ru-catalyzed oxidation of stilbenes,[9] (d) coupling of iodobenzene with phenyl propiolic acid in the presence of CuI/ $Cu(OTf)_2$,[10] (e) $Ru(bpy)_2Cl_2$,[9] $VOCl_3$,[11] Fe_3O_4,[12] $Bi(NO_3)_3$/$Cu(OAc)_2$[13] catalyzed oxidation of α-halo or α-hydroxy ketones, (f) conversion of 1,3-diketones to 1,2-diketones in the presence of Lewis acid ($FeCl_3$) and TBN or I_2/DMSO,[14, 15] (g) $PdBr_2$/ $CuBr_2$,[16-19] $PdCl_2$,[20] CuI,[21] Ru,[22] or $KMnO_4$[23] catalyzed Wacker-type oxidation of internal alkynes, (h) SmI_2 catalyzed transformation of N-acylbenzotriazoles to 1,2-diketones.[24, 25] Additionally, few metal-free synthesis of 1,2-diketones have also been reported.[26, 27]



Scheme 1. Literature methods and our new method for preparation of 1,2-diketones

Although several methods are reported, most of them have one or other drawback such as: (a) expensive metal catalysts,[9, 11, 13, 16-19] (b) prior synthesis of starting materials (phenyl propiolic acids and diphenyl alkynes,[10, 16-19, 23] α-haloketones,[9, 11, 13] and 1,3-diketones[14, 15]) is required, and (c) many involve vigorous and harsh reaction conditions. In this context, we thought of exploiting terminal alkynes towards the synthesis of diaryl 1,2-diketones *via* transition metal catalyzed C(sp)-H bond functionalization.

Transition metal-catalyzed coupling of sp C−H bond of alkynes is perhaps one of the most synthetically useful C−H bond functionalization reactions.[28-32] Among various transition metal-catalyzed C-H bond functionalizations, cobalt-mediated C−H bond functionalization has met with recent success for C-C bond formation reactions.[32] Herein, we employed the strategy to utilize a phenyl hydrazine as a phenyl radical source,[33-38] for coupling with activated C−H of phenyl acetylene to yield diphenyl 1,2-

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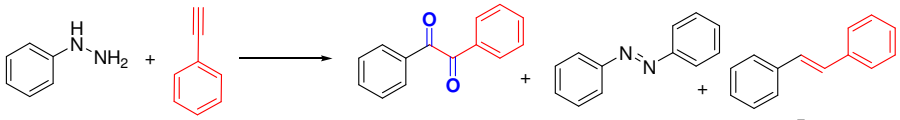
Table 1. Optimization studies[a]



1a **2a** **3a** **4a** **5a**

Entry	Oxidant (mol%)	Catalyst (mol%)	Solvent	Temp.	Time (h)	**3a** yield[b]
1	Air	None	DMF[c]	rt	0.5	20
2	Air	None	DMSO	rt	8	5
3	Air	None	DMF	rt	8	25
4	O_2	None	DMF	rt	0.5	16
5	O_2	None	DMF	rt	8	23
6	none[d]	None	DMF	rt	8	traces[e]
7	Air, $K_2S_2O_8$ (50)	None	DMF	rt	8	5
8	Air, $Na_2S_2O_8$ (50)	None	DMF	rt	8	5
9	Air, BQ (50)	None	DMF	rt	8	35
10	Air, MnO_2 (50)	None	DMF	rt	8	32
11	Air, $PhI(OAc)_2$ (50)	None	DMF	rt	8	30
12	Air, AgOAc (50)	None	DMF	rt	8	30
13	Air, Ag_2CO_3 (50)	None	DMF	rt	8	20
14	Air, Ag_2O (50)	None	DMF	rt	8	38
15	O_2, Ag_2O (50)	None	DMF	rt	8	38
16	Air, Ag_2O (10)	None	DMF	rt	0.5	35
17	Air, Ag_2O (10)	None	DMF	rt	8	40[f]
18[g]	Air	$CuCl_2$ (10)	DMF	rt	8	0
19	Air	CuBr (10)	DMF	rt	8	0
20	Air	CuI (10)	DMF	rt	8	0
21	Air	$Cu(OTf)_2$ (10)	DMF	rt	8	0
22	**Air**	$Cu(OTf)_2$ (10), $Fe(NO_3)_3$ (10), DABCO (3 equiv.)	DMF	0	8	50
23	Air	Co(acetate) (10)	DMF	rt	8	58
24	Air	$Co(acac)_2$ (10)	DMF	rt	8	64
25[h]	**Air, Ag_2O (10)**	**$Co(acac)_2$ (10)**	**DMF**	**rt**	**8**	**70**[g]
26	Air, Ag_2O (10)	$Co(acac)_2$ (10)	DMF	70	8	35
27	Air, Ag_2O (10)	$Co(acac)_2$ (10)	DMF: H_2O (9:1)	rt	8	68

