Data in Brief 15 (2017) 174–202

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Dataset on the synthesis and characterization of boron fenbufen and its F-18 labeled homolog

Chun-Nan Yeh [a], Chi-Wei Chang [b], Yi-Hsiu Chung [c], Shi-Wei Tien [d], Yong-Ren Chen [d], Tsung-Wen Chen [a], Ying-Cheng Huang [e], Hsin-Ell Wang [f], You-Cheng Chou [d], Ming-Huang Chen [g], Kun-Chun Chiang [h], Wen-Sheng Huang [b], Chung-Shan Yu [d,i]

[a] *Department of Surgery, Liver Research Center, Chang-Gung Memorial Hospital at Linkou, Chang Gung University, Taiwan*
[b] *Department of Nuclear Medicine, Veterans General Hospital at Taipei, Taiwan*
[c] *Center for Advanced Molecular Imaging and Translation, Chang Gung Memorial Hospital, Taiwan*
[d] *Department of Biomedical Engineering and Environmental Sciences, National Tsinghua University, Hsinchu 300, Taiwan*
[e] *Department of Neurosurgery, Chang-Gung Memorial Hospital at Linkou, Chang Gung University, Taiwan*
[f] *Department of Biomedical Imaging and Radiological Sciences, National Yang-Ming University, Taipei, Taiwan*
[g] *Department of Medical Radiology, Yang-Ming University at Taipei, Taiwan*
[h] *Department of Surgery, Chang-Gung Memorial Hospital at Keelung, Chang Gung University, Taiwan*
[i] *Institute of Nuclear Engineering and Science, National Tsing-Hua University, Hsinchu 300, Taiwan*

ARTICLE INFO

Article history:
Received 17 July 2017
Received in revised form
8 August 2017
Accepted 30 August 2017
Available online 5 September 2017

Keywords:
Setup
NMR spectra
Coupling constant
Binding
Survival

ABSTRACT

The data presented in this article are related to the research article entitled "Synthesis and Characterization of Boron Fenbufen and its F-18 Labeled Homolog for Boron Neutron Capture Therapy of COX-2 Overexpressed Cholangiocarcinoma". The contents of the data article include 1) the set up for performing *in vitro* binding assay, 2) ^{1}H-, ^{13}C- and ^{19}F-NMR of compounds described in main text, 3) HPLC chromatogram of the fluorination mixtures, 4) data of *in vitro* stability test, cell survival assay, western blot and PCR analysis, 5) the modules for fixing the two CCA rats for BNCT, and 6) bar diagram for tumor reduction using [^{18}F]FDG-PET 24 h post treatment with BNCT.

DOI of original article: http://dx.doi.org/10.1016/j.ejps.2017.07.019
E-mail address: csyu@mx.nthu.edu.tw (C.-S. Yu).

http://dx.doi.org/10.1016/j.dib.2017.08.048

Specifications Table

Subject area	Chemistry, Biology
More specific subject area	Spectroscopy, Chromatography, Bioassay
Type of data	Table, Chromatogram (HPLC), Illustration, Graph, Figure
How data was acquired	Spectra of NMR of ^{1}H, ^{13}C and ^{19}F were generated from NMR experiments. Survival assay was performed by MTT protocol. Statistical analysis of PET imaging was analyzed. Setup for binding assay and BNCT module was described. Data of mRNA and protein expression level were described.
Data format	Raw, Analyzed.
Experimental factors	Samples have been well prepared, purified and characterized.
Experimental features	The relevant data of cell survival assay, HPLC chromatogram and analytic data were determined.
Data source location	Hsinchu, Taoyuan and Taipei, Taiwan
Data accessibility	All the data is with this article.

Value of the data

- NMR spectra of the target compounds and intermediates are useful for structural characterization.
- Set up for binding assay is useful for other researchers to perform the relevant binding assay design.
- Expression level of protein and mRNA of COX-2 in HuCCT1 is useful for future selection of patients for BNCT study.
- Module for performing neutron irradiation is useful for ensuring the measurement correctness.

1. Data

The data set of this article provides information on structural data, separation data, and setup. Figs. 1 and 8 show the binding and BNCT irradiation setups, respectively. Fig. 2 shows the HPLC chromatogram. Figs. 4–7 show the bioassay data. Fig. 9 shows the statistics of imaging data. Fig. 3 and the rest data show the NMR and mass data.

2. Experimental design, materials and methods

Chemical synthesis and radiochemical synthesis provided the target compounds. Chemical structures were characterized using ^{1}H-, ^{13}C- and ^{19}F-NMR and low-resolution and high-resolution mass spectrometry (LR-MS, HR-MS). Meta- and ortho-fluoro fenbufen compounds are differentiated based on ^{13}C-^{19}F coupling constants. Radiofluorination gave the meta- and ortho-FFBPin, ***m*-6** and *o*-FFBPin, ***o*-6**. The two isomers were obtained in limited amounts of less than 3 mg. ^{1}H-NMR were not easily used to identify the $J_{F,H}$ of aromatic couplings because they are similar to the values of $J_{H,H}$. The ^{13}C-^{19}F coupling constants from different bond ranges could be used to identify the fluoro position. Binding assay using the set up as shown in Fig. 1 was performed in a compact manner through a team work. One member is responsible for mixing the enzyme, tracer and ligand and for transferring the mixture. The other member pumped the mixture through the silica cartridge. The third member was responsible for controlling the timing. The rest work regarding the counting of the activity was done by the fourth member. The binding experiments were performed for COX-1 and COX-2, sequentially. The laborious pumping of the mixture for