

## Supplementary Information

### Synthesis and characterization of $^{18}\text{F}$ -labeled hydrazinocurcumin derivatives for tumor imaging

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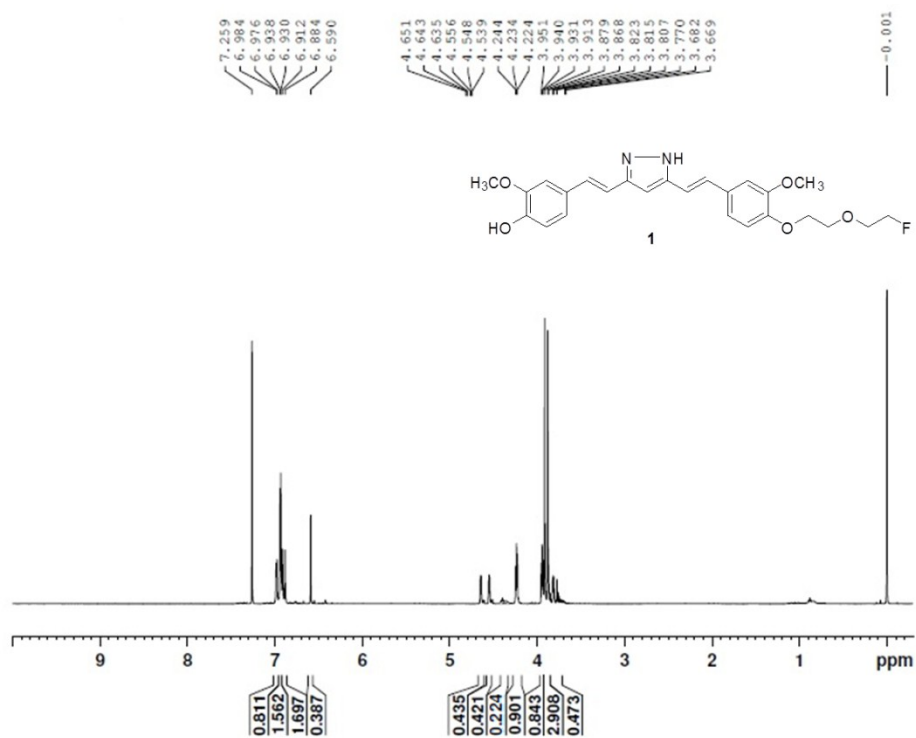
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135-710, Korea

#### Contents:

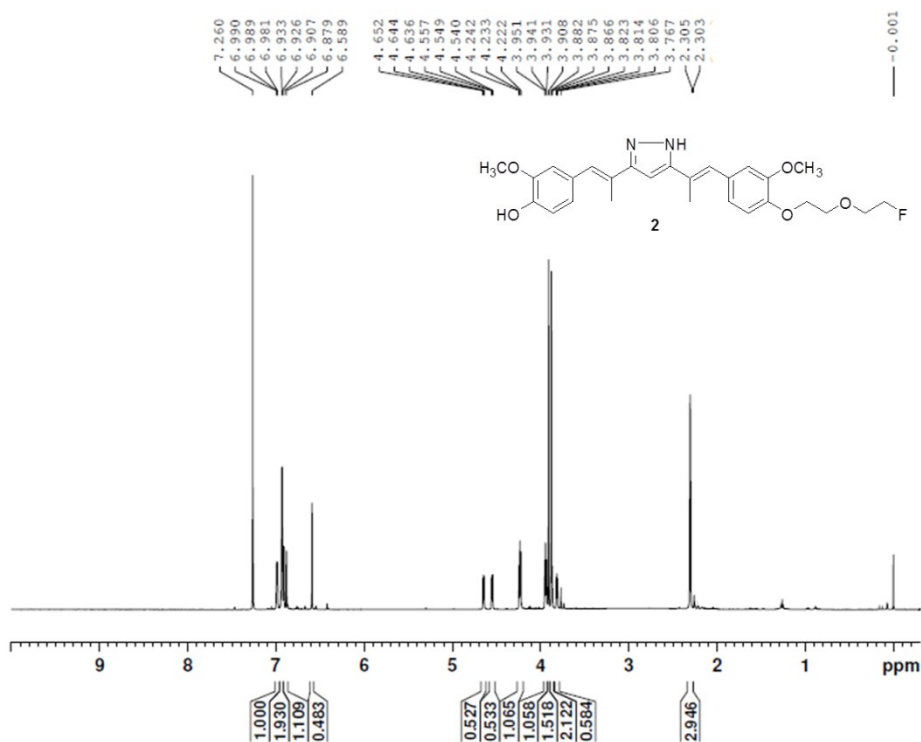
1.  $^1\text{H}$  NMR spectra of compounds **1-6** and precursors (**26** and **27**) ..... S2 - S5
2. HPLC chromatograms of compounds **1-6** and precursors (**26** and **27**) ..... S6 - S9
3. HPLC chromatograms of the radioligands ..... S10
4. 2D ROESY spectra of **2** ..... S11

# 1. <sup>1</sup>H NMR spectra of compounds 1-6 and precursors

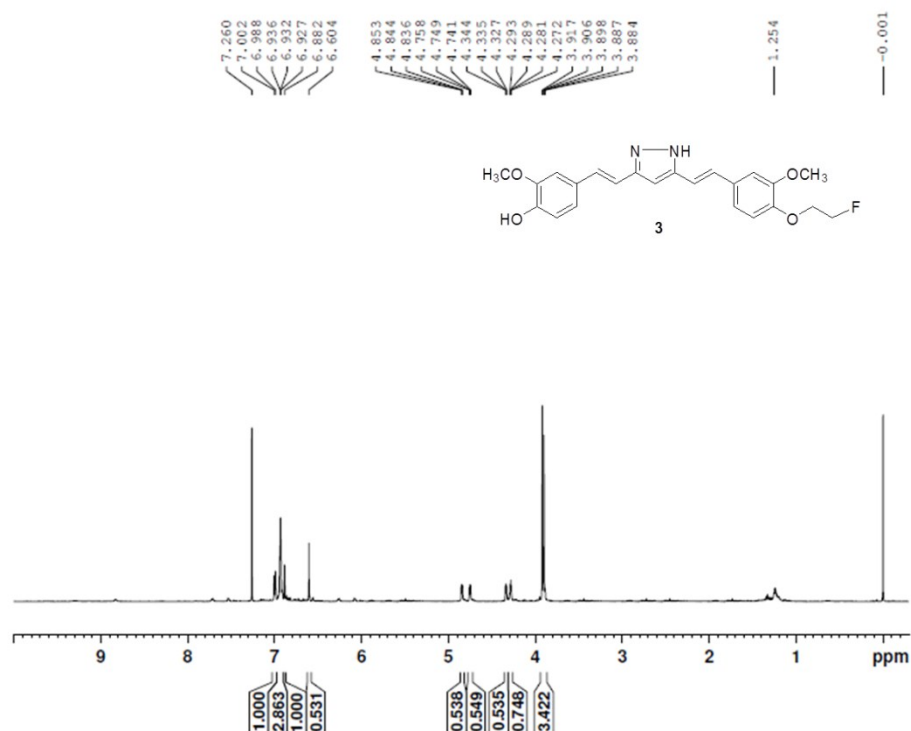
## Compound 1



## Compound 2



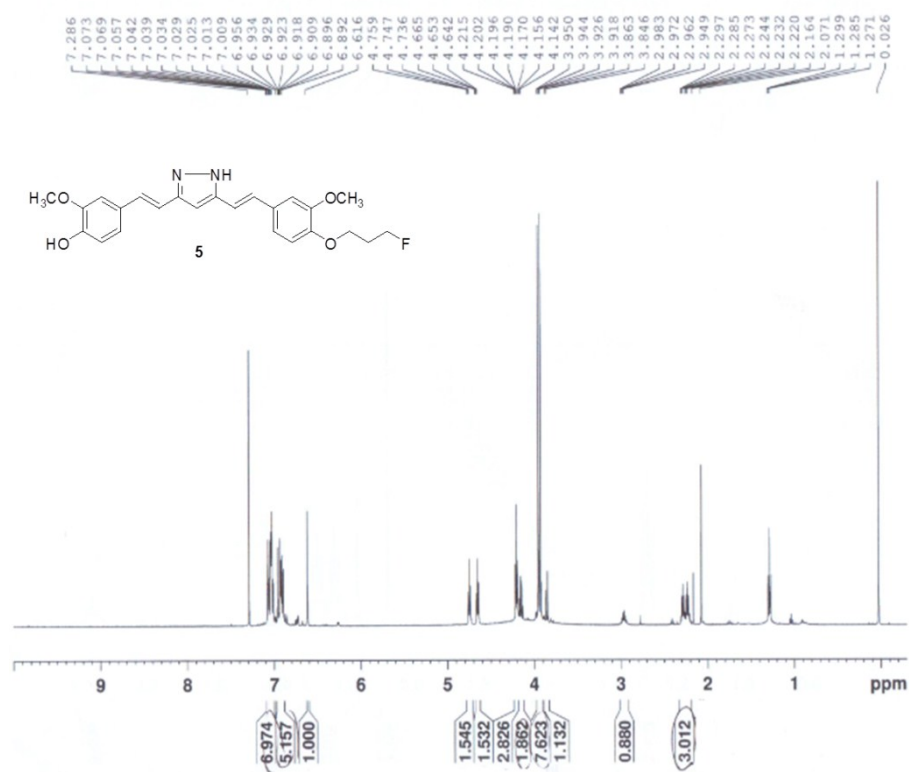
# Compound 3



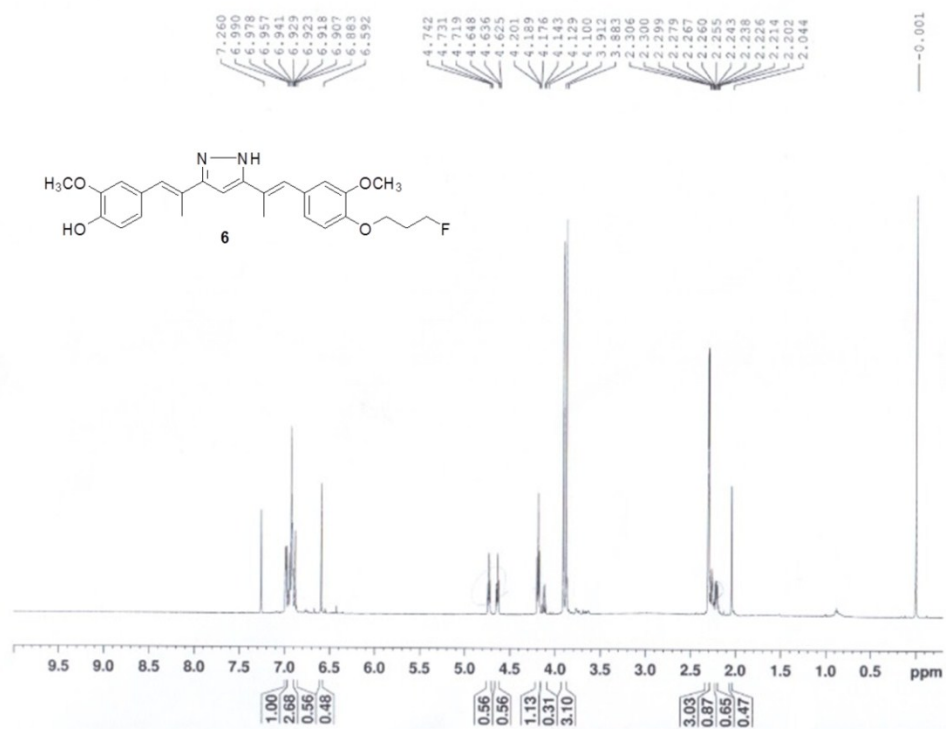
# Compound 4



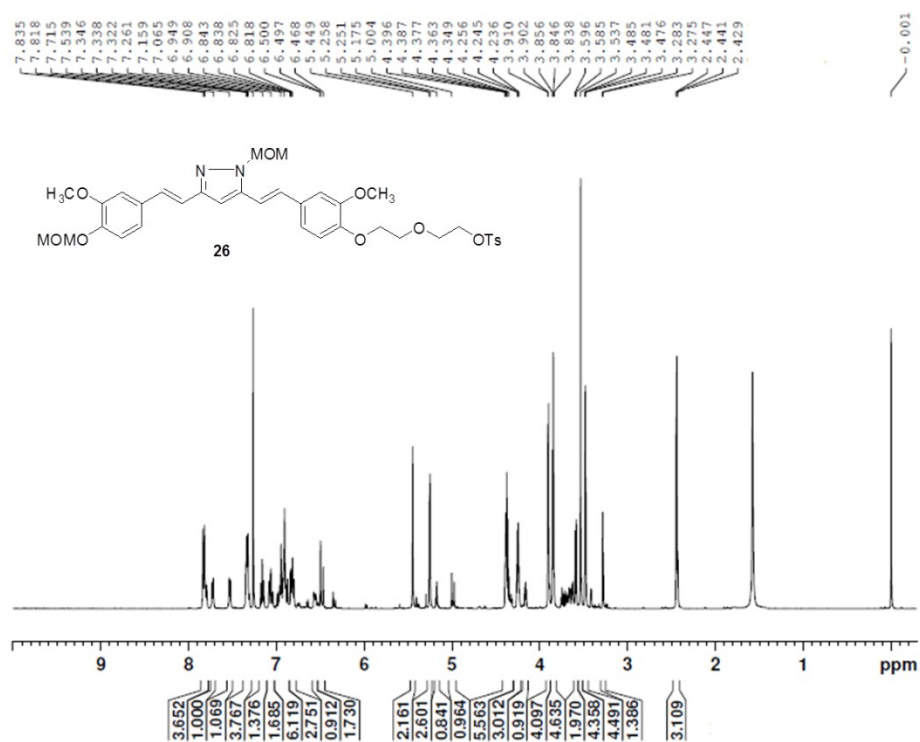
## Compound 5



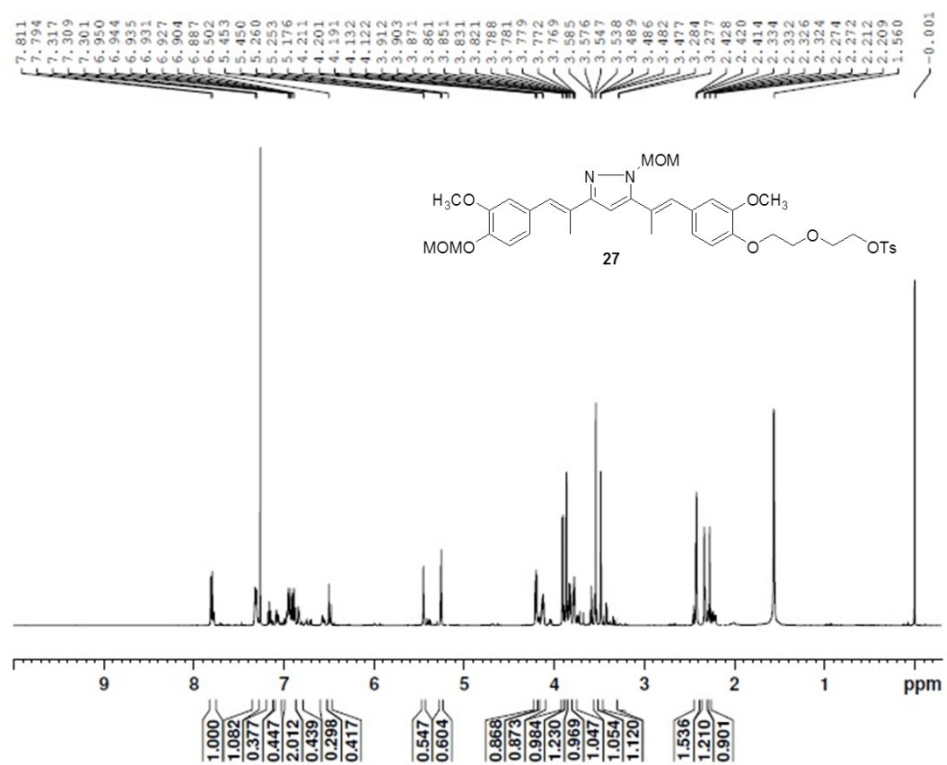
## Compound 6



## Precursor 26



## Precursor 27



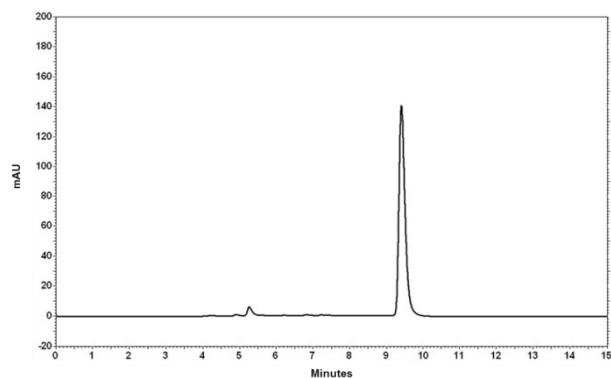
