Supporting Information

A New Generation of Radiofluorinated Pyrimidine-2,4,6-triones as MMP-targeted Radiotracers for Positron Emission Tomography

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General Methods. All chemicals, reagents and solvents were analytical grade, purchased from commercial suppliers and used without further purification unless otherwise specified. Melting points were measured on a Stuart Scientific SMP3 capillary melting point apparatus and are uncorrected. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded in $CDCl_3$ or in DMSO-d_6 on Bruker AV400, AV300 or Varian Unity plus 600 spectrometers with the corresponding solvent signals as an internal standard. For ^{19}F NMR shift values $CFCl_3$ was the internal standard. Chemical shifts are reported in δ (ppm). Values of the coupling constant J are given in Hertz (Hz); the following abbreviations are used for the description of ^{1}H NMR spectra: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd), doublet of triplets (dt), broad singlet (br s). The chemical shifts of complex multiplets are given as the range of their occurrence. Exact mass analyses were conducted on a Bruker MicroTof apparatus. Reactions were monitored by thin layer chromatography (TLC, performed on silica gel-coated polyester backed TLC plates, SIL G/UV_{254}, Macherey-Nagel) using solvent mixtures of cyclohexane (CH), ethyl acetate (EtOAc), methanol (MeOH), and triethyl amine (TEA). The ≥ 95% purities of each new nonradioactive compound were assessed by elementary analysis or analytical reversed phase HPLC on HPLC system **I**: Two Smartline 1000 pumps and a Smartline UV detector 2500 (Knauer), a GabiStar γ-detector (Raytest Isotopenmessgeräte GmbH) and a Nucleosil Eurosphere 100-5 C-18 column (250 mm x 4.6 mm). The recorded data were processed by the GINA Star software (Raytest Isotopenmessgeräte GmbH). The HPLC system **I** started with a linear gradient from 10% to 90% CH_3CN in water (0.1% TFA) over 9 min, followed by a linear gradient from 90% to 10% CH_3CN in water (0.1% TFA) over 6 min, with a flow rate of 1 $mL \cdot min^{-1}$ (unless otherwise specified).

Synthesis of compounds 16-20, 5, 22 and 23

2-(2-{2-[2-(2-{2-[2-(2-Trityloxy-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethanol (16). A solution of Tetraethylene glycol (60.4 mL, 348 mmol) and *t*-BuOK (39.1 g, 348 mmol) in dry *t*-BuOH (1.5 L) was refluxed for 30 min. After addition of PEG derivatives **15** (59.7 g, 116 mmol)**,** the reaction mixture was refluxed for 17 h. The mixture was then cooled to rt and washed with brine. The solvent was evaporated *in vacuo* and the crude product was purified by silica gel chromatography (CH/EtOAc 1/1) to give **16** as a colourless oil (58.8 g, 83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.11 (br s, 1H, O*H*), 3.20 (t, ^{3}J = 5.2 Hz, 2H, CH_2), 3.56-3.70 (m, 30H, CH_2), 7.17-7.21 (m, 3H, H_{Aryl}), 7.24-7.28 (m, 6H, H_{Aryl}), 7.41-7.44 (m, 6H, H_{Aryl}) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ 61.81, 63.44, 70.35, 70.60, 70.62, 70.64, 70.66, 70.71, 70.77, 70.79, 70.89, 72.79, 86.65, 127.03, 127.87, 128.83, 144.24 ppm. HRMS-ESI: calcd for $C_{35}H_{48}O_9Na$ ([M+Na]$^+$), 635.3191; found 635.3186. The purity of **16** was determined by analytical HPLC to be ≥ 98%, t_R = 10.72 ± 0.02 min (n = 3).

1,1,1-Triphenyl-2,5,8,11,14,17,20,23,26-nonaoxanonacos-28-yne (17). Compound **16** (58.7 g, 96 mmol) was dissolved in THF (450 ml) and the solution was cooled to 0°C. After sodium hydride (60% suspension in oil, 4.6 mg, 115 mmol) was added slowly, the mixture was stirred at 0°C for 30 min, followed by a dropwise addition of propargyl bromide (80% wt in toluene, 12.8 mL, 115 mmol). The mixture was stirred at rt overnight, then evaporated to dryness and the residue was purified by silica gel chromatography (CH/EtOAc 1/2) to afford **17** as a colourless oil (58.8 g, 94%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.43 (t, ^{4}J = 2.4 Hz, 1H, C≡C*H*), 3.23 (t, ^{3}J = 5.2 Hz, 2H, CH_2), 3.63-3.69 (m, 30H, CH_2), 4.20 (d, ^{4}J = 2.4 Hz, 2H, CH_2-C≡CH), 7.19-7.24 (m, 3H, H_{Aryl}), 7.28-7.31 (m, 6H, H_{Aryl}), 7.44-7.48 (m, 6H, H_{Aryl}) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 58.52, 63.45, 69.24, 70.53, 70.69, 70.74, 70.80, 70.83, 70.91, 74.65, 79.79, 86.65, 127.03, 127.87, 128.84, 144.25 ppm. HRMS-ESI: calcd for $C_{38}H_{50}O_9Na$ ([M+Na]$^+$), 673.3347; found 673.3347. The purity of **17** was determined by analytical HPLC to be > 99%, t_R = 11.24 ± 0.01 min (n = 3).

2-(2-{2-[2-(2-{2-[2-(2-Prop-2-ynyloxy-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethanol (**18**). To a solution of **17** (58.7 g, 90 mmol) in 500 mL MeOH was added p-toluenesulfonic acid monohydrate (1.7 g, 9 mmol). The mixture was refluxed for 24 h. After cooling to rt, sodium carbonate (19.1 g, 180 mmol) was added and the mixture was stirred for 10 min. The solvent was evaporated *in vacuo* and the residue was redissolved in CH_2Cl_2. The resulting suspension was filtered and concentrated. The residue was purified by silica gel chromatography (EtOAc/MeOH 9/1) to give pure **18** (30.2 g, 82 %). ^{1}H NMR (300

MHz, $CDCl_3$): δ 2.42 (t, ^4J = 2.3 Hz, 1H, C≡C*H*), 2.74 (br s, 1H, O*H*), 3.55-3.67 (m, 32H, CH_2), 4.17 (d, ^4J = 2.4 Hz, 2H, CH_2-C≡CH) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 58.44, 61.75, 69.15, 70.38, 70.45, 70.61, 70.66, 72.59, 74.63, 79.72 ppm. HRMS-ESI: calcd for $C_{19}H_{36}O_9Na$ ([M+Na]$^+$), 431.2252; found 431.2250.

Toluene-4-sulfonic acid 2-(2-{2-[2-(2-{2-[2-(2-prop-2-ynyloxy-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethyl ester (19). A solution of *p*-toluenesulfonyl chloride (18.7 g, 98 mmol) in CH_2Cl_2 (50 mL) was added dropwise to a solution of **18** (20.0 g, 49 mmol) and TEA (10.2 mL, 74 mmol) in CH_2Cl_2 (200 mL) at 0°C. The reaction mixture was allowed to warm to rt and stirred overnight. The solvent was evaporated *in vacuo* and the residue was purified by silica gel chromatography (EtOAc/MeOH 9/1) to afford a colourless oil (23.1 g, 84%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.41-2.43 (m, 4H, C≡C*H* and CH_3), 3.56-3.68 (m, 30H, CH_2), 4.12-4.16 (m, 2H, CH_2), 4.18 (d, ^4J = 2.4 Hz, 2H, CH_2-C≡CH), 7.31-7.34 (m, 2H, H_{Aryl}), 7.76-7.80 (m, 2H, H_{Aryl}) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 21.74, 58.49, 68.77, 69.20, 69.34, 70.50, 70.61, 70.66, 70.70, 70.84, 74.64, 79.77, 128.08, 129.92, 133.11, 144.88 ppm. HRMS-ESI: calcd for $C_{26}H_{42}O_{11}SNa$ ([M+Na]$^+$), 585.2340; found 585.2342. Anal. calcd for $C_{26}H_{42}O_{11}S$: C 55.50, H 7.52, found: C 55.21, H 7.51.

4-[2-(2-{2-[2-(2-{2-[2-(2-Prop-2-ynyloxy-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethyl]-piperazine-1-carboxylic acid *tert*-butyl ester (20). *N*-Boc piperazine (9.1 g, 49 mmol) was added to a solution of PEG derivative **19** (23.0 g, 41 mmol) and TEA (11.4 mL, 82 mmol) in CH_3CN (200 mL). After refluxing overnight, the mixture was concentrated. Silica gel chromatography (EtOAc/MeOH 9/1) gave compound **20** as a colourless oil (10.1 g, 43%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.44 (s, 9H, CH_3), 2.42-2.45 (m, 5H, C≡C*H* and N-CH_2), 2.59 (t, ^3J = 5.8 Hz, 2H, N-CH_2), 3.41-3.44 (m, 4H, N-CH_2), 3.58-3.68 (m, 30H, CH_2), 4.19 (d, ^4J = 2.4 Hz, 2H, CH_2-C≡CH) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ 28.54, 53.48, 57.93, 58.52, 68.93, 69.22, 70.50, 70.52, 70.69, 70.72, 74.67, 79.70, 79.78, 154.84 ppm. HRMS-ESI: calcd for $C_{28}H_{53}N_2O_{10}$ ([M+H]$^+$), 577.3695; found 577.3677.

4-[2-(2-{2-[2-(2-{2-[2-(2-prop-2-ynyloxy-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethoxy]-ethoxy}-ethoxy)-ethyl]-piperazin-1-ium-trifluoro-acetate (5). Compound **20** (9.65 g, 16.7 mmol) was dissolved in CH_2Cl_2 (200 ml) and the solution was cooled to 0°C. After TFA (19.0 g, 167 mmol) was added dropwise, the mixture was allowed to warm to rt and stirred overnight. After evaporation to dryness, the residue was purified by silica gel chromatography (EtOAc/MeOH 2/1) to afford **5** as a yellow oil (7.43 g, 75%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.45 (t, ^4J = 2.3 Hz, 1H, C≡C*H*), 2.77-2.80 (m, 2H, N-CH_2), 2.95-3.02 (m, 4H, N-CH_2), 3.28-

3.33 (m, 4H, N-CH_2), 3.63-3.69 (m, 32H, CH_2), 4.18 (d, ^4J = 2.3 Hz, 2H, CH_2-C≡CH) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 43.00, 49.80, 57.17, 58.43, 67.70, 68.99, 70.17, 70.20, 70.26, 70.31, 70.40, 70.43, 74.88, 79.65 ppm. HRMS-ESI: calcd for $C_{23}H_{45}N_2O_8$ ($[M]^+$), 477.3170; found 477.3169. Anal. calcd for $C_{23}H_{45}N_2O_8$·2TFA: C 45.96, H 6.71, N 3.97 found: C 45.53, H 7.00, N 3.95.

3-(2-{2-[2-(2-Azido-ethoxy)-ethoxy]-ethoxy}-ethoxy)-2-nitro-pyridine (22). Sodium hydride (60% suspension in oil, 250 mg, 6.3 mmol) was dissolved in DMF (15 ml) and the resulting suspension was cooled to 0°C. A solution of 3-hydroxy-2-nitropyridine (701 mg, 5.0 mmol) in DMF (5 ml) was added slowly, followed by dropwise addition of Toluene-4-sulfonic acid 2-{2-[2-(2-azido-ethoxy)-ethoxy]-ethoxy}-ethyl ester (2.24 g, 6.0 mmol). The suspension was held at 0°C for 10 min, then stirred at rt for 2h and heated to 60°C for 72 h. After cooling to rt, the reaction mixture was quenched with water and subsequently extracted with EtOAc (2x). The combined organic extracts were washed with brine, dried ($MgSO_4$), filtered and concentrated. The crude product was purified by silica gel chromatography (CH/EtOAc 2/1 to 1/1) to yield a light yellow solid (1.16 g, 68%). Mp: 35°C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.35-3.38 (m, 2H, CH_2), 3.63-3.68 (m, 10H, CH_2), 3.87-3.89 (m, 2H, CH_2), 4.27-4.30 (m, 2H, CH_2), 7.50 (dd, 1H, ^{3}J = 4.4 Hz, ^{3}J = 8.4 Hz, $H_{\text{Pyridinyl}}$), 7.59 (dd, 1H, ^{4}J = 1.4 Hz, ^{3}J = 8.4 Hz, $H_{\text{Pyridinyl}}$), 8.07 (dd, 1H, ^{4}J = 1.4 Hz, ^{3}J = 4.4 Hz, $H_{\text{Pyridinyl}}$) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 50.75, 69.31, 69.90, 70.08, 70.67, 70.73, 71.14, 124.46, 128.65, 139.50, 147.39, 149.15 ppm. HRMS-ESI: calcd for $C_{13}H_{19}N_5O_6$ ($[M+Na]^+$), 364.1228; found 364.1228. Anal. calcd for $C_{13}H_{19}N_5O_6$: C 45.75, H 5.61, N 20.52, found: C 45.74, H 5.62, N 20.41.

3-(2-{2-[2-(2-Azido-ethoxy)-ethoxy]-ethoxy}-ethoxy)-2-fluoro-pyridine (23).

Nitropyridine derivative **22** (1.0 g, 2.9 mmol) in 1:1 THF:DMF (30 ml) was treated with *tert*-butylammonium fluoride (1.8 g, 5.8 mmol). After stirring for 24 h at 90°C, the reaction mixture was poured into water and extracted with EtOAc (2x). The combined organic extracts were washed with water and brine, dried ($MgSO_4$), filtered and concentrated. Purification by silica gel chromatography (cyclohexane/EtOAc 1/1) afforded **23** as a colourless oil (549 mg, 60 %). ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.37-3.41 (m, 2H, CH_2), 3.65-3.76 (m, 10H, CH_2), 3.88-3.91 (m, 2H, CH_2), 4.20-4.23 (m, 2H, CH_2), 7.08-7.13 (m, 1H, $H_{\text{Pyridinyl}}$), 7.30-7.37 (m, 1H, $H_{\text{Pyridinyl}}$), 7.74-7.77 (m, 1H, $H_{\text{Pyridinyl}}$) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 50.77, 69.14, 69.55, 70.13, 70.76, 70.79, 71.08, 121.80 (d, ^{4}J = 4.3 Hz), 123.47 (d, ^{3}J = 4.4 Hz), 137.73 (d, ^{3}J = 13.3 Hz), 142.33 (d, ^{2}J = 25.5 Hz), 153.98 (d, ^{1}J = 239 Hz) ppm. ^{19}F NMR (282 MHz,

$CDCl_3$): δ -83.60 ppm. HRMS-ESI: calcd for $C_{13}H_{19}FN_4O_4$ ($[M+H]^+$), 315.1463; found 315.1462. Anal. calcd for $C_{13}H_{19}FN_4O_4$: C 49.68, H 6.09, N 17.83, found: C 49.53, H 6.04, N 17.60.

NMR Data of Compounds 28–36.

compound	NMR
28	^{1}H NMR (300 MHz, DMSO-d_6): δ 3.28 (t, 1H, ^{3}J = 7.1 Hz, N*H*-CH_2), 3.47-3.57 (m, 9H, CH_2), 3.65-3.67 (m, 1H, O-CH_2-CH_2-F), 3.73 (d, ^{3}J = 6.9 Hz, 2H, NH-CH_2), 3.80 (t, 2H, ^{3}J = 5.3 Hz, N-CH_2-CH_2), 4.39-4.42 (m, 1H, CH_2-F), 4.49 (t, 2H, ^{3}J = 5.2 Hz $N_{Triazole}$-CH_2), 4.55-4.58 (m, 1H, CH_2-F), 7.01-7.06 (m, 4H, H_{Aryl}), 7.14-7.20 (m, 1H, H_{Aryl}), 7.37-7.43 (m, 2H, H_{Aryl}), 7.44-7.49 (m, 2H, H_{Aryl}), 7.97 (s, 1H, $H_{Triazole}$), 11.60 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, DMSO-d_6): δ 45.67, 49.32, 68.79, 69.58, 69.65, 69.66 (d, ^{2}J = 18.8 Hz), 69.75, 69.82, 83.05 (d, ^{1}J = 166 Hz), 118.31, 119.15, 123.26, 124.00, 128.28, 130.18, 132.32, 145.44, 149.70, 155.95, 157.29, 170.67 ppm. ^{19}F NMR (282 MHz, DMSO-d_6): δ -221.30 ppm.
29	^{1}H NMR (300 MHz, DMSO-d_6): δ 3.26 (t, 1H, ^{3}J = 6.9 Hz, N*H*-CH_2), 3.48-3.57 (m, 8H, CH_2), 3.71-3.76 (m, 4H, NH-CH_2 and CH_2), 3. 80 (t, 2H, ^{3}J = 5.2 Hz, $N_{Triazole}$-CH_2-CH_2), 4.18-4.21 (m, 2H, CH_2), 4.48 (t, 2H, ^{3}J = 5.2 Hz $N_{Triazole}$-CH_2), 7.00-7.04 (m, 4H, H_{Aryl}), 7.14-7.19 (m, 1H, H_{Aryl}), 7.24-7.28 (m, 1H, $H_{Pyridinyl}$), 7.37-7.42 (m, 2H, H_{Aryl}), 7.45-7.48 (m, 2H, H_{Aryl}), 7.60-7.67 (m, 1H, $H_{Pyridinyl}$), 7.71-7.72 (m, 1H, $H_{Pyridinyl}$), 7.96 (s, 1H, $H_{Triazole}$), 11.56 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, DMSO-d_6): δ 45.68, 49.25, 68.36, 68.58, 68.72, 69.53, 69.60, 69.68, 69.70, 69.89, 118.24, 119.07, 122.56 (d, ^{4}J = 3.8 Hz), 123.16, 123.77 (d, ^{3}J = 3.8 Hz), 123.91, 128.20, 130.09, 132.18, 136.77 (d, ^{3}J = 13.6 Hz), 141.58 (d, ^{2}J = 25.7 Hz), 145.37, 149.61, 152.72 (d, ^{1}J = 235 Hz), 155.90, 157.23, 170.57 ppm. ^{19}F NMR (282 MHz, DMSO-d_6): δ -85.31 ppm.
30	^{1}H NMR (300 MHz, $CDCl_3$): δ 2.71-2.77 (m, 10H, N-CH_2), 3.52-3.68 (m, 14H, CH_2), 4.63 (dm, 2H, CH_2-CH_2-F, ^{3}J = 27.1 Hz), 4.70 (s, 2H, O-CH_2-$C_{Triazole}$), 4.74 (dm, 2H, CH_2-F, ^{2}J = 47.1 Hz), 6.93-7.01 (m, 4H, H_{Aryl}), 7.09-7.14 (m, 1H, H_{Aryl}), 7.30-7.37 (m, 2H, H_{Aryl}), 7.47-7.50(m, 2H, H_{Aryl}), 7.72 (s, 1H, $H_{Triazole}$), 9.44 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 47.08, 50.64 (d, ^{2}J = 20.6 Hz), 53.54, 57.45, 64.46, 67.55, 69.79, 70.38, 70.47, 70.65, 70.74, 74.07, 81.64 (d, ^{1}J = 172 Hz), 118.30, 119.56, 123.91, 123.95, 129.05, 129.97, 130.21, 145.50, 149.72, 156.50, 158.17, 169.67 ppm. ^{19}F NMR (282 MHz, $CDCl_3$): δ -221.51 ppm.

31	^{1}H NMR (400 MHz, DMSO): δ 2.43-2.58 (m, 10H, N-C*H*$_2$), 3.45-3.57 (m, 30H, C*H*$_2$), 4.53 (s, 2H, O-C*H*$_2$-C$_{Triazole}$), 4.70 (dm, 2H, C*H*$_2$-CH$_2$-F, ^{3}J = 27.9 Hz), 4.81 (dm, 2H, C*H*$_2$-F, ^{2}J = 47.0 Hz), 7.00-7.06 (m, 4H, *H*$_{Aryl}$), 7.15-7.19 (m, 1H, *H*$_{Aryl}$), 7.39-7.43 (m, 4H, *H*$_{Aryl}$), 8.12 (s, 1H, *H*$_{Triazole}$), 11.62 (br s, 2H, N*H*) ppm. ^{13}C NMR (101 MHz, DMSO): δ 47.25, 49.93 (d, ^{2}J = 19.5 Hz), 53.69, 57.08, 63.47, 69.00, 69.63, 69.69, 69.73, 69.77, 73.93, 81.91 (d, ^{1}J = 168 Hz), 118.07, 119.27, 124.05, 124.30, 129.64, 129.68, 130.18, 144.16, 149.40, 155.81, 157.39, 169.95 ppm. ^{19}F NMR (282 MHz, DMSO): δ -222.18 ppm.
32	^{1}H NMR (300 MHz, $CDCl_3$): δ 2.69-2.78 (m, 10 H, N-C*H*$_2$), 3.54-3.71 (m, 22H, C*H*$_2$), 3.85-3.88 (m, 4H, C*H*$_2$), 4.17-4.20 (m, 2H, C*H*$_2$), 4.50 (t, 2H, ^{3}J = 5.1 Hz, N$_{Triazole}$-C*H*$_2$), 4.66 (s, 2H, O-C*H*$_2$-C$_{Triazole}$), 6.69 (br s, 2H, N*H*), 6.92-7.01 (m, 4H, H$_{Aryl}$), 7.07-7.14 (m, 2H, *H*$_{Aryl}$ and *H*$_{Pyridinyl}$), 7.30-7.36 (m, 3H, *H*$_{Aryl}$ and *H*$_{Pyridinyl}$), 7.46-7.49 (m, 2H, *H*$_{Aryl}$), 7.72-7.74 (m, 1H, *H*$_{Pyridinyl}$), 7.76 (s, 1H, *H*$_{Triazole}$) ppm. ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 46.97, 50.24, 53.53, 57.27, 64.32, 67.55, 69.02, 69.44, 69.55, 70.29, 70.35, 70.42, 70.49, 70.55, 70.96, 74.21, 118.27, 119.52, 121.85 (d, ^{4}J = 4.2 Hz), 123.41 (d, ^{3}J = 4.3 Hz), 123.93, 124.09, 128.98, 129.93, 130.07, 137.61 (d, ^{3}J = 13.1 Hz), 142.22 (d, ^{2}J = 25 Hz), 144.75, 149.87, 153.86 (d, ^{1}J = 239 Hz), 156.35, 158.16, 170.01 ppm. ^{19}F NMR (282 MHz, $CDCl_3$): δ -83.87 ppm.
33	^{1}H NMR (300 MHz, DMSO): δ 2.41-2.57 (m, 10H, N-C*H*$_2$), 3.43-3.53 (m, 10H, C*H*$_2$), 3.81 (t, 2H, ^{3}J = 5.2 Hz, C*H*$_2$-CH$_2$-N$_{Triazole}$), 4.53 (t, 2H, ^{3}J = 5.2 Hz, CH$_2$-C*H*$_2$-N$_{Triazole}$), 5.39 (s, 2H, C$_{Triazole}$-C*H*$_2$-O), 6.99-7.06 (m, 4H, *H*$_{Aryl}$), 7.14-7.20 (m, 1H, *H*$_{Aryl}$), 7.30-7.43 (m, 6H, *H*$_{Aryl}$), 7.98-8.05 (m, 2H, *H*$_{Aryl}$), 8.21 (s, 1H, *H*$_{Triazole}$), 11.59 ppm (br s, 2H, N*H*). ^{13}C NMR (75.5 MHz, DMSO-*d*$_6$): δ 47.26, 49.45, 53.68, 57.06, 58.11, 68.06, 68.61, 69.55, 69.61, 69.67, 73.94, 115.94 (d, ^{2}J = 22.2 Hz), 118.06, 119.28, 124.05, 125.32, 125.97 (d, ^{4}J = 2.9 Hz), 129.64, 129.67, 130.17, 132.16 (d, ^{3}J = 9.6 Hz), 141.57, 149.41, 155.80, 157.38, 164.52, 165.20 (d, ^{1}J = 252 Hz) 169.96 ppm. ^{19}F NMR (282 MHz, DMSO): δ -100.86 ppm.

