Supplementary material for Kristian A, et al. Positron emission tomography and pharmacokinetics of 2-[¹⁸F]-fluoroethyl choline for metabolic studies in breast cancer xenografts. Acta Oncol 2014; 53:1086–92.

Supplementary Figure 1. (a) A two-tissue compartment model applied for kinetic modeling for timeframe from 0 to 90 minutes. C_B , concentration of bound tracer in tissue; C_F , concentration of the free tracer in tissue; C_P , concentration of tracer in the plasma; C_T , concentration of tracer in tissue. k_1 , k_2 , k_3 and k_4 are rate constant for tracer transfer between compartments as indicated on the scheme. The rates constant are numerical estimated by solving a set of two differential equations. (b) An equation for linear regression analysis of tracer kinetics for a timeframe from 20 to 90 minutes. K_P is a Patlak slope, V is an intercept.

Supplementary Appendix

Production of 2-[¹⁸F]-fluoroethyl choline

The automated process was implemented on a Scintomics HotBox III synthesis module. [¹⁸F]fluoride ions were produced via the ¹⁸O(p, n)¹⁸F nuclear reaction by irradiation of a H₂¹⁸O water target using a GE Healthcare PETtrace cyclotron.

The ¹⁸F radioactivity was extracted from the target water using an anion exchange cartridge (Waters SepPak Accell plus QMA light). The trapped ¹⁸F was eluted with a solution of Kryptofix 2.2.2 (35 μmol) and potassium hydrogen carbonate (15 μmol) in acetonitrile-water (4:1, 500 μl). The eluate was concentrated to dryness under reduced pressure (200 mbar) with gentle heating (75°C) to obtain the potassium crypt-222 cryptate ¹⁸F-complex ([K⁺ 2.2.2]¹⁸F⁻). Two cycles of addition of anhydrous acetonitrile (500 μl) followed by evaporation were conducted to remove excess water from the dried residue. The reactor was cooled to room temperature and ethylene ditosylate (7.5 mg) in acetonitrile (500 μl) was added and heated to 75°C for 4.5 minutes to obtain 2-[¹⁸F]fluoroethyltosylate ([¹⁸F]FETs). Subsequently, the reactor was cooled

Supplementary Figure 2. In vitro uptake of [¹⁸F]FECh in the MAS98.06 and MAS98.12 cell suspension after 90 minutes incubation at 37°C.

and aqueous acetic acid (3 ml, 0.0066 M) was added to selectively precipitate unreacted ethylene ditosylate.

The obtained suspension was filtered through a 0.54 μm membrane filter and chromatographed through a stack of two C18 cartridges (Sep-Pak C18 Plus Short) using 35% MeOH in water (35 ml). The [¹⁸F]FETs peak (10–20 mL) was identified using an online radioactivity detector and diverted through a Strata X cartridge to immobilized the product. The Strata X was dried in a stream of nitrogen. [¹⁸F]FETs was eluted in DMSO (500 μl) into a reactor containing N,N-dimethyl aminoethanol (50 μl) and heated to 110°C for 10 minutes. The reactor was cooled to r.t. and water (4 ml) was added. The opaque mixture was loaded onto a cation-exchange cartridge (Accell CM plus) and the cartridge was washed with EtOH (10 ml) followed by water (10 ml).

The product was eluted from the cartridge in 0.9% NaCl solution, passed through a Millex sterile filter and collected in a multi injection vial. Identity and purity of the product were determined using radioTLC (Merck Silica Gel 60, MeOH-water) and radioHPLC (Partisil HPLC Column 10 SCX, 10 μm particle size, L×I.D. 25 cm×4.6 mm, phosphate buffer).