[a]**1a** (1.0 mmol), **2a** (1.2 mmol) and oxidizing agent and/ or catalyst (wherever mentioned) in a mentioned solvent at rt; [b]Isolated yields after silica gel column chromatography; [c]reaction does not proceed in other solvents such as ACN, DCE, dioxane, ethanol, methanol, toluene and NMP; [d]reaction under N_2 atmosphere; [e] 1.3% yield, determined by GCMS; [f] under this reaction condition, we have also isolated side products azobenzene **4a** (14%) and stilbene **5a** (13%); [g] Reactions does not proceed in presence of iron acetate, iron bromide, gold chloride and palladium acetate catalysts (10 mol%), under air, DMF, rt, 8 h reaction condition; [h] bold entry indicates optimized reaction condition for synthesis of 1,2-diketones; BQ: benzoquinone.

diaryl ketones. To the best of our knowledge, there has been no previous report on the direct synthesis of 1,2-diketones from terminal alkynes and phenyl hydrazines. In the present communication, we report $Co(acac)_2$ catalyzed synthesis of diaryl 1,2-diketones using atmospheric oxygen and Ag_2O as a mixed oxidizing system (Scheme 1). The developed method showed good substrate scope for variety of substituted phenyl hydrazines and phenyl acetylenes.

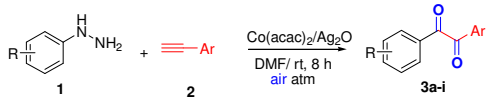
The study was initiated with the preliminary reaction of phenyl hydrazine **1a** with phenylacetylene **2a** in an open air atmosphere using various solvents. Among various solvents investigated, DMF was the best solvent for this reaction. Reaction of **1a** with **2a** in DMF at room temperature for 30 min led to the formation of diphenyl 1,2-diketone **3a** in 20% yield (Table 1, entry 1). Intriguingly, this result does not involve the use of any metal catalysts or oxidizing agent; however, the poor yields warranted optimization of the reaction conditions. When the open air catalyst-free reaction was continued further for 8 h, the desired product was formed in 25% yield (entry 3). When the reaction was performed with molecular oxygen, the desired product **3a** was formed in similar yields to that of atmospheric air (entries 1 and 3 *versus* 4-5). Interestingly, under N_2 atmosphere in dry DMF, only trace amount of product was formed (1.3%, entry 6), which indicated the role of oxygen for the progress of the reaction. Next, we investigated the reaction in the presence of various oxidants such as $K_2S_2O_8$, $Na_2S_2O_8$, benzoquinone, MnO_2, $PhI(OAc)_2$ and silver catalysts AgOAc, Ag_2CO_3 and Ag_2O in DMF (entries 7-17). Reactions performed in the presence of benzoquinone, MnO_2, $PhI(OAc)_2$, AgOAc and Ag_2O showed formation of diphenyl 1,2-diketone **3a** in 30-40% yield. The 10 mol% of Ag_2O was found to be optimal for efficient formation of desired product (entry 17). We further made attempts to improve the product yield beyond 40% under catalyst and oxidant free reaction conditions, by varying the relative equivalents of both the substrates; however all such attempts were unsuccessful.

Next, we tried to improve the reaction yield by using various catalysts such as iron acetate, iron bromide, gold chloride and palladium acetate, Cu-based catalysts $CuCl_2$, CuBr, CuI, $Cu(OTf)_2$, Co(acetate) and $Co(acac)_2$ (entries 18-21 and 23-24). The copper triflate/ ferric nitrate,[7] which was used earlier for the synthesis of 1,2-diketones from phenyl hydrazines and styrenes, was also investigated for our reaction. Under this condition (entry 22), desired 1,2-diketone **3a** was formed in 50% yield. However, with the use of only copper triflate, it did not led to the product formation (entry 21). Among various catalysts attempted, $Co(acac)_2$ in the presence of Ag_2O provided best results (70% yield of **3a**) (entry 25). When the entry 25 condition, was attempted under heating (70 °C), the product yield was decreased

from 70 to 35% (entry 25 *versus* 26). Next, in order to check whether addition of water as an additional oxygen source results in the improvement of product yield, reaction was performed in the mixture of DMF and water. Reaction in DMF: water (9:1) led to the formation of equivalent yield of the desired product **3a** to that of optimized condition (entry 27 *versus* 25). Thus, we used entry 25 as an optimized reaction for further experiments.

With the optimized reaction condition in hand, we explored the utility of this approach for oxidative coupling of various substituted phenyl hydrazines with phenylacetylene. As shown in Table 2, various substituted phenyl hydrazines were well tolerated in the reaction. The phenyl hydrazines substituted with various electron-withdrawing groups such as F, Cl, Br, I, CF_3 (entries 2, 5, 12, 13, 15) as well as electron-donating groups such as OCF_3, *t*-Bu groups (entries 3 and 10) gave corresponding 1,2-diketones in good yields. In order to check whether the reaction works with –CN, -NO_2 substituents on aromatic rings, the reaction between 4-cyano phenyl hydrazine and 3-nitro phenyl hydrazine with phenylacetylene was attempted, however desired products were not obtained (entries 29-30 in Table 2). The phenylacetylenes substituted with various electron-donating groups (e.g. methyl, ethyl, propyl, OMe, acetylene, tert-butyl; entries 6-9 and 21-26), as well as electron withdrawing groups (e.g. F, Cl, Br; entries 11, 14, 16), participated well in the reaction. Reaction of 2-ethynylpyridine (entry 31) was also attempted, however the product was not formed. However, the reaction was also well tolerated for thiophene heterocycle (entries 17 and 27), bicyclic (entries 18 and 28), tricyclic (entry 19) and biphenyl (entry 20) acetylenes, producing desired products in good yields All our attempts with aliphatic alkynes such as 1-hexyne, 1-heptyne, 1-octyne failed to give desired 1,2-diketones; wherein primarily the azobenzene **4a** and styryl products were formed.

