

SUPPORTING INFORMATION

Title: Radiosynthesis and evaluation of [¹¹C]HD-800, a high affinity brain penetrant PET tracer for imaging microtubules

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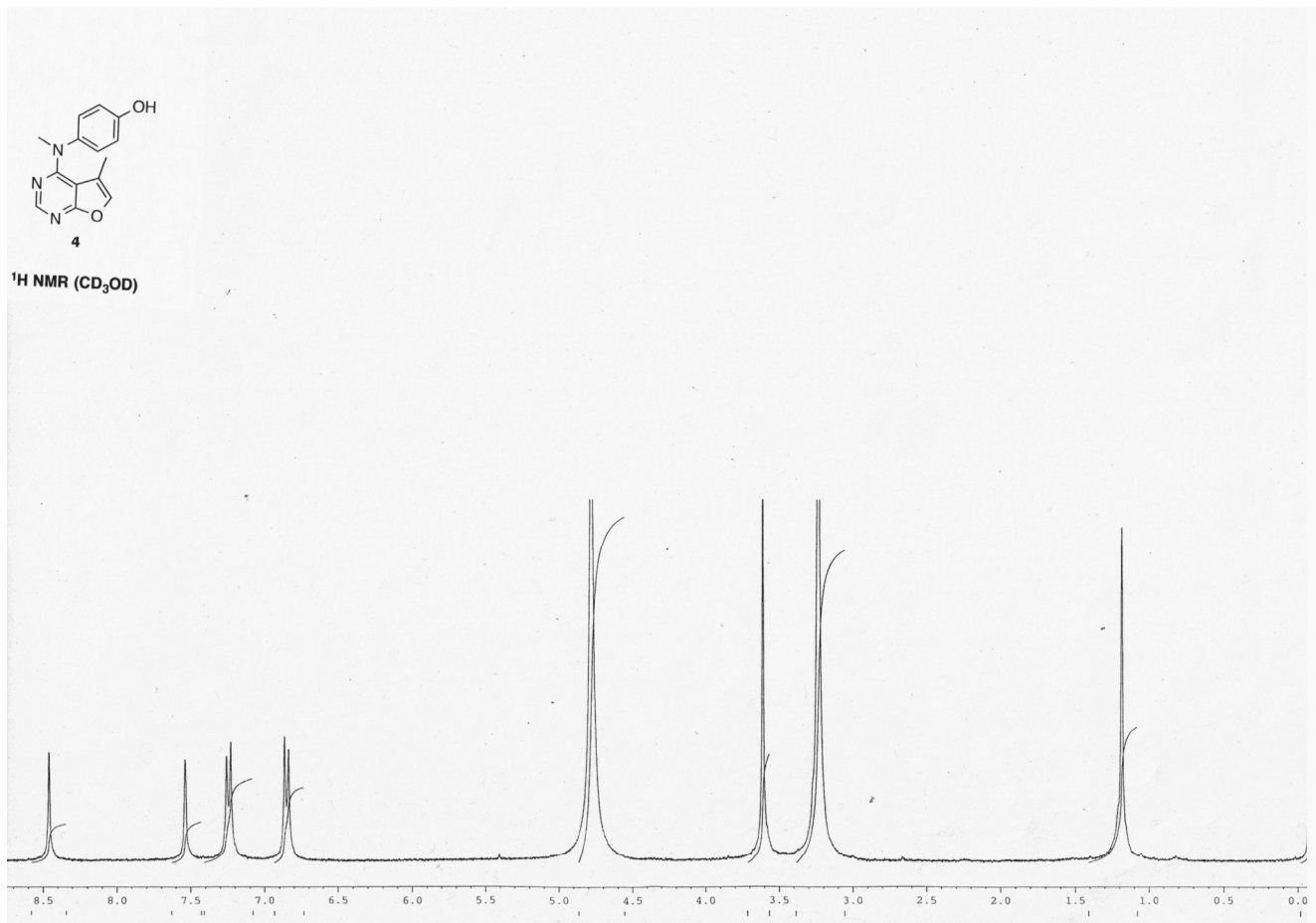
#1. Molecular formula strings of key chemicals