## 2. HPLC chromatograms of target compounds and precursors

HPLC column: YMC-Pack C18 (4.6 x 250 mm, 5  $\mu$ m)

Flow rate: 1 mL/min

Detection: UV detector (254 nm)

### Compound 1

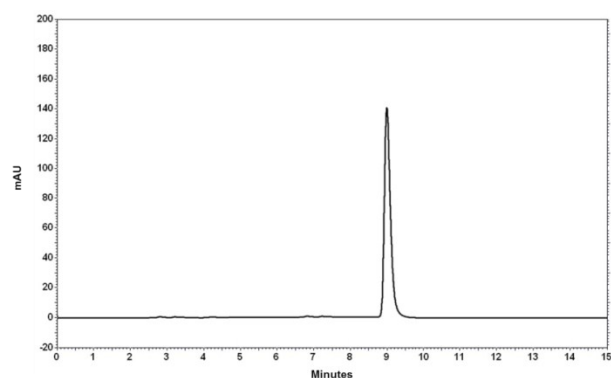


HPLC solvents: 30:70 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 9.40 min

Chemical purity: 98.99%

### Compound 2

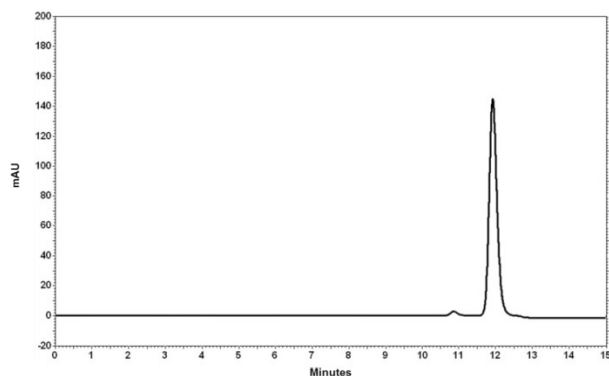


HPLC solvents: 25:75 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 9.08 min

