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SUPPLEMENTARY MATERIAL TO

Electrogenerated base-promoted synthesis of 4-aryl-5-benzoyl--2-hydroxy-6-(trifluoromethyl)-1,4-dihydropyridine-3--carbonitriles nanoparticles by three-component condensation of aromatic aldehydes, malononitrile and 4,4,4-trifluoro--1-phenylbutane-1,3-dione

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ANALYTICAL DATA FOR COMPOUNDS

*5-Benzoyl-2-hydroxy-4-(4-nitrophenyl)-6-(trifluoromethyl)-1,4-dihydropyridine-3-carbonitrile (**4a**)*. White powder (85 %), m.p. 173–175 °C. IR (KBr) (ν_{max}, cm^{-1}): 3498, 3396 (NH, OH), 2217 (CN), 1655 (C=O). Anal. Calcd. for $C_{20}H_{12}F_3N_3O_4$: C, 57.84; H, 2.91; N, 10.12 %. Found: C, 57.69; H, 2.85; N, 10.31 %. MS (*m*/*z*): 415 (9). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 4.49 (1H, *s*, CH), 7.32–7.92 (10H, *m*, arom. and NH), 9.65 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 53.05 (CH), 90.05, 97.65, 104.90, 120.67, 125.47, 127.64, 129.01, 132.40, 134.14, 139.07, 143.80, 161.88, 170.98 (C arom., olefine and CN), 116.22 (*q*, $^1J_{FC}$ = 285 Hz, CF_3), 188.48 (C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$), δ = –75.61 (CF_3) ppm.

*5-Benzoyl-2-hydroxy-4-(3-nitrophenyl)-6-(trifluoromethyl)-1,4-dihydropyridine-3-carbonitrile (**4b**)*. White powder (70 %), m.p. 174–176 °C. IR (KBr) (ν_{max}, cm^{-1}): 3522, 3311 (NH, OH), 2247 (CN), 1637 (C=O). Anal. Calcd. for $C_{20}H_{12}F_3N_3O_4$: C, 57.84; H, 2.91; N, 10.12 %. Found: C, 57.98; H, 2.68; N, 10.28 %. MS (*m*/*z*): 415 (11). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 4.64 (1H, *s*, CH), 7.08–8.25 (10H, *m*, arom. and NH), 9.73 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 53.88 (CH), 90.04, 114.15, 120.67, 125.32, 127.64, 128.41, 129.01, 131.65, 132.94, 136.35, 139.08, 148.51, 159.78, 170.87, 172.60 (C arom., olefine and CN), 119.40 (*q*, $^1J_{FC}$ = 286 Hz, CF_3), 188.48 (C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –75.91 (CF_3) ppm.

*5-Benzoyl-2-hydroxy-4-(4-hydroxyphenyl)-6-(trifluoromethyl)-1,4-dihydropyridine-3-carbonitrile (**4c**)*. White powder (65 %), m.p. 175–177 °C. IR (KBr)

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(ν_{max}, cm^{-1}): 3495, 3399 (NH, OH), 2246 (CN), 1637 (C=O). Anal. Calcd. for $C_{20}H_{13}F_3N_2O_3$: C, 62.18; H, 3.39; N, 7.25 %. Found: C, 62.31; H, 3.21; N, 7.39 %. MS (*m*/*z*): 386 (12). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 4.49 (1H, *s*, CH), 34 7.07–7.97 (10H, *m*, arom., NH), 9.81 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 52.06 (CH), 90.03, 94.48, 105.93, 123.37, 127.63, 129.01, 129.12, 130.32, 132.39, 134.01, 139.07, 149.82, 160.61 (C arom., olefine and CN), 119.39 (*q*, $^1J_{FC}$ = 286 Hz, CF_3), 188.47 (C=O) ppm. ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –75.43 (CF_3) ppm.

5-Benzoyl-4-(4-chlorophenyl)-2-hydroxy-6-(trifluoromethyl)-1,4-dihydro-pyridine-3-carbonitrile (***4d***). White powder (70 %), m.p. 182–184 °C. IR (KBr) (ν_{max}, cm^{-1}): 3522, 3341 (NH), 2251 (CN), 1635 (C=O). Anal. Calcd. for $C_{20}H_{12}ClF_3N_2O_2$: C, 59.35; H, 2.99; N, 6.92 %. Found: C, 59.20; H, 2.81; N, 6.69 %. MS (*m*/*z*): 404 (7). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 4.62 (1H, *s*, CH), 7.10–8.04 (10H, *m*, arom., NH), 9.61 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 54.81 (CH), 90.04, 96.27, 113.21, 120.68, 121.33, 127.63, 129.01, 132.39, 137.04, 139.08, 146.82, 151.85, 170.89 (C arom., olefine and CN), 118.40 (*q*, $^1J_{FC}$ = 289 H, CF_3), 188.48 (C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –76.56 (CF_3) ppm.

