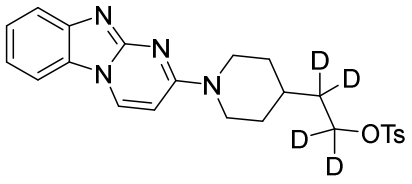
WHAT IS CLAIMED:

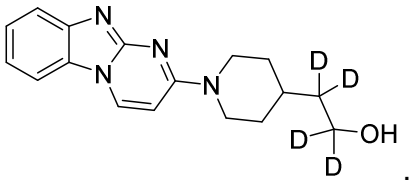
1. A compound of formula:



.

2. The compound of claim 1, having a deuterium enrichment factor of 3,000 or greater at each deuterium atom.

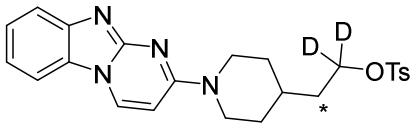
3. A compound of formula:



.

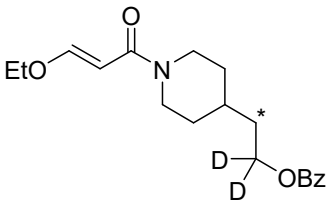
4. The compound of claim 3, having a deuterium enrichment factor of 3,000 or greater at each deuterium atom.

5. A method of synthesizing the compound of formula (I), the method comprising:

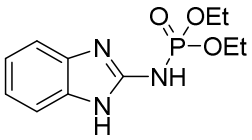


(I)

coupling a compound of formula (II) with a compound of formula (III)

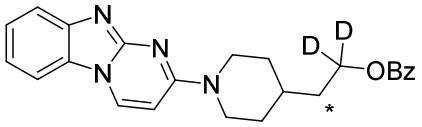


(II)



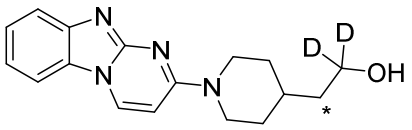
(III)

in the presence of $POCl_3$ and Et_3N in a non-aqueous solvent to give a first precursor (I-P1);



(I-P1)

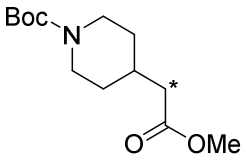
removing the benzoate group in I-P1 to give second precursor (I-P2); and



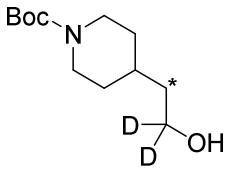
(I-P2)

replacing the hydroxyl group in I-P2 by a tosyl group to give compound (I), wherein, in formulae (I), (II), (I-P1) and (I-P2), the carbon atom labeled (*) is optionally doubly-deuterated.

6. The method of claim 5, wherein the compound of formula (II) is synthesized by a method comprising:

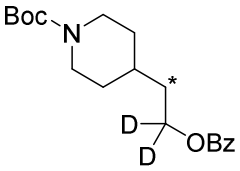
reacting 

with a first deuterating agent to produce a compound of formula (II-P1);



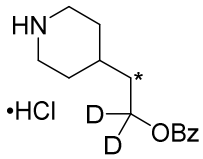
(II-P1);

introducing a benzoyl group to the hydroxyl group of (II-P1) to produce a compound of formula (II-P2);

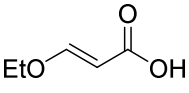


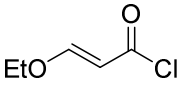
(II-P2)

removing the Boc protecting group from (II-P2) to produce a hydrochloride salt (II-P3); and



(II-P3)

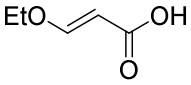
reacting (II-P3) with 

(IV) or 

(IVa) to produce the compound of formula (II).

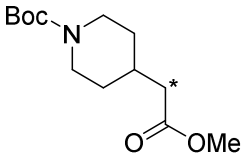
7. The method of claim 6, wherein the first deuterating agent comprises $LiAlD_4$.

8. The method of claim 6, wherein the first deuterating agent comprises D_2 gas.

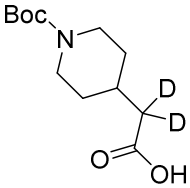
9. The method of claim 6, wherein compound (IVa) is formed by reacting 

with $SOCl_2$.

10. The method of claim 6, wherein the carbon atom labeled (*) is doubly deuterated, and wherein compound (II-P1) is created by:

reacting 

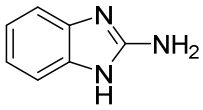
with a second deuterating agent to produce a compound of formula (II-P0); and



(II-P0)

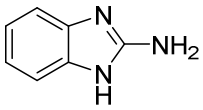
reacting the first deuterating agent with (II-P0) to form d_4-(II-P1).

11. The method of claim 5 wherein the compound of formula (III) is synthesized by a method comprising:

reacting  with $PCl(O)(OEt)_2$, in the presence of N-methylimidazole, and MeCN.

12. The method of claim 11, wherein the $PCl(O)(OEt)_2$ is formed *in situ* by reacting diethyl hydrogen phosphate with 1,3,5-trichloro-1,3,5-triazinane-2,4,6-trione.

13. The method of claim 11, wherein the compound of formula (III) is formed by:

charging a reactor under nitrogen with  and MeCN;

adding N-methylimidazole followed by MeCN to the mixture; and

adding $ClP(O)(OEt)_2$ dropwise for 1 hour at a temperature between 20 and 30 °C.

14. The method of claim 11, wherein the compound of formula (III) