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Supporting Information

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Experimental Information

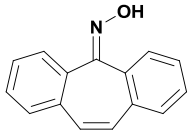
General

All reactions were carried out in oven dried glassware unless otherwise specified. Lys[3]-bombesin was purchased from Sigma-Aldrich and used as received as were all other chemicals unless specified otherwise. ^{1}H- and ^{13}C-NMR spectra were recorded on a Varian AMX400 (400 and 100.59 MHz) using $CDCl_3$ as solvent unless otherwise indicated. Chemical shift values are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: δ 7.26 for ^{1}H and δ 77.0 for ^{13}C). Data are reported as follows: chemical shifts, multiplicity (s=singlet, d=doublet, t=triplet, q=quartet, dd=doublet of doublets, dt=doublet of triplets, td=triplet of doublets, m=multiplet, br=broad), coupling constants (Hz), and integration. Flash chromatography was performed on silica gel. All thin layer chromatography was performed on Merck F-254 silica gel plates. Visualization of the TLC plates was performed with $KMnO_4$ staining reagent and UV light (254 nm). Mass spectra were recorded on an AEI-MS-902 mass spectrometer by EI (70 eV) measurements. Melting points are uncorrected. ^{1}H and ^{13}C NMR data are provided for all synthesized compounds. Spectra were in accordance with published experimental data and references are provided for known compounds. HRMS mass data is provided for all new compounds. Reversed phase-HPLC analyses were performed on a Shimadzu LC-20AD VP, Waters Xterra MS C18 column (3.0 x 150 mm, partciel size 3.5 μm) using a gradient of MeCN/H_2O (0.1 % formic acid) at a flow of 0.5 mL/min.

Safety

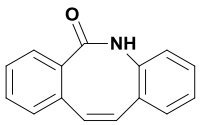
Working with azides should always be done carefully. Organic azides, particularly those of low molecular weight, or with high nitrogen content, are potentially explosive. Heat, light and pressure can cause decomposition of the azides. Furthermore, the azide ion is toxic, and sodium azide should always be handled while protected with gloves. Heavy metal azides are particularly unstable, and may explode if heated or shaken.

Characterization of substrates and reference compounds



5*H*-dibenzo[7]annulen-5-one oxime (2)

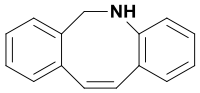
A solution of hydroxylamine was prepared by dissolving 15.6 g (0.22 mol, 3.1 eq) of $NH_2OH{\cdot}HCl$ in a hot mixture of absolute alcohol (100.0 mL) and pyridine (75.0 mL). To this solution was added 15.0 g (0.073 mmol, 1.0 eq) of dibenzosuberenone and 20.0 mL of pyridine. The reaction mixture was heated at reflux for three hours, and the disappearance of starting material was monitored by thin layer chromatography. After completion of the reaction, the solvent was evaporated under reduced pressure, and the product was precipitated with water. The solid was filtered, washed with water (3 x 50 mL), dissolved in chloroform, and the organic layer was washed one further time with water. The organic layer was dried over $MgSO_4$ and the solvent evaporated to yield a pale yellow solid (15.3 g). Yield=95 %. mp 187 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.10 (s, 1H), 7.67 (m, 1H), 7.57 (m, 1H), 7.28-7.37 (m, 6H), 6.86 (dd, *J*=28.0, 4.0 Hz, 2H); ^{13}C NMR (100.59 MHz, $CDCl_3$): 156.3, 135.4, 134.5, 133.8, 130.8, 130.6, 130.5, 129.4, 129.2, 129.1, 128.9 (2C), 128.8, 127.8, 127.6. HRMS (ESI+) (m/z) calculated for $C_{15}H_{12}NO$ $[M + H]^+$ 222.0913, measured 222.0903.