34	^{1}H NMR (300 MHz, DMSO): δ 2.45-2.58 (m, 10H, N-C*H*$_2$), 3.39-3.48 (m, 10H, C*H*$_2$), 3.73 (t, 2H, ^{3}J = 5.1 Hz, C*H*$_2$-CH$_2$-N$_{Triazole}$), 4.05 (d, 2H, ^{3}J = 5.3 Hz, C$_{Triazole}$-C*H*$_2$-NH), 4.43 (t, 2H, ^{3}J = 5.1 Hz, CH$_2$-C*H*$_2$-N$_{Triazole}$), 6.99-7.06 (m, 4H, *H*$_{Aryl}$), 7.14-7.19 (m, 1H, *H*$_{Aryl}$), 7.35-7.41 (m, 6H, *H*$_{Aryl}$), 7.80-7.85 (m, 2H, *H*$_{Aryl}$), 8.24 (s, 1H, *H*$_{Triazole}$), 11.64 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, DMSO-*d*$_6$): δ 38.16, 47.25, 49.36, 53.73, 57.07, 68.00, 68.77, 69.65, 69.70, 69.77, 74.03, 116.28 (d, ^{2}J = 22.6 Hz), 118.16, 119.36, 123.71, 124.15, 129.67 (d, ^{3}J = 9.5 Hz), 129.71, 129.76, 130.26, 136.94 (d, ^{4}J = 3.0 Hz), 143.17, 149.55, 155.88, 157.50, 164.15 (d, ^{1}J = 251 Hz) 170.08 ppm. ^{19}F NMR (282 MHz, DMSO): δ -109.64 ppm.
35	^{1}H NMR (300 MHz, DMSO): δ 2.45-2.58 (m, 10H, N-C*H*$_2$), 2.65 (s, 3H, N-C*H*$_3$), 3.45-3.48 (m, 10H, C*H*$_2$), 3.76 (t, 2H, ^{3}J = 5.2 Hz, C*H*$_2$-CH$_2$-N$_{Triazole}$), 4.27 (s, 2H, C$_{Triazole}$-C*H*$_2$-N), 4.47 (t, 2H, ^{3}J = 5.1 Hz, CH$_2$-C*H*$_2$-N$_{Triazole}$), 6.98-7.05 (m, 4H, *H*$_{Aryl}$), 7.14-7.19 (m, 1H, *H*$_{Aryl}$), 7.36-7.46 (m, 6H, *H*$_{Aryl}$), 7.81-7.87 (m, 2H, *H*$_{Aryl}$), 7.99 (s, 1H, *H*$_{Triazole}$), 11.63 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, DMSO-*d*$_6$): δ 34.72, 44.90, 47.25, 49.47, 53.72, 57.07, 67.99, 68.70, 69.65, 69.70, 69.76, 74.03, 116.58 (d, ^{2}J = 22.7 Hz), 118.15, 119.36, 124.16, 124.51, 129.70, 129.75, 130.27, 130.42 (d, ^{3}J = 9.6 Hz), 133.32 (d, ^{4}J = 3.0 Hz), 141.41, 149.53, 155.87, 157.50, 164.56 (d, ^{1}J = 252 Hz) 170.07 ppm. ^{19}F NMR (282 MHz, DMSO): δ -106.10 ppm.
36	^{1}H NMR (300 MHz, DMSO): δ 1.71-1.81 (m, 4H, C*H*$_2$), 2.42-2.70 (m, 10H, N-C*H*$_2$), 3.34-3.51 (m, 12H, C*H*$_2$), 3.77 (t, 2H, ^{3}J = 5.3 Hz, C*H*$_2$-CH$_2$-N$_{Triazole}$), 4.11 (t, 2H, ^{3}J = 6.0 Hz, C*H*$_2$), 4.45 (t, 2H, ^{3}J = 5.2 Hz, CH$_2$-C*H*$_2$-N$_{Triazole}$), 7.00-7.07 (m, 4H, *H*$_{Aryl}$), 7.15-7.20 (m, 1H, *H*$_{Pyridinyl}$), 7.25-7.29 (m, 1H, H$_{Aryl}$), 7.37-7.43 (m, 4H, *H*$_{Aryl}$), 7.59-7.66 (m, 1H, *H*$_{Pyridinyl}$), 7.71-7.72 (m, 1H, *H*$_{Pyridinyl}$), 7.83 (s, 1H, *H*$_{Triazole}$), 11.61 (br s, 2H, N*H*) ppm. ^{13}C NMR (75.5 MHz, DMSO-*d*$_6$): δ 24.65, 25.46, 27.91, 47.25, 49.26, 53.70, 57.06, 68.07, 68.46, 68.82, 69.55, 69.62, 69.66, 69.71, 73.94, 118.11, 119.33, 122.30, 122.72 (d, ^{4}J = 4.1 Hz), 123.51 (d, ^{3}J = 4.3 Hz),124.12, 129.66, 129.72, 130.23, 136.58 (d, ^{3}J = 13.4 Hz), 141.75 (d, ^{2}J = 25.6 Hz), 146.44, 149.47, 152.76 (d, ^{1}J = 235 Hz), 155.84, 157.44, 170.02 ppm. ^{19}F NMR (282 MHz, DMSO): δ -85.73 ppm.