Table 2. Substrate scope for the synthesis of diaryl 1,2-diketones[a]

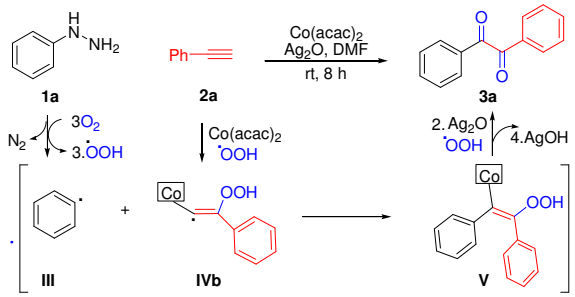


1 2 3a-i

Entry	R	Ar	Product	% yield[b]
1	H	-Ph	**3a**	70
2	*p*-CF_3	-Ph	**3b**	65
3	*p*-OCF_3	-Ph	**3c**	68
4	*m*-CF_3	-Ph	**3d**	68
5	p-I	-Ph	**3e**	72
6	H	-Ph(*p*-Me)	**3f**	70
7	H	-Ph(*p*-C≡CH)	**3g**	64
8	H	-Ph(*p*-$CH_2CH_2CH_3$)	**3h**	60
9	H	-Ph(*p*-tBu)	**3i**	68
10	*p*-tBu	-Ph	**3i**	70
11	H	-Ph(*p*-F)	**3j**	68
12	*p*-F	-Ph	**3j**	70
13	*p*-Cl	-Ph	**3k**	62
14	H	-Ph(*p*-Cl)	**3k**	67
15	*p*-Br	-Ph	**3l**	68
16	H	-Ph(*p*-Br)	**3l**	66
17	H	-thiophen-3-yl	**3m**	62
18	H	-naphthalen-1-yl	**3n**	72
19	H	-anthracen-10-yl	**3o**	64
20	H	-Ph(*p*-Ph)	**3p**	64
21	*p*-OCF_3	-Ph(*p*-OMe)	**3q**	62
22	*p*-CF_3	-Ph(*p*-Me)	**3r**	65
23	*p*-CF_3	-Ph(*p*-Et)	**3s**	68
24	*p*-tBu	-Ph(*p*-Me)	**3t**	63
25	*p*-F	-Ph(*p*-OMe)	**3u**	66
26	*p*-I	-Ph(*p*-OMe)	**3v**	65
27	*p*-Br	-thiophen-3-yl	**3w**	63
28	*p*-F	-naphthalen-1-yl	**3x**	68
29	*p*-CN	-Ph	**3y**	0
30	*m*-NO_2	-Ph	**3z**	0
31	H	-pyridin-2-yl	**3aa**	0

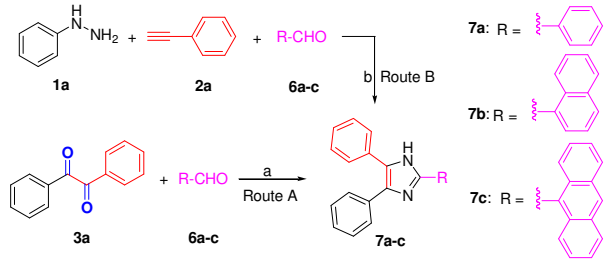
[a]Reagents and conditions: **1** (1.0 mmol), **2** (1.2 mmol), Co(acac)$_2$/Ag_2O (10 mol% each), DMF, rt, 8 h. [b]Isolated yields after silica gel column chromatography.

The possibility of free-radical mechanism was investigated by performing reaction in the presence of free-radical quencher TEMPO. Reaction performed in the presence of TEMPO produced trace amounts of product **3a**, which indicated that the reaction involves free-radical mechanism. As confirmed by TEMPO experiment and quantum chemical calculations (details provided in section S6 of ESI), the reaction pathway possibly involves a radical mechanism. The reaction mechanism showing key possible reaction intermediates is depicted in Scheme 2.



Scheme 2. Plausible reaction mechanism

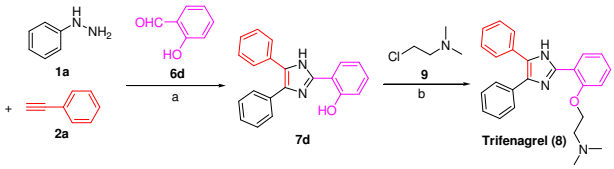
Next, utility of the protocol for the synthesis of imidazoles was investigated. The treatment of 1,2-diketone **3a** with aldehydes **6a-c** in acetic acid produced imidazoles **7a-c** in 60-70% yields (Scheme 3, route A). It is noteworthy to mention that the one-pot synthesis of 2,4,5-trisubstituted imidazoles **7a-c** directly from phenylacetylene **2a** and phenyl hydrazine **1a** was also successful (Scheme 3, route B).



Scheme 3. Synthesis of imidazoles **7a-c**. Reagents and conditions: (a). AcOH, NH_4OAc, 120 °C, 2 h, 60-70%; (b) Co(acac)$_2$, Ag_2O/DMF, air atm, AcOH, NH_4OAc, 120 °C, 2 h, 55-65%.

Trifenagrel (**8**), a 2,4,5-triaryl imidazole is a potent platelet aggregation inhibitor.[39] The present method was utilized for the synthesis of this inhibitor as depicted in Scheme 4. It is noteworthy to mention that we could prepare imidazole **7d** using a one-pot manner directly from precursors **1a**, **2a** and **6d**. Treatment of phenyl hydrazine **1a**, phenylacetylene **2a** and 2-

formyl phenol **6d** in one-pot in presence of the Co(II)/Ag_2O/air catalytic system and NH_4OAc/ AcOH produced imidazole **7d**. Treatment of intermediate **7d** with 2-chloro-N,N-dimethylethanamine (**9**) in the presence of K_2CO_3 produced trifenagrel (**8**) in 70% yield.



Scheme 4. Synthesis of trifenagrel (**8**). Reagents and conditions: (a). 10 mol% $Co(acac)_2$, 10 mol% Ag_2O/DMF, air atm, AcOH, NH_4OAc, 120 °C, 2 h, 55%; (b) K_2CO_3, rt, 6 h, 70%.

Conclusion

In summary, we have successfully developed new cobalt (II) catalyzed synthesis of 1,2-diketones using air/Ag_2O as a mixed oxidizing system. This is the first report on the synthesis of 1,2-diketones from terminal alkynes. Developed method is operationally simple and could be used efficiently for the preparation of variety of biologically important heterocycles as demonstrated by the synthesis of trifenagrel. This protocol may serve as an excellent method for C–H activation of terminal alkynes to study its scope in other reactions.

Experimental section

General. All chemicals were obtained from Sigma-Aldrich Company and used as received. ^1H, ^{13}C and DEPT NMR spectra were recorded on Brucker-Avance DPX FT-NMR 500 and 400 MHz instruments. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$, 7.26 ppm). Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 125 MHz or 100 MHz: chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent ($CDCl_3$, 77 ppm). ESI-MS and HR-ESIMS spectra were recorded on Agilent 1100 LC-Q-TOF and HRMS-6540-UHD machines. IR spectra were recorded on Perkin-Elmer IR spectrophotometer. Melting points were recorded on digital melting point apparatus.

General procedure for synthesis of diaryl 1,2-diketones 3a-x. To the mixture of phenyl hydrazine (1.0 equiv.) and phenyl acetylene (1.2 equiv.) in dimethylformamide was added 10 mol% of cobalt acetylacetanoate $Co(acac)_2$, 10 mol% silver oxide (Ag_2O) and reaction was stirred at room temperature for 8 h. After completion of the reaction (monitored by TLC), reaction mixture was filtered using whatman filter paper and then was extracted with ethyl acetate. The combined organic layers were dried over anhydrous sodium sulphate and evaporated on vacuo rotavapor to get crude product. The crude product was purified by silica gel (#100-200) column chromatography using *n*-hexane and ethyl acetate as an eluent to get pure products **3a-3x** in 60-72% yield.

Benzil (***3a***)*:*[7] Yellow solid; m.p. 94-96 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.99 (d, *J* = 8.0 Hz, 4H), 7.66 (t, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 8.0 Hz, 4H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 194.6, 135.0, 133.0, 129.9, 129.1; IR ($CHCl_3$): ν_{max} 3438, 2923, 1725, 1682, 1596, 1581, 1449 cm^{-1}; GC-MS: *m/z* (EI) 210 (M^+, 7), 105 (100), 77 (64), 51 (17).

1-Phenyl-2-(4-(trifluoromethyl) phenyl) ethane-1,2-dione (***3b***)*:*[7] Brown sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, *J* = 8.0 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.69 (t, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.5, 193.1, 136.0 (t, $^2J_{CF}$ = 32.69 Hz), 135.6, 135.3, 132.6, 130.3, 130.0, 129.2, 126.2; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.36 (s, 3F); IR ($CHCl_3$): ν_{max} 3435, 2922, 1737, 1674, 1596, 1450 cm^{-1}; GC-MS: *m/z* (EI) 278 (M^+, 1), 173 (16), 145 (22), 125 (5), 105 (100), 77 (31), 51 (6).

1-Phenyl-2-(4-(trifluoromethoxy) phenyl) ethane-1,2-dione (***3c***)*:*[7] Brown sticky oil; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.8, 192.7, 153.9, 135.2, 132.7, 132.1, 130.0, 129.1, 128.8 (t, $^1J_{CF}$ = 32.69 Hz), 120.7 ; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -57.54 (s, 3F); IR ($CHCl_3$): ν_{max} 3437, 1674, 1599, 1259, 1211, 1167 cm^{-1}; GC-MS: *m/z* (EI) 294 (M^+, 2), 189 (55), 105 (100), 95 (9), 77 (26), 63 (7), 50 (3).