Dibenzo[b,f]azocin-6(5H)-one (3)

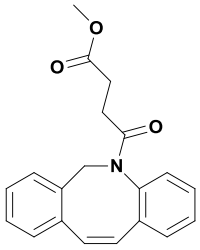
Trichlorotriazine (834.0 mg, 4.52 mmol) was added to 1.0 mL DMF in a sample vial. The solution was stirred, and white precipitate formed. The formation of the catalyst was monitored by thin layer chromatography until all of the TCT had been consumed. To this solution was added oxime **2** along with 10.0 mL DMF. The reaction mixture was

stirred at room temperature for 24-72 h (depending on the amount of oxime in a given reaction). DMF was added if needed in cases where no solvent remained (depending on the scale of the reaction). The reaction was quenched with water and DCM was added to the solution. The organic phase was washed with saturated aqueous Na_2CO_3 (2 x 10 mL), 1 N aqueous HCl (2 x 10 mL) and brine (2 x 10 mL). The organic layer was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The crude reaction mixture was purified by column chromatography (3:1 pentane:ethyl acetate, R_f: 0.65) to give a pale yellow solid (650.0 mg). Yield=65 %. mp 141-142 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (s, 1 H), 7.70-7.72 (m, 1H), 7.57-7.60 (m, 1H), 7.42-7.51 (m, 6H), 6.96 (s, 2H); ^{13}C NMR (100.59 MHz, $CDCl_3$):163.5, 134.3, 133.0, 130.4, 130.2, 129.7, 129.5, 129.2, 129.0, 128.7, 128.5, 128.0, 127.7. HRMS (ESI+) (m/z) calculated for $C_{15}H_{12}NO$ $[M + H]^+$ 222.0913, measured 222.0901.



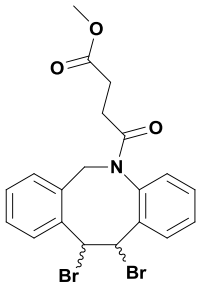
5,6-dihydrodibenzo[b,f]azocine (4)

Amide 3 (2.00 g, 9.0 mmol) was dissolved in 25.0 mL dry CH_2Cl_2 and 45.0 mL of a 1.0 M solution of Dibal-H in CH_2Cl_2 was added dropwise to the solution at room temperature with stirring. The reaction was stirred under N_2 at room temperature and the conversion followed by thin layer chromatography until all of the starting material was consumed. The reaction was then carefully quenched with an aqueous solution of ammonium chloride. An aqueous solution of Rochelle salts was subsequently added and the mixture was stirred vigorously for 45 min. A further 50 mL of DCM was added and the organic layer collected and washed with brine. After drying over $MgSO_4$ the solvent was removed under reduced pressure to yield a yellow oil which was purified by column chromatography (2:1 pentane:ethyl acetate, R_f: 0.8). The resulting compound was a yellow solid (1.40 g). Yield=75 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.62 (m, 1 H), 7.16-7.24 (m, 3H), 6.97 (d, *J*=8.0 Hz, 1H), 6.88 (t, *J*=8.0 Hz, 1H), 6.60 (t, *J*=7.2 Hz, 1H), 6.54 (d, *J*=12.8 Hz, 1H), 6.47 (d, *J*=8.4 Hz, 1H), 6.36 (d, *J*=13.2 Hz, 1H), 4.59 (s, 2H), 4.29 (br s, 2H); ^{13}C NMR (100.59 MHz, $CDCl_3$): 147.1, 138.1, 136.2, 134.7, 132.7, 130.1, 128.8, 127.9, 127.6, 127.4, 127.3, 121.7, 117.9, 117.7, 49.6.