Chemical purity: 99.64%

### Compound 3

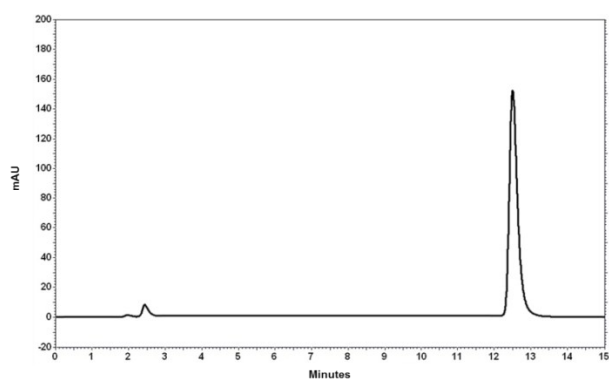


HPLC solvents: 55:45 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 12.08 min

Chemical purity: 99.01%

### Compound 4

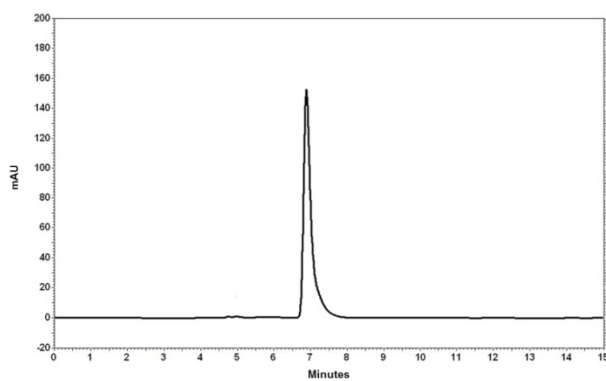


HPLC solvents: 55:45 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 12.54 min

Chemical purity: 98.94%

## Compound 5

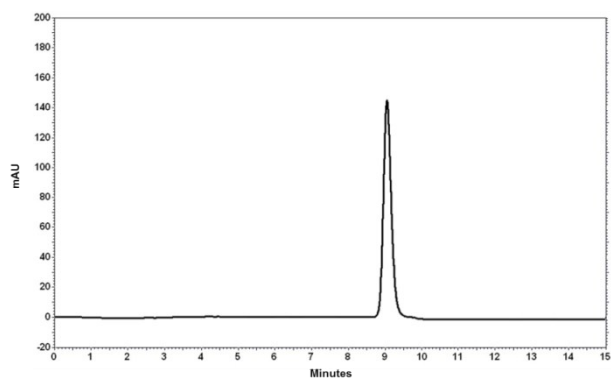


HPLC solvents: 45:55 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 6.97 min

Chemical purity: 99.84%

## Compound 6



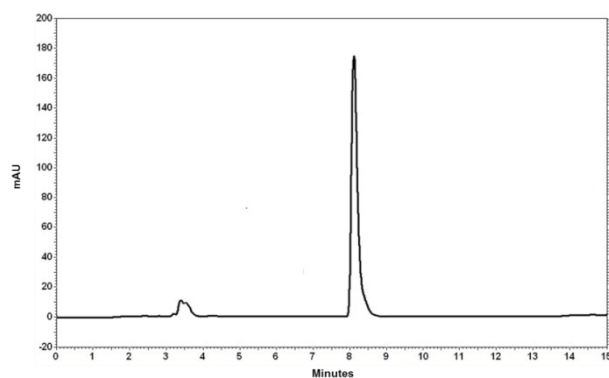
HPLC solvents: 45:55 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 9.09 min

Chemical purity: 99.96%



## Precursor 26

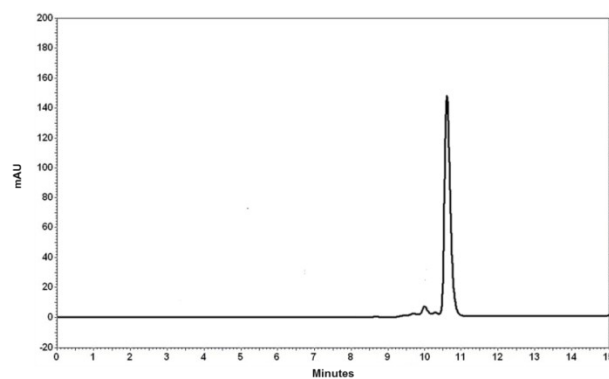


HPLC solvents: 20:80 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 8.24 min

Chemical purity: 96.54%

## Precursor 27



HPLC solvents: 20:80 H<sub>2</sub>O (0.1% trifluoroacetic acid)-CH<sub>3</sub>CN

Retention time: 10.78 min

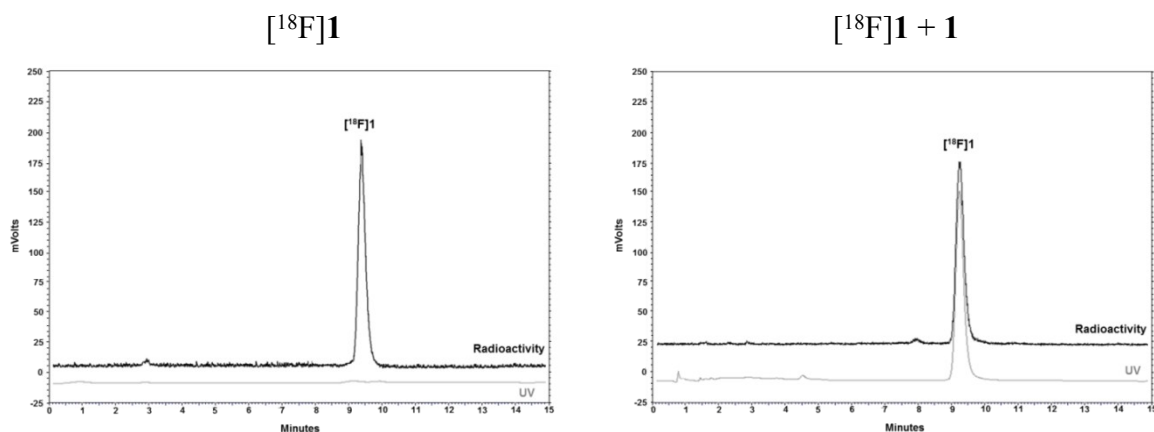
Chemical purity: 99.03%

**3. HPLC chromatograms of final radioligands ( $[^{18}\text{F}]1$  and  $[^{18}\text{F}]2$ ) and after co-injection of the radioligands with the corresponding cold ligands**

HPLC column: YMC-Pack C18 (4.6 x 250 mm, 5  $\mu\text{m}$ )