1-Phenyl-2-(3-(trifluoromethyl) phenyl) ethane-1,2-dione (***3d***)*:*[7] Brown sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.28 (s, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.71-7.64 (m, 2H), 7.54 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.3, 192.6, 135.3, 133.6, 133.2, 132.6, 132.0 (t, $^2J_{CF}$ = 41.50 Hz), 131.2, 130.0, 129.7, 129.2, 126.5; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -62.93 (s, 3F); IR ($CHCl_3$): ν_{max} 3438, 2924, 1686, 1674, 1611, 1556, 1450 cm^{-1}; GC-MS: *m/z* (EI) 278 (M^+ 1), 259 (4), 173 (18), 145 (19), 125 (4), 105 (10), 95 (1), 77 (7), 51 (1).

1-(4-Iodophenyl)-2-phenylethane-1,2-dione (***3e***)*:*[40] Yellow solid; m.p. 79-80 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.97 (d, *J* = 8.0 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.69-7.66 (m, 3H), 7.52 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.9, 193.7, 138.4, 135.1, 132.8, 132.3, 131.0, 130.0, 129.1, 103.7; IR ($CHCl_3$): ν_{max} 3437, 2924, 1671, 1581, 702 cm^{-1}; GC-MS: *m/z* (EI) 336 (M^+ 7), 231 (69), 209 (8), 203 (15), 105 (100), 77 (54), 50 (16).

1-Phenyl-2-(p-tolyl)ethane-1,2-dione (***3f***)*:*[7] Yellow solid; m.p. 94-96 ^0C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 194.8, 194.4, 146.3, 134.8, 133.1, 130.6, 130.1, 129.9, 129.8, 129.1, 22.0 ; IR ($CHCl_3$): ν_{max} 3436, 2923, 1726, 1671, 1450, 1216 cm^{-1}; GC-MS: *m/z* (EI) 224 (M^+ 5), 119 (100), 105 (22), 91 (28), 77 (19), 65 (12), 51 (7).

1-(4-Ethynylphenyl)-2-phenylethane-1,2-dione (***3g***)*:* Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.98-7.93 (m, 4H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 8.0 Hz, 2H), 3.32 (s, 1H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 194.1, 193.6, 135.1, 132.8, 132.7, 130.0, 129.7, 129.1, 128.8, 128.5,

82.5, 81.7; IR ($CHCl_3$): ν_{max} 3440, 2921, 1665, 1617, 1450 cm^{-1}; GC-MS: *m/z* (EI) 234 (M^+ 6), 206 (32), 129 (100), 105 (88), 101 (35), 77 (50), 75 (22), 51 (17).

*1-Phenyl-2-(4-propylphenyl) ethane-1,2-dione (**3h**):* Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.99-7.88 (m, 4H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 2.66 (t, *J* = 8.0 Hz, 2H), 1.70-1.59 (m, 2H), 0.95 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 194.8, 194.4, 150.9, 134.8, 130.8, 130.1, 129.9, 129.2, 129.0, 128.8, 38.3, 24.2, 13.8; IR ($CHCl_3$): ν_{max} 3439, 2923, 1721, 1668, 1604, 1450, 1049 cm^{-1}; GC-MS: *m/z* (EI) 252 (M^+, 2), 147 (100), 119 (4), 91 (18), 51 (5).

*1-(4-(Tert-butyl)phenyl)-2-phenylethane-1,2-dione (**3i**):*[7] Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.99 (d, *J* = 8.0 Hz, 2H), 7.92 (d, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.54-7.49 (m, 4H), 1.34 (s, 9H);^{13}C NMR ($CDCl_3$, 100 MHz): δ 194.8, 194.3, 159.1, 134.8, 133.1, 130.5, 129.9, 130.0, 126.1, 31.0; IR ($CHCl_3$): ν_{max} 3449, 1733, 1669, 1598, 1217, 1177 cm^{-1}; GC-MS: *m/z* (EI) 266 (M^+, 2), 161 (100), 146 (10), 105 (20), 77 (20), 51 (6).

*1-(4-Fluorophenyl)-2-phenylethane-1,2-dione: (**3j**):*[7] Brown solid, m.p. 68-70 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.04 (dd, *J* = 4.0 & 4.0 Hz, 2H), 7.98 (d, *J* = 4.0 Hz, 2H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 2H); 7.19 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 194.1, 192.7, 168.1, (d, $^1J_{CF}$ = 258 Hz), 135.1, 132.9, 132.8, 132.7, 130.0, 129.1, 116.5, (d, $^2J_{CF}$ = 22.13 Hz); ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -101.18 (s, 1F); IR ($CHCl_3$): ν_{max} 3440, 1657, 1643, 1633, 1452, 718 cm^{-1}; GC-MS: *m/z* (EI) 228 (M^+, 6), 123 (60), 105 (100), 77 (50), 51 (15).

*1-(4-Chlorophenyl)-2-phenylethane-1,2-dione (**3k**):*[7] Yellow solid, m.p. 66-67°C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.98-7.92 (m, 4H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.54-7.48 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.9, 193.2, 141.9, 135.1, 131.3, 131.2, 130.0, 129.5, 129.4, 129.1; IR ($CHCl_3$): ν_{max} 3436, 2923, 1721, 1676, 1587, 1208, 837 cm^{-1}; GC-MS: *m/z* (EI) 244 (M^+, 2), 209 (4), 139 (41), 111 (20), 105 (100), 77 (50), 51 (13).