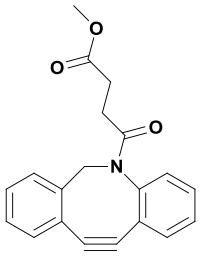


Methyl 4-(dibenzo[b,f]azocin-5(6H)-yl)-4-oxobutanoate (5)

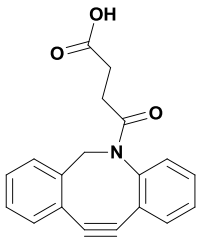
Amide 4 (2.00g, 9.65 mmol) was dissolved in 25.0 mL dry DCM under a N_2 atmosphere. To the stirred solution was added triethylamine (2.67 mL, 19.3 mmol) and the mixture cooled to 0 °C whereupon methyl succinyl chloride (1.78 mL, 14.4 mmol) was added dropwise. The reaction was allowed to warm to room temperature, and stirred overnight. The reaction mixture was quenched with water and the mixture diluted with a further 20.0 mL of DCM. The organic layer was washed with 2 M aqueous NaOH (2 x 15 mL), 2 M aqueous HCl (2 x 15 mL), water (2 x 15 mL) and brine (1 x 10 mL). The organic layer was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography (4:1 pentane:ethyl acetate, R_f: 0.4) to yield a yellow-white solid (2.70 g). Yield=87%. mp 108 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.26 (m, 5H), 7.12-7.16 (m, 3H), 6.79 (d, *J*=17.2 Hz, 1H), 6.61 (d, *J*=17.2 Hz, 1H), 5.51 (d, *J*=20.0 Hz, 1H), 4.25 (d, *J*=20.8, 1H), 3.61 (s, 3H), 2.55-2.60 (m, 1H), 2.39-2.48 (m, 2H), 1.99-2.10 (m, 1H); ^{13}C NMR (100.59 MHz, $CDCl_3$): 177.4, 170.8, 140.5, 136.4, 135.8, 134.5, 132.6, 131.8, 130.8, 130.1, 128.5, 128.2, 128.0, 127.2, 126.9, 54.4, 51.6, 29.5, 29.0. HRMS (ESI+) (m/z) calculated for $C_{20}H_{19}NO_3$ $[M + Na]^+$ 344.1257, measured 344.1250.



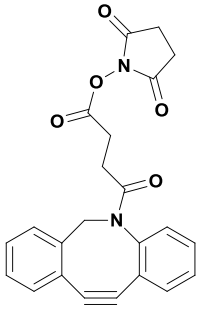
Methyl 4-(11,12-dibromo-11,12-dihydrodibenzo[b,f]azocin-5(6H)-yl)-4-oxobutanoate (6)
Compound 5 (1.87 g, 5.82 mmol) was dissolved in dry CH_2Cl_2 (100.0 mL) under a N_2 atmosphere and the reaction vessel was cooled to 0 °C.Br_2 (0.93 g, 5.82 mmol) dissolved in 5.0 mL of dry CH_2Cl_2 was added dropwise to the cooled solution and the reaction mixture was allowed to stir for 1 h while at 0 °C. After 1 h, the reaction was quenched with aqueous saturated Na_2SO_3 (10 mL) and the mixture diluted with a further 50.0 mL of CH_2Cl_2. The organic layer was washed with saturated aqueous Na_2SO_3 (3 x 15 mL), water (2 x 15 mL) and brine (1 x 15 mL). The organic layer was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The compound was purified by column chromatography (3:1 pentane:ethyl acetate, R_f: 0.3) to yield a dark solid (2.46 g). Yield=88%. mp 108 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J*=7.6 Hz, 1H), 7.00-7.25 (m, 6H), 6.86 (d, *J*=7.6 Hz, 1H), 5.90 (d, *J*=9.6 Hz, 1H), 5.80 (d, *J*=14.8 Hz, 1H), 5.15 (d, *J*=10.0 Hz, 1H), 4.17 (d, *J*=14.8 Hz, 1H), 3.66 (s, 3H), 2.80-2.86 (m, 1H), 2.57-2.64 (m, 2H), 2.43-2.55 (m, 1H). ^{13}C NMR (100.59 MHz, $CDCl_3$): 173.5, 172.0, 138.3, 137.0, 136.9, 132.8, 130.8, 130.7, 130.6, 129.6, 129.5, 128.9, 128.8, 128.6, 60.0, 55.5, 52.5, 51.7, 30.6, 29.2. HRMS (ESI+) (m/z) calculated for $C_{20}H_{19}Br_2NO_3$ $[M + Na]^+$ 503.9603, measured 503.9606.



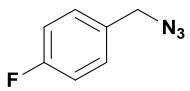
Methyl 4-(11,12-didehydrodibenzo[b,f]azocin-5(6H)-yl)-4-oxobutanoate (7)
To a cold solution (-40 ºC) of compound 6 (245.0 mg, 0.512 mmol) dissolved in 17.0 mL freshly distilled THF under Ar atmosphere was added dropwise 1.02 mL of a commercial solution of *t*BuOK (1.0 M in THF). The progress of the reaction was monitored by GC-MS. After 3 h, a further 0.4 mL of *t*BuOK solution was added and the mixture left to react for a further hour. The mixture was poured onto water (15 mL) and extracted with CH_2Cl_2 (3 x 30 mL). The combined organic layers were washed with brine (2 x 25 mL) and water (1 x 10 mL). A mixture of methyl ester, and *tert*-butyl ester products were detected in the crude ^{1}H NMR. The desired methyl ester product was isolated by column chromatography (3:1 pentane:ethyl acetate, R_f: 0.2) to give a clear yellow oil (109.5 mg). Yield=67 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J*=7.2 Hz, 1H), 7.48-7.50 (m, 1H), 7.27-7.49 (m, 6H), 5.16 (d, *J*=14.0 Hz, 1H), 3.67 (d, *J*=13.6 Hz, 1H), 3.56 (s, 3H), 2.68-2.74 (m, 1H), 2.58-2.63 (m, 1H), 2.35-2.38 (m, 1H), 1.93-1.97 (m, 1H). ^{13}C NMR (100.59 MHz, $CDCl_3$): δ 173.3, 171.7, 151.4, 148.0, 132.3, 129.3, 128.8, 128.5, 128.1, 127.7, 127.1, 125.5, 123.1, 122.6, 114.9, 107.7, 55.4, 51.6, 29.6, 29.0. HRMS (ESI+) (m/z) calculated for $C_{20}H_{17}NO_3$ $[M + Na]^+$ 342.1101, measured 342.1102.



4-(11,12-Didehydrodibenzo[b,f]azocin-5(6H)-yl)-4-oxobutanoic acid (8)
Compound 7 (42.5 mg, 0.13 mmol) was dissolved in 1.7 mL dry THF. A solution of LiOH (6.4 mg, 0.26 mmol) in 0.6 mL H_2O was added dropwise to the stirred reaction mixture. The progress of the reaction was monitored by thin layer chromatography and upon full conversion, a further 6.0 mL of H_2O was added. The reaction mixture was then made basic to a pH of 14 using 2 M aqueous NaOH. The water layer was washed with CH_2Cl_2 (3 x 10 mL) and then acidified to a pH of 2 using 2 M aqueous HCl. The aqueous layer was then extracted with CH_2Cl_2 (3 x 15 mL) and the resulting organic layers of this extraction procedure were combined, dried over $MgSO_4$ and the solvent was removed under reduced pressure. Pure product was obtained as a white solid (30.6 mg). Yield= 77 %. mp 163-164 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J*=7.2 Hz, 1H), 7.25-7.43 (m, 7H), 5.16 (d, *J*=13.6 Hz, 1H), 3.67 (d, *J*=13.6 Hz, 1H), 2.68-2.74 (m, 1H), 2.56-2.63 (m, 1H), 2.32-2.40 (m, 1H), 1.94-2.00 (m, 1H). ^{13}C NMR (100.59 MHz, $CDCl_3$): δ 177.8, 172.6, 151.2, 147.9, 132.5, 129.3, 128.7, 128.5, 128.1, 127.6, 127.4, 125.8, 123.2, 122.9, 115.3, 107.7, 55.9, 29.7, 29.6. HRMS (ESI+) (m/z) calculated for $C_{19}H_{15}NO_3$ $[M + Na]^+$ 328.0944, measured 328.0949.