Compound 3: CN(C1=CC=C(OC)C=C1)C2=C3C(OC=C3C)=NC=N2

Compound [¹¹C]3: CN(C1=CC=C(O[11CH3])C=C1)C2=C3C(OC=C3C)=NC=N2

Compound 4: CN(C1=CC=C(O)C=C1)C2=C3C(OC=C3C)=NC=N2

#2. ^1H NMR spectra of compound 4



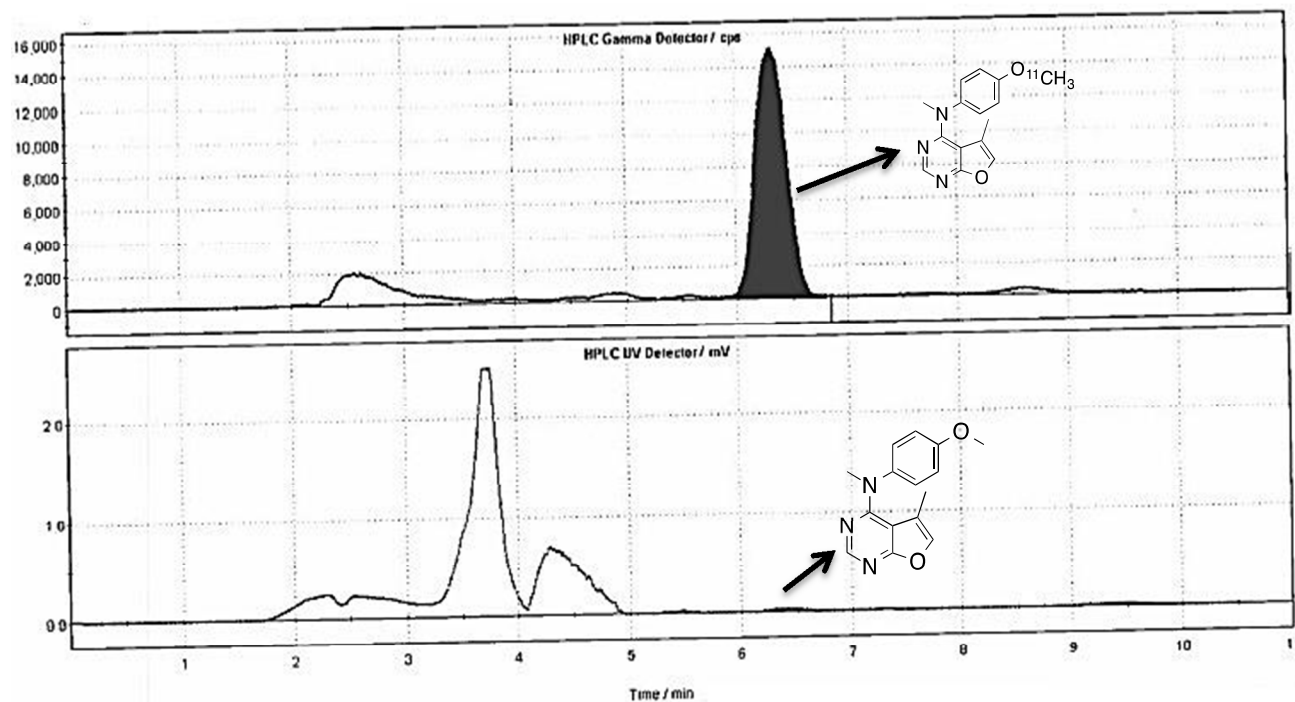
#3. Binding affinity of HD-800 to brain targets (Table 1)

Table 1. Affinity of HD-800 to brain targets.

