

Materials List for:

# Technical Aspect of the Automated Synthesis and Real-Time Kinetic Evaluation of [<sup>11</sup>C]SNAP-7941

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## Materials

| Name   | Company  | Catalog Number | Comments                                     |
|--|--|----------------|--|
| <b>Table 1: List of materials and instrumentation of the fully automated radiosynthesis of [<sup>11</sup>C]SNAP-7941</b> |  |                |  |
| Ni catalyst  | Shimadzu, Kyoto, Japan                         |                | Shimaliite Ni reduced, 80/100 mesh           |
| Iodine   | Merck, Darmstadt, Germany                      |                | 1.04761.0100                                 |
| Acetonitrile   | Merck, Darmstadt, Germany                      |                | for DNA synthesis, < 10 ppm H <sub>2</sub> O |
| Acetonitrile   | Sigma-Aldrich, St. Louis, MO, USA              |                | HPLC grade                                   |
| Ammonium acetate   | Merck, Darmstadt, Germany                      |                |  |
| Acetic acid  | Merck, Darmstadt, Germany                      |                | glacial                                      |
| Ethanol  | Merck, Darmstadt, Germany                      |                | 96%  |
| NaCl   | B. Braun, Melsungen, Germany                   |                | 0.9%   |
| Tetrabutylammonium hydroxide   | Sigma-Aldrich, St. Louis, MO, USA              |                |  |
| Methanol   | Sigma-Aldrich, St. Louis, MO, USA              |                | HPLC grade                                   |
| SPE cartridge  | Waters, Milford, MA, USA                       |                | SepPak C18plus                               |
| Semi-preparative RP-HPLC column  | Merck, Darmstadt, Germany                      |                | Chromolith SemiPrep RP-18e, 100-10 mm        |
| Precolumn  | Merck, Darmstadt, Germany                      |                | Chromolith Guard RP-18e, 5-4.6 mm            |
| Precursor  | University of Vienna, Austria                  |                | SNAP-acid                                    |
| Reference compound   | University of Vienna, Austria                  |                | SNAP-7941                                    |
| Silver trifluoromethanesulfonate   | Sigma-Aldrich, St. Louis, MO, USA              |                |  |
| Graphpa GC   | Alltech, Deerfield, IL, USA                    |                | 80/100 mesh                                  |
| PET trace 860 cyclotron  | GE Healthcare, Uppsala, Sweden                 |                |  |
| [ <sup>11</sup> C]CO <sub>2</sub> high pressure target   | Air Liquide, Vienna, Austria                   |                |  |
| TRACERlabFX2 C   | GE Healthcare, Uppsala, Sweden                 |                |  |
| N <sub>2</sub> + 1% O <sub>2</sub>   | Air Liquide, Vienna, Austria                   |                | Target gas                                   |
| Name   | Company  | Catalog Number | Comments                                     |
| <b>Table 2: List of materials and instrumentation of the quality control of [<sup>11</sup>C]SNAP-7941.</b>               |  |                |  |
| Merck Hitachi LaChrom, L-7100  | Hitachi Vantara Austria GmbH (Vienna, Austria) |                | HPLC pump                                    |

|   |  |                       |   |
|---|--|-----------------------|---|
| Merck Hitachi, L7400  | Hitachi Vantara Austria GmbH (Tokyo, Japan)                |                       | UV-detector   |
| Nal-radiodetector   | Raytest (Straubenhardt, Germany)                           |                       | Nal-radiodetector   |
| Chromolith Performance RP-18e, 100-4.6 mm   | Merck (Darmstadt, Germany)                                 |                       | HPLC column   |
| 430-GC  | Bruker (Bremen, Germany)                                   |                       | Gas chromatograph   |
| Capillary column ID-BP20; 12 mx0.22 mmx0.25 mm  | SGE Ananalytical Science Pty. Ltd. (Victoria, Australia)   |                       | Gas capillary   |
| Wesco, osmometer Vapro 5600   | Sanoya Medical Systems (Vienna, Austria)                   |                       | Osmometer   |
| g-spectrometer  |  |                       | g-spectrometer  |
| Gas chromatography controlling software   | VARIAN (Palo Alto, California, U.S.A)                      |                       | Galaxie Version 1.9.302.952   |
| Gamma spectrometer controlling software   | ORTEC (Oak Ridge, Tennessee, U.S.A.)                       |                       | Maestro for windows Version 6.06  |
| Gamma spectrum recalling software   | ORTEC (Oak Ridge, Tennessee, U.S.A.)                       |                       | Winplots version 3.21   |
| HPLC controlling software   | Raytest (Straubenhardt, Germany)                           |                       | Gina Star Version 5.9   |
| inolab 740  | WTW (Weilheim, Germany)                                    |                       | pH meter  |
| <b>Name</b>   | <b>Company</b>   | <b>Catalog Number</b> | <b>Comments</b>   |
| <b>Table 3: List of materials and instrumentation for the evaluation of the real-time kinetic behaviour of [<sup>11</sup>C]SNAP-7941.</b> |  |                       |   |
| Madin-Darby Canine Kidney cell line (MDCKII-hMDR1)  | Netherlands Cancer Institute (NKI, Amsterdam, Netherlands) |                       | Expressing the human P-glycoprotein (hMDR1)                             |
| Madin-Darby Canine Kidney cell line (MDCKII-WT)   | Netherlands Cancer Institute (NKI, Amsterdam, Netherlands) |                       | Wildtype (WT)   |
| DMEM GlutaMAX   | VWR International GmbH, Vienna, Austria                    |                       | Gibco 61965-026   |
| Fetal Calf Serum (FCS)  | VWR International GmbH, Vienna, Austria                    |                       | Gibco 10270-106   |
| Penicillin/Streptomycin   | VWR International GmbH, Vienna, Austria                    |                       | Gibco 15140   |
| Cell culture dish   | Greiner Bio-One GmbH, Frickenhausen, Germany               |                       | Cellstar 100 mm x 20 mm, Mfr.No. 664160                                 |
| <i>In vitro</i> experiments   |  |                       |   |
| DMEM GlutaMAX   | VWR International GmbH, Vienna, Austria                    |                       | Gibco 61965-026   |
| (±)-Verapamil hydrochloride   | Sigma Aldrich (St. Louis, Missouri, USA)                   |                       |   |
| DMSO  | Sigma Aldrich (St. Louis, Missouri, USA)                   |                       | 276855-100 mL   |
| Cell culture dish   | Greiner Bio-One GmbH, Frickenhausen, Germany               |                       | Cellstar 100 mm x 20 mm, Mfr.No. 664160                                 |
| Sterile disposable plastic pipettes   | VWR International GmbH, Vienna, Austria                    |                       | Sterilin, 5 mL – 25 mL  |
| Sterile pipette tips  | VWR International GmbH, Vienna, Austria                    |                       | Eppendorf epT.I.P.S. Biopur 20 µL – 200 µL                              |
| Cell culture flasks   | Greiner Bio-One GmbH, Frickenhausen, Germany               |                       | Cellstar 250 mL, 75 cm <sup>2</sup> red filter screw cap, Mfr.No.658175 |
| LigandTracer control Version 2.2.2  | Ridgeview Instruments AB, Uppsala, Sweden.                 |                       |   |

|                                 |   |  |   |
|---------------------------------|---|--|---|
| LigandTracer Yellow             | Ridgeview Instruments AB,<br>Uppsala, Sweden. |  |   |
| LigandTracer White              | Ridgeview Instruments AB,<br>Uppsala, Sweden. |  |   |
| GraphPad Prism 6.0              | GraphPad Software, Inc.                       |  |   |
| Handheld automated Cell Counter | Millipore Corporation Billerica<br>MA01821    |  | Scepter (Cat.No. PHC00000)                    |
| Cell Counter Sensors            | Millipore Corporation Billerica<br>MA01821    |  | Scepter Sensor 60 $\mu$ m (Cat.No. PHCC60050) |