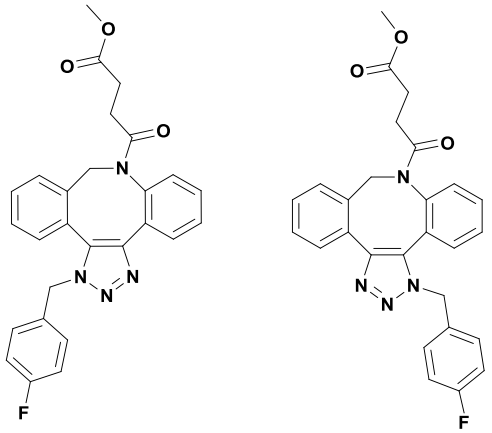


2,5-dioxopyrrolidin-1-yl 4-(didehydrodibenzo[b,f]azocin-5(6H)-yl)-4-oxobutanoate (9)
Carboxylic acid 8 (26.0 mg, 0.085 mmol) was dissolved in 5.0 mL dry CH_2Cl_2. To this solution was added 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) (0.02 mL, 0.094 mmol) and *N*-hydroxysuccinimide (10.8 mg, 0.094 mmol). The reaction mixture was allowed to stir overnight at room temperature after which time it was diluted with a further 10 mL of CH_2Cl_2. The reaction mixture was washed with citric acid (5 %, 2 x 5 mL) and with saturated aqueous $NaHCO_3$ (2 x 5 mL) and brine (1 x 10 mL). The compound was then purified by column chromatography (1:1 pentane:ethyl acetate, R_f: 0.5) to yield the pure compound as a yellow oil (28.0 mg). Yield=82 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J*=7.6 Hz, 1H), 7.24-7.41 (m, 7H), 5.17 (d, *J*=14.0 Hz, 1H), 3.69 (d, *J*=14.0 Hz, 1H), 2.92-2.99 (m, 1H), 2.72-2.77 (m, 1H), 2.78 (s, 4H), 2.61-2.68 (m, 1H), 2.05-2.10 (m, 1H). ^{13}C NMR (100.59 MHz, $CDCl_3$): δ 170.2, 168.9, 168.3, 151.0, 147.8, 132.3, 129.1, 128.6, 128.3, 127.8, 127.2, 125.5, 123.0, 122.7, 115.0, 107.5, 55.6, 29.2, 26.4, 25.5. HRMS (ESI+) (m/z) calculated for $C_{23}H_{18}N_2O_5$ $[M + Na]^+$ 425.1108, measured 425.1121.



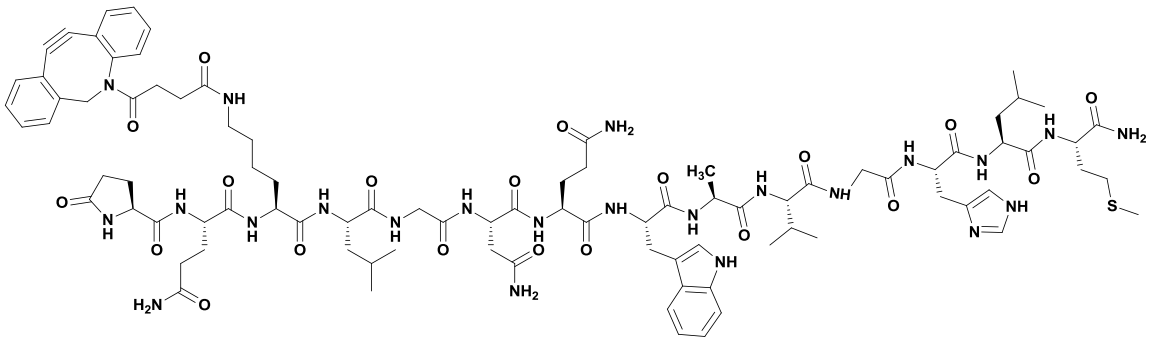
1-(Azidomethyl)-4-fluorobenzene.
To a stirred solution of 1-(bromomethyl)-4-fluorobenzene (472.6 mg, 2.5 mmol) in a water/acetone mixture (1:4) was added NaN_3 (1.5 eq). The resulting suspension was stirred at room temperature for 24 h. DCM was added to the mixture and the organic layer was separated. The aqueous layer was extracted with DCM (3 x 10 mL) and the combined organic layers were dried over $MgSO_4$. Solvent was removed under reduced pressure to give the product