*1-(4-Bromophenyl)-2-phenylethane-1,2-dione (**3l**):*[7] Yellow solid, m.p. 86-88 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 3H), 7.53 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.8, 193.3, 135.1, 132.8, 132.5, 131.8, 131.3, 130.5, 130.0, 129.1; IR ($CHCl_3$): ν_{max} 3443, 1633, 1456, 1420 cm^{-1}; GC-MS: *m/z* (EI) 290 (M^+, 2), 209 (5), 185 (24), 157 (10), 105 (100), 77 (52).

*1-Phenyl-2-(thiophen-3-yl)ethane-1,2-dione (**3m**):*[41] Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.22 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.68-7.64 (m, 2H), 7.51 (t, *J* = 8.0 Hz, 2H); 7.41 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.3, 187.3, 138.1, 137.0, 134.8, 132.8, 130.2, 129.0, 127.2, 127.1; IR ($CHCl_3$): ν_{max} 3435, 1737, 1617, 1577, 1465 cm^{-1}; GC-MS: *m/z* (EI) 216 (M^+, 18), 105 (99), 77 (71), 51 (21), (4).

*1-(Naphthalen-1-yl)-2-phenylethane-1,2-dione (**3n**):*[42] Yellow solid, m.p. 100-102 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 9.32 (d, *J* = 8.0 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 2H), 7.96 (dd, *J* = 8.0 & 8.0 Hz, 2H); 7.75 (t, *J* = 8.0 Hz, 1H), 7.68-7.62 (m, 2H), 7.54-7.48 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 197.2, 194.8, 136.0, 135.0, 134.7, 130.0, 129.5, 129.0, 128.8, 128.7, 127.1, 126.0, 124.4; IR ($CHCl_3$): ν_{max} 3443, 1633, 1452, 1120 cm^{-1}; GC-MS: *m/z* (EI) 260 (M^+ 6), 155 (100), 127 (54), 105 (15), 77 (29), 51 (9).

*1-(Anthracen-9-yl)-2-phenylethane-1,2-dione (**3o**):* Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 9.30 (d, *J* = 8.0 Hz, 1H), 8.70 (d, *J* = 8.0 Hz, 1H), 8.64 (d, *J* = 12.0 Hz, 1H), 8.16 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 2H), 7.81 (d, *J* = 12.0 Hz, 1H), 7.75-7.69 (m, 3H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.1, 194.5, 138.8, 134.8, 133.2, 131.0, 130.1, 129.5, 129.1, 128.4, 127.7, 127.4, 126.9, 122.8; IR ($CHCl_3$): ν_{max} 3443, 1757, 1633, 1453 cm^{-1}; ESI-MS: *m/z* 311.10 [M+H^+]; HRMS: *m/z* 311.1093 (ESI) calcd for $C_{22}H_{15}O_2$ (311.1093).

*1-([1,1'-Biphenyl]-4-yl)-2-phenylethane-1,2-dione (**3p**):*[10] Yellow solid, m.p. 103-105 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.06 (dd, *J* = 8.0 Hz, 4H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.68-7.62 (m, 2H), 7.55-7.42 (m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 194.6, 194.2, 147.7, 139.5, 134.9, 133.1, 131.7, 130.5, 130.0, 129.1, 128.7, 127.7, 127.4; IR ($CHCl_3$): ν_{max} 3443, 1639, 1449, 1321 cm^{-1}; GC-MS: *m/z* (EI) 286 (M^+ 2), 181 (100), 152 (41), 105 (14), 77 (21), 51 (7).

*1-(4-Methoxyphenyl)-2-(4-(trifluoromethoxy) phenyl) ethane-1,2-dione (**3q**):* Yellow sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, *J* = 12.0 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 193.0, 192.4, 165.2, 153.7, 132.5, (d, $^1J_{CF}$ = 55.33 Hz), 131.3, 125.8, 120.6, 114.5, 55.7 ; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -57.53 (s, 3F); IR ($CHCl_3$): ν_{max} 3437, 2925, 1726, 1667, 1599, 1424, 1260 cm^{-1}; GC-MS: *m/z* (EI) 324 (M^+, 1), 189 (10), 135 (100), 107 (7), 92 (13), 77 (16), 63 (8).

*1-(P-Tolyl)-2-(4-(trifluoromethyl) phenyl) ethane-1,2-dione (**3r**):* Brown solid; m.p. 77-78 °C; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.11 (d, *J* = 8.0 Hz, 2H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 12.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 193.2, 193.1, 146.7, 136.0, (t, $^2J_{CF}$ = 15.0 Hz), 135.6, 130.3, 130.2, 130.1, 129.9, 126.1, 21.9; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.35 (s, 1F); IR ($CHCl_3$): ν_{max} 3436, 2924, 1677, 1664, 1605, 1117 cm^{-1}; GC-MS: *m/z* (EI) 292 (M^+, 1), 173 (9), 145 (17), 119 (100), 91 (40), 65 (17).

*1-(4-Ethylphenyl)-2-(4-(trifluoromethyl) phenyl) ethane-1,2-dione (**3s**):* Brown sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 8.11 (d, *J* = 8.0 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 12.0 Hz, 2H), 2.77-2.71 (quartet, *J* = 8.0 Hz, 2H), 1.27 (t, *J* = 4.0 Hz, 3H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 193.3, 193.2, 152.8, 135.9, (t, $^2J_{CF}$ = 17.1 Hz), 135.6, 130.4, 130.3, 130.2, 128.7, 126.0, 124.7, 29.2, 15.0; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.35 (s, 3F); IR ($CHCl_3$): ν_{max} 3437, 2925, 1672, 1604, 1325, 1068 cm^{-1}.

*1-(4-(Tert-butyl) phenyl)-2-(p-tolyl)ethane-1,2-dione (**3t**):* Brown sticky solid; ^1H NMR ($CDCl_3$, 400 MHz): δ 7.91-7.85 (m, 4H), 7.54 (t, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H), 1.35 (s, 9H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 193.4, 157.7, 144.9, 129.5, 129.3, 128.9, 128.7, 128.5, 124.8, 121.2, 30.1, 28.5, 20.8; IR ($CHCl_3$): ν_{max} 1725, 1671, 1604, 1542, 1463, 1410 cm^{-1};

GC-MS: *m/z* (EI) 280 (M^+4), 161 (100), 146 (9), 119 (48), 91 (28), 65 (10).

*1-(4-Fluorophenyl)-2-(4-methoxyphenyl) ethane-1,2-dione (**3u**):*[43] Yellow solid, m.p. 68-70 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.03-7.94 (m, 4H), 7.18 (t, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$,100 MHz): δ 193.0, 192.6, 168.0 (d, $^1J_{CF}$ = 257 Hz), 165.1, 132.8, 132.7, 132.4, 116.4, (d, $^2J_{CF}$ = 22.13 Hz),114.4, 55.6; ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -101.64 (s, 1F); IR ($CHCl_3$): ν_{max} 3440, 1650, 1643, 1633, 1599, 749 cm^{-1}.

*1-(4-Iodophenyl)-2-(4-methoxyphenyl) ethane-1,2-dione (**3v**):* Yellow sticky solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94-7.87 (m, 4H), 7.69 (d, *J* = 12.0 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 193.7, 192.0, 134.5, 132.2, 130.5, 130.2, 129.7, 128.9, 128.6, 127.4, 126.8, 49.6; IR ($CHCl_3$): ν_{max} 3441, 1733, 1675, 1593, 1018 cm^{-1}.

*1-(4-Bromophenyl)-2-(thiophen-3-yl)ethane-1,2-dione (**3w**):* Pale yellow sticky solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.24 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 3H), 7.42 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 186.4, 137.8, 137.3, 132.4, 131.5, 130.5, 127.3, 127.2; IR ($CHCl_3$): ν_{max} 3443, 1633, 1449, 1417, 748 cm^{-1}; GC-MS: *m/z* (EI) 294 (M^+, 3), 185 (24), 111 (100), 76 (11), 50 (7).

*1-(4-Fluorophenyl)-2-(naphthalen-1-yl)ethane-1,2-dione (**3x**):*[19] Pale yellow solid; m.p. 68-70 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.29 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.07 (t, *J* = 8.0 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 196.7, 192.9, 168.0, (d, $^1J_{CF}$ = 258 Hz), 136.1, 135.1, 134.1, 132.9, 132.8, 129.5, 128.9, 127.2, 125.9, 124.4, 116.5, (d, $^2J_{CF}$ = 22.13 Hz); ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -101.64 (s, 1F); IR ($CHCl_3$): ν_{max} 3444, 1667, 1650, 1597, 1411, 776, cm^{-1}; GC-MS: *m/z* (EI) 278 (M^+ 5), 155 (100), 127 (62), 95 (17), 75 (16), 50 (3).

General procedure for synthesis of imidazoles 7a-c from 1,2-diketones. Benzil (0.2 equiv.), benzaldehyde (0.2 equiv.), and ammonium acetate (2.0 equiv.) were mixed together and were dissolved in 1.0 mL of AcOH in a round bottom flask containing a magnetic stir bar. Reaction mixture was then refluxed at 100 °C for 3 h. Then, concentrated NH_4OH solution was added to the reaction mixture at 0 °C, which resulted in formation of a white precipitate which was collected by filtration and washed with H_2O. The solid was dried in a vacuum oven for 18 h at 50 °C to afford as imidazoles **7a-c** bright white solids.

General one-pot procedure for synthesis of imidazoles 7a-c from phenylacetylenes. To the mixture of phenyl hydrazine (1.0 equiv.) and phenylacetylene (1.2 equiv.) in DMF was added 10 mol% of cobalt acetylacetanoate and 10 mol% silver oxide. Reaction mixture was stirred at room temperature for 8 h. Aldehyde (1 equiv.), ammonium acetate (2 equiv.) and acetic acid (2 ml) were then added to the reaction mixture and it was refluxed at 100 °C for 3 h. After completion of the reaction (monitored by TLC), reaction mixture was filtered, and filtrate was extracted with ethyl acetate. The combined organic layers were dried over anhydrous sodium sulphate and evaporated on vacuo rotavapor to get crude product. The crude product was purified by silica gel (#100-200) column chromatography using *n*-hexane and ethyl acetate as an eluent to get pure product **7a-d** in 55-65% yield.