Targets	Affinity (nM)	Targets	Affinity (nM)
MT	IC50 3.235	5-HT1A-1E	>10,000
MT	GI50 <1035		
5-HT2A-2C	>10,000	5-HT3-7	>10,000
5-HT2A-2C	>10,000	A	>10,000
5-HT3-7	>10,000	α1A-1C	>10,000
α ₂ -2C	>10,000	β ₂ -3	>10,000
AMPA	>10,000	BZP	>10000
Ca ⁺ channel	>10,000	CB1, CB2	>10,000
D1-D5	>10,000	DAT	>10,000
DOR	>10,000	H1	>10,000
H2	>10,000	H3, H4	>10,000
HERG	>10,000	GABA	>10,000
EP	>10,000	I	>10,000
KOR	>10,000	KA	>10,000
M	>10,000	mGluR	>10,000
MDR1	>10,000	MOR	>10,000
NET	>10,000	NK	>10,000
NPY	>10,000	NOP	>10,000
NT	>10,000	Oxytocin	>10,000
PBR	2364	PKC	>10,000
SERT	>10,000	Sigma1	>10,000
Sigma 2	>10,000	Na ⁺ Channel	>10,000
Smoothened	>10,000	VMAT 1,2	>10,000

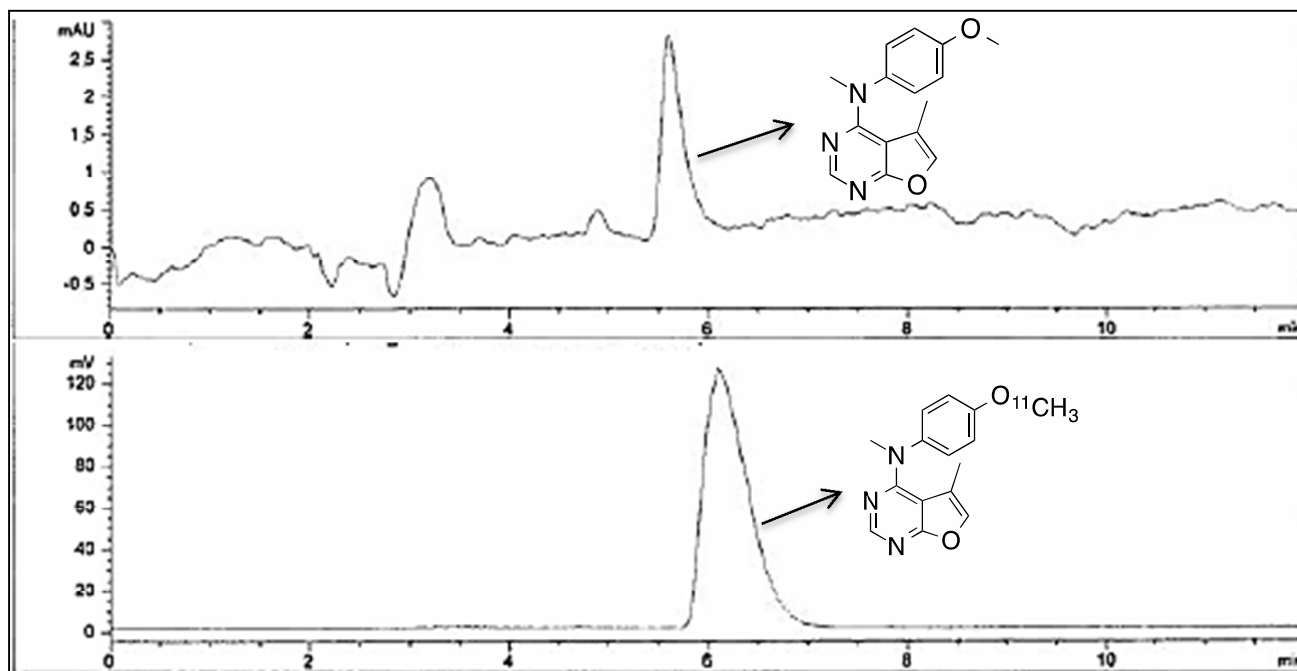
MT: microtubule; 5-HT: 5-hydroxytryptamin; A: adenosine; α: alpha; β: beta; BZP: benzodiazepine; AMPA: R-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid; CB: cannabinoid; D: dopamine; DAT: dopamine transporters; DOR: delta opioid receptors; EP: prostanoid receptors; GABA: gamma-amino butyric acid; H: histamine; hERG: human ether-a-go-go; KA: Kainate; KOR: kappa opioid receptors; M: muscarinic; MDR: multidrug resistance; MOR: mu opioid receptor; mGluR: metabotropic glutamate receptors; NMDA: N-methyl-D-aspartic acid; NK: neurokinin; NET: norepinephrine transporter; NT: neurotrophin; PKC: Protein kinase C; SERT: serotonin transporter; V: vasopressin; VMAT: vesicular monoamine transporter