as a pale yellow oil, sufficiently pure to use without further purification (374.0 mg). Yield= 99%. Spectroscopic data is in accordance with literature values.[1] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.39 (m, 2H), 7.00-7.11 (m, 2H), 4.30 (s, 2H); ^{13}C (100.59 MHz, $CDCl_3$): δ 162.5 (d, *J*=130.7 Hz), 131.4, 129.9 (d, J= 45.2 Hz), 115.7 (d, *J*=110.0 Hz), 54.0; ^{19}F NMR (200 MHz, $CDCl_3$): δ -112.3.



Methyl 4-(1-(4-fluorobenzyl)-1*H*-dibenzo[*b,f*][1,2,3]triazolo[4,5-*d*]azocin-8(9*H*-yl)-4-oxobutanoate (10)
To a solution of aza-dibenzocyclooctyne 9 (80 mg, 0.25 mmol) dissolved in 5.0 mL CH_2Cl_2 was added 1-(azidomethyl)-4-fluorobenzene (57 mg, 0.38 mmol). The reaction mixture was allowed to stir for 1 h at room temperature, after which the solvent was evaporated and the crude product was purified by column chromatography (1:1 pentane:ethyl acetate) to yield the product as a white solid (94.1 mg). Yield=80 %. Two isomers are formed as determined by ^{1}H NMR (1:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67-7.73 (m, 1H), 7.44-7.49 (m, 2H), 7.38-7.42 (m, 1H), 7.24-7.31 (m, 1H), 7.17-7.24 (m, 2H), 6.93-7.10 (m, 5H), 5.99 (d, *J*=16.9 Hz, 1H), 5.58 (s, 2H), 4.33 (d, *J*=16.9 Hz, 1H), 3.60 (s, 3H), 2.44 (m, 1H), 2.23 (m, 1H), 2.09 (m, 1H), 1.80 (m, 1H). ^{13}C NMR (100.59 MHz, $CDCl_3$): δ173.2, 171.3, 163.7, 161.3, 143.1, 140.0, 135.9, 134.9, 131.8, 131.2, 130.7, 128.9, 129.6, 129.3, 129.1, 129.0, 127.9, 127.1, 124.3, 116.0, 115.8, 52.0, 51.6, 51.4, 29.2, 28.9. HRMS (ESI+) (m/z) calculated for $C_{27}H_{23}N_4O_3F$ [M + H]$^+$ 471.1827, measured 471.1789; (ESI+) (m/z) calculated for $C_{27}H_{23}N_4O_3F$ [M + Na]$^+$ 493.1646, measured 493.1606.

Peptide Chemistry



Aza-DBCO-BN.
Lys[3]-bombesin (0.18 mg, 1.0 eq) was weighed into a 2.0 mL Eppendorf tube along with 9 (0.5 mg, 5.0 eq). 200 µL of dry DMF and 10.0 eq of diisopropylethyl amine were added and the resulting solution was stirred at room temperature for 24 h. The solvent was removed by lyophilization. Full conversion of lys[3]-bombesin could be observed by RP-HPLC. The product was purified by preparative RP-HPLC yielding Aza-DBCO-BBN in 25 % yield. HRMS (ESI+) (m/z) calculated for $C_{90}H_{123}N_{23}O_{20}S$ [M + H]$^+$ 1878.9108, measured 1878.9078. Retention time=32.0 min.

Radiochemistry General

[^{18}F] fluoride was obtained by proton bombardment of an [^{18}O] enriched water target via the $^{18}O(p,n)^{18}F$ reaction. The radioactivity was trapped by passing the target water through a preactivated Sep-Pak light QMA cartridge (Waters). A 1 mL H_2O solution of K_2CO_3 (4.5 mg) and Kryptofix 222 (20 mg) was used to elute the [^{18}F]-fluoride from the cartridge into a conical glass vial. This eluate was evaporated to dryness by three consecutive azeotropic distillations after with acetonitrile (3 × 500 μL) under a gentle stream of nitrogen gas (130 °C). Analytical as well as semipreparative RP-HPLC was performed for monitoring and purification. Isolation of radiolabeled peptides was performed using a reversed-phase RP-C18 column (4.6 mm × 250 mm, 10 μm). The flow was set at 2.5 mL/min using a gradient system starting from 90% solvent A (0.01 M phosphate buffer, pH=6.0) and 10% solvent B (acetonitrile) (0-2 min) and ramped to 45% solvent A and 55% solvent B at 35 min. The analytic HPLC was performed using the same gradient system but with a reversed-phase Grace Smart RP-C18 column (4.6 mm × 250 mm, 5 μm) and a flow of 1 mL/min.

Synthesis and radiolabelling

The reaction with cyclooctyne modified bombesin was performed in DMF at room temperature and proceeded to completion in 15 min. The resulting tracer was also purified by RP-HPLC yielding the desired triazole tracers: [**^{18}F]-BnTOxBN** (retention time=16 min), [**^{18}F]-BuTOxBN** (retention time=19 min) and [**^{18}F]-PEGTOxBN** (retention time=22 min) with radiochemical yields of 31%, 37% and 19% respectively. The specific activities were 62 GBq/µmol, 57 GBq/µmol , 60 GBq/µmol.

Cell culture: The GRPR-positive PC-3 human prostate cancer cell line (ATCC, Manassas, Virginia, USA) was cultured at 37 °C in a humidified 5 % CO_2 atmosphere. The cells were cultured in RPMI 1640 (Lonza, Verviers, France) supplemented with 10 % fetal calf serum (Thermo Fisher Scientific Inc., Logan, Utah, USA) and subcultured twice a week after detaching with trypsin-EDTA.

***In Vitro* Competitive Receptor-Binding Assay:** *In vitro* GRPR binding affinities and specificities of BN(1-14) were assessed via a competitive displacement assay Experiments were performed with PC-3 human prostate cancer cells according to a method previously described.[2] The 50% inhibitory concentration (IC_{50}) values were calculated by fitting the data with nonlinear regression using GraphPad Prism 5.0 (GraphPad Software, San Diego, California, USA). Experiments were performed with triplicate samples. Results were plotted in sigmoidal curves for the displacement of [**^{18}F]-BnTOxBN**, [**^{18}F]-BuTOxBN** and [**^{18}F]-PEGTOxBN** as a function of increasing concentration of BN(1-14). The tracers displayed high affinity for binding to GRPRs within PC-3 cell with IC_{50} values of 29 nM , 30 nM and 40 nM for [**^{18}F]-BnTOxBN**, [**^{18}F]-BuTOxBN** and [**^{18}F]-PEGTOxBN**, respectively.