Flow rate: 1 mL/min

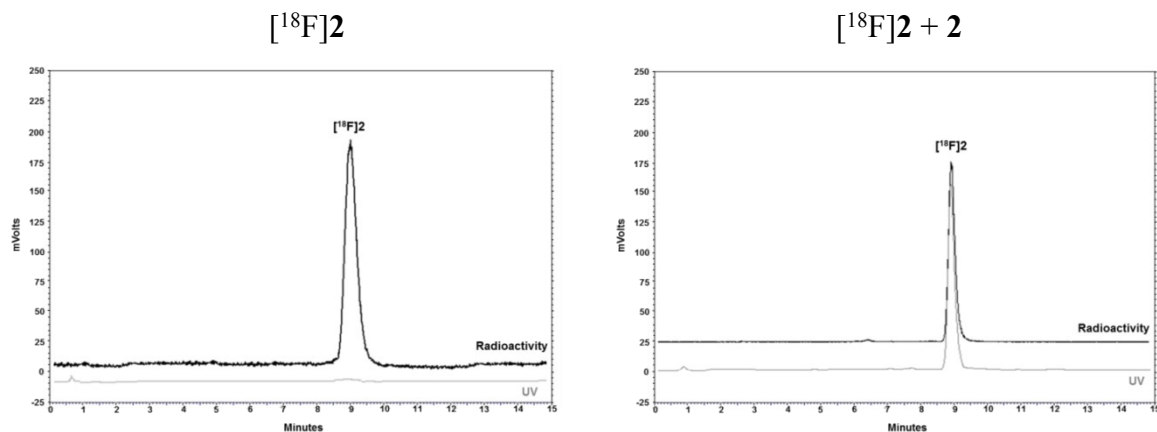
Detection: NaI(Tl) radioactivity detector (black) and UV detector (grey)



Retention time: 9.42 min

Radiochemical purity: 98.20%

HPLC solvents: 30:70  $\text{H}_2\text{O}$  (0.1% trifluoroacetic acid)- $\text{CH}_3\text{CN}$

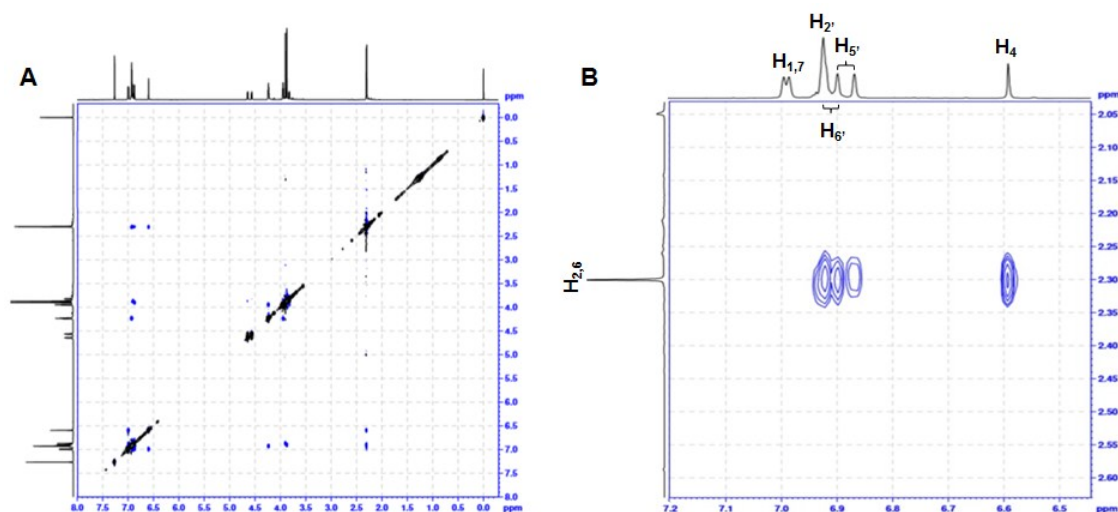


Retention time: 9.02 min

Radiochemical purity: 99.56%

HPLC solvents: 25:75  $\text{H}_2\text{O}$  (0.1% trifluoroacetic acid)- $\text{CH}_3\text{CN}$

#### 4. 2D ROESY spectra of **2**



(A) Full spectrum; (B) partially enlarged spectrum of (A); Methyl groups at C2 and C6 positions of **2** are confirmed to have *E,E*-configurations, as no cross-peaks were detected between methyl protons at C2 and C6 positions, indicated as H<sub>2,6</sub> (2.30 ppm), and olefinic protons at C1 and C7 positions, indicated as H<sub>1,7</sub> (6.98 and 6.99 ppm). The numbers with a prime symbol indicate the positions of aromatic carbons.