#4. Semipreparative HPLC chromatogram of [¹¹C]HD-800



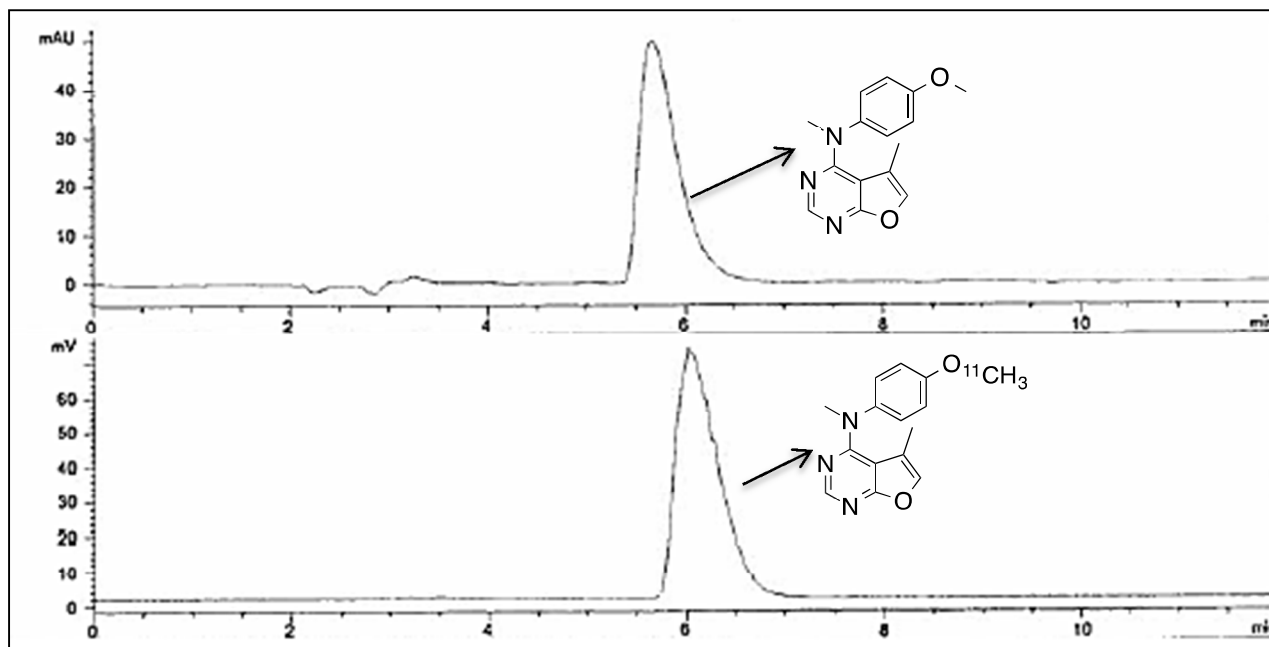
	Retention time	Component
UV detector @ 254 nm	6.4 min	HD800
Rad detector	6.3 min	[¹¹ C]HD800

#5. Analytical HPLC chromatogram of [¹¹C]HD-800



	Retention time	Component
UV detector @ 254 nm	5.67 min	HD800
Rad detector	6.01 min	[¹¹ C]HD800

#6. Analytical HPLC chromatograms of [¹¹C]HD-800 and unlabeled HD-800



	Retention time	Component
UV detector @ 254 nm	5.67 min	HD800
Rad detector	6.01 min	[¹¹ C]HD800