*2,4,5-Triphenyl-1H-imidazole (**7a**):*[1] White solid; m.p. 274-276 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 12.71 (s, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 7.56-7.23 (m, 13H); ^{13}C NMR (DMSO-d_6,100 MHz): δ 145.0, 134.6, 130.5, 129.8, 128.1, 127.9, 127.7, 127.6, 127.2, 126.5, 126.0, 124.6; IR ($CHCl_3$): ν_{max} 3417, 1658, 1644, 1633, 1503, 1460 cm^{-1}; ESI-MS: *m/z* 297.00 [M+H^+]; HRMS: *m/z* 297.1417 (ESI) calcd for $C_{21}H_{17}N_2$ (297.1417).

*2-(Naphthalen-1-yl)-4,5-diphenyl-1H-imidazole (**7b**):*[44] Brown solid, m.p. 220-222 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 12.88, (s, 1H), 8.63 (s, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.03-7.94 (m, 4H), 7.58-7.34 (m, 11H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 145.5, 133.0, 132.7, 128.5, 128.4, 128.2, 128.1, 127.8, 127.7, 127.1, 126.7, 126.3, 123.7, 123.5; IR ($CHCl_3$): ν_{max} 3357, 1652, 1600, 1502, 1446 cm^{-1}; ESI-MS: *m/z* 347.00 [M+H]$^+$; HRMS: *m/z* 347.9528 (ESI) calcd for $C_{25}H_{18}N_2$ (347.9528).

*2-(Anthracen-9-yl)-4,5-diphenyl-1H-imidazole (**7c**):*[45] Brown solid, m.p.166-168 °C; ^{1}H NMR (DMSO, 400 MHz): δ 12.96 (s, 1H), 8.81 (s, 1H), 8.22 (d, *J* = 12.0 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 4.0 Hz, 6H), 7.45 (t, *J* = 4.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 3H), 7.27 (t, *J* = 4.0 Hz, 1H); ^{13}C NMR (DMSO,100 MHz): δ 143.3, 136.9, 135.4, 131.1, 130.9, 130.8, 128.7, 128.4, 128.2, 127.9, 127.3, 126.6, 126.0, 125.5; IR ($CHCl_3$): ν_{max} 3391, 1666, 1602, 1533, 1483, 1444, 1266 cm^{-1}; ESI-MS: *m/z* 397.00 [M+H]$^+$; HRMS: *m/z* 397.1709 (ESI) calcd for $C_{29}H_{21}N_2$ (397.1709).

Procedure for synthesis of trifenagrel (8): To the mixture of phenyl hydrazine (**1a**, 1.0 equiv.) and phenylacetylene (**2a**, 1.2 equiv.) in DMF was added 10 mol% of cobalt acetylacetanoate and 10 mol% silver oxide. Reaction mixture was then stirred at room temperature for 8 h. Salicyladehyde (**6d**, 1 equiv.), ammonium acetate and acetic acid (2 mL) was added to the reaction mixture and it was refluxed at 100 °C for 3 h. After completion of the reaction (monitored by TLC), reaction mixture was filtered, and filtrate was extracted with ethyl acetate and the combined organic layers were dried over anhydrous sodium sulphate. Solvent was evaporated on vacuo rotavapor to get the crude product. The crude product was purified by silica gel (#100-200) column chromatography using *n*-hexane-EtOAc as an eluent to get imidazole **7d** in 55% yield. Compound **7d** (1 equiv.) was then treated with 2-chloro-N,N-dimethylethanamine (1.5 equiv.) in presence of K_2CO_3 (2 equiv.) in dry acetone for 6 h at room temparature, resulting in formation of trifenagrel (**8**) in 70% yield.

*2-(4,5-Diphenyl-1H-imidazol-2-yl)phenol (**7d**):*[46] Yellow solid; m.p. 170-172 °C; ^{1}H NMR (acetone-d_6, 400 MHz): δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 4H), 7.43-7.28 (m, 7H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.93 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (acetone-d_6, 100 MHz): δ 158.5, 147.3, 131.0, 129.5, 128.8, 128.5, 125.8, 119.7, 118.0, 113.9; IR ($CHCl_3$): ν_{max} 3436, 1629, 1604, 1488, 1444 cm^{-1}; ESI-MS: *m/z* 313.10 [M+H]$^+$; HRMS: *m/z* 313.1350 (ESI) calcd for $C_{21}H_{16}N_2O$ (313.1350).

*Trifenagrel (**8**).*[1] White solid; m.p. 132-134 °C ^{1}H NMR ($CDCl_3$, 400 MHz): δ 12.33 (s, 1H), 8.48 (d, *J* = 8.0 Hz, 1H), 7.75-7.40 (m, 4H), 7.35-7.20 (m, 7H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 4.22 (t, *J* = 4.0 Hz, 2H), 2.66 (t, *J* = 4.0 Hz, 2H), 1.97 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.1, 143.7, 129.0, 128.9, 128.3, 127.1, 124.0, 123.5, 122.2, 120.3, 115.9, 113.6, 65.7, 58.1, 44.5; IR ($CHCl_3$): ν_{max} 3225, 2923, 1603, 1587, 1481, 1465, 1261, 765 cm^{-1}; ESI-MS: *m/z* 384.2070 $[M+H]^+$.

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