Octanol/Water Partition Coefficient Study. Water partition coefficients were determined at pH =7.4. 5 μL containing 500 kBq of the radiolabeled compound in PBS was added to a vial containing 1.2 mL 1-octanol and PBS (1:1). After vortexing for 1 min, the vial was centrifuged for 5 min at 10 000 rpm to ensure complete separation of layers. Then, 40 μL of each layer was taken in a pre-weighed vial and measured in the γ-counter. Counts per unit weight of sample were calculated. The lop P values were found to be 1.27, 0.26 and -0.43 for [**^{18}F]-BnTOxBN**, [**^{18}F]-BuTOxBN** and [**^{18}F]-PEGTOxBN**, respectively.

Figure S1. Competitive Binding Assay on PC-3 cells with **[^{18}F]-BuTOxBN**

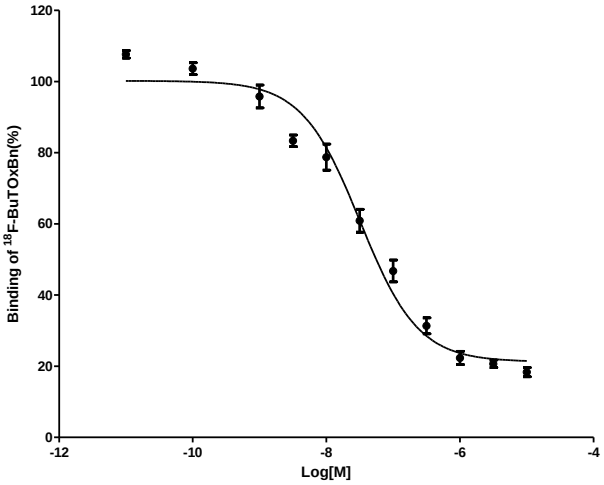


Figure S2. Competitive Binding Assay on PC-3 cells with **[^{18}F]-BnTOxBN**

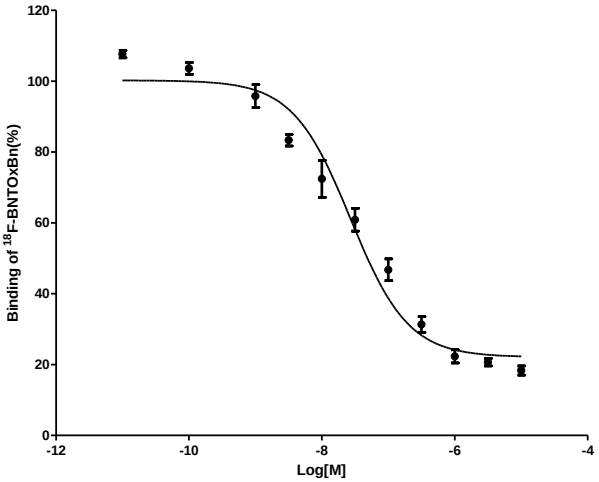
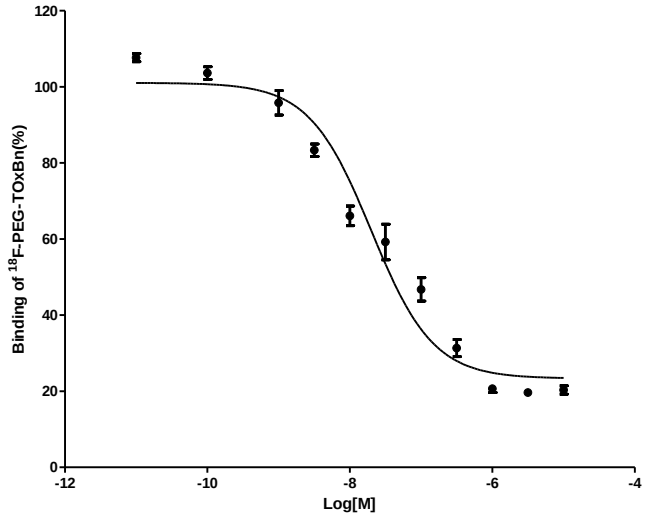


Figure S3. Competitive Binding Assay on PC-3 cells with **[^{18}F]-PEGTOxBN**



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