5-Benzoyl-4-(2,4-dimethoxyphenyl)-2-hydroxy-6-(trifluoromethyl)-1,4--dihydropyridine-3-carbonitrile (***4e***). White powder (72 %), m.p. 172–174 °C. IR (KBr) (ν_{max}, cm^{-1}): 3505, 3329 (NH, OH), 2226 (CN), 1622 (C=O). Anal. Calcd. for $C_{22}H_{17}F_3N_2O_4$: C, 61.40; H, 3.98; N, 6.51 %. Found: C, 61.55; H, 3.78; N, 6.40 %. MS (*m*/*z*): 430 (9). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 3.92, 3.93 (6H, 2*s*, $2OCH_3$), 4.39 (1H, *s*, CH), 6.44–8.22 (9H, *m*, arom., NH), 9.70 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 53.47 (CH), 53.47, 55.53 ($2OCH_3$), 79.98, 90.04, 97.70, 108.95, 125.67, 54 126.87, 127.62, 129.01, 130,21, 132.38, 135,50, 139.08, 149.42, 153.34, 161.47 (C arom., olefine and CN), 114.13 (*q*, $^1J_{FC}$ = 286 Hz, CF_3), 188.47 C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –75.90 (CF_3) ppm.

5-Benzoyl-4-(3,5-dimethoxyphenyl)-2-hydroxy-6-(trifluoromethyl)-1,4--dihydropyridine-3-carbonitrile (***4f***). White powder (65 %), m.p. 165–167 °C. IR (KBr) (ν_{max}, cm^{-1}): 3516, 3330 (NH, OH), 2239 (CN), 1631 (C=O). Anal. Calcd. for $C_{22}H_{17}F_3N_2O_4$: C, 61.40; H, 3.98; N, 6.51%. Found: C, 61.76; H, 3.75; N, 6.66 %. MS (*m*/*z*): 430 (11). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 3.82 (6H, 2*s*, $2OCH_3$), 4.37 (1H, *s*, CH), 6.77–8.39 (9H, *m*, arom., NH), 9.79 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 52.05 (CH), 56.63, 56.80 ($2OCH_3$), 90.03, 98.83, 100.01, 108.21, 110.06, 113.62, 127.63, 129.01, 132.39, 139.08, 144.22, 154.38, 167.27 (C arom., olefine and CN), 116.06 (*q*, $^1J_{FC}$ = 284 Hz, CF_3), 188.32(C=O) ppm. ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –76.45 (CF_3) ppm.

*5-Benzoyl-4-(4-bromophenyl)-2-hydroxy-6-(trifluorom)-ethyl-1,4-dihydro-pyridine-3-carbonitrile (**4g**)*. White powder (70 %), m.p. 174–176 °C. IR (KBr) (ν_{max}, cm^{-1}): 3507, 3324 (NH, OH), 2246 (CN), 1640 (C=O). Anal. Calcd. for $C_{20}H_{12}BrF_3N_2O_2$: C, 53.47; H, 2.69; N, 6.24 %. Found: C, 53.35; H, 2.52; N, 6.18 %. MS (*m*/*z*): 448 (7). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 4.39 (1H, *s*, CH), 7.17–7.92 (10H, *m*, arom., NH), 9.09 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 57.80 72 (CH), 90.04, 98.78, 107.59, 120.68, 127.63, 128.88, 129.01, 132.40, 139.08, 145.68, 152.58, 163.60 (C arom., olefine and CN), 118.40 (*q*, $^1J_{FC}$ = 286 Hz, CF_3), 188.48 (C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –75.61 (CF_3) ppm.

*5-Benzoyl-2-hydroxy-4-o-tolyl-6-(trifluoromethyl)-1,4-dihydropyridine-3-carbonitrile (**4h**)*. White powder (65%), m.p. 171–173 °C. IR (KBr) (ν_{max}, cm^{-1}): 3457, 3320 (NH_2), 2225 (CN), 1651 (C=O). Anal. Calcd. for $C_{21}H_{15}F_3N_2O_2$: C, 65.62; H, 3.93; N, 7.29 %. Found: C, 65.75; H, 3.86; 78 N, 7.41 %. MS (*m*/*z*): 384 (9). ^{1}H-NMR (500.1 MHz, DMSO) δ / ppm: 2.17 (3H, *s*, OCH_3), 4.51 (1H, *s*, CH), 7.08–7.80 (10H, *m*, arom., NH), 9.86 (1H, *s*, OH). ^{13}C-NMR (125.77 MHz, DMSO) δ / ppm: 19.17 (CH_3), 53.99 (CH), 63.87, 90.03, 110.00, 120.60, 125.60, 126.67, 127.58, 81 127.61, 127.75, 127.77, 128.44, 128.98, 132,34, 134.77, 139.13, 171.14 (C arom., olefine and CN), 115.08 (*q*, $^1J_{FC}$ = 288 Hz, CF_3), 189.48 (C=O). ^{19}F-NMR (470.56 MHz, $CDCl_3$) δ = –76.56 (CF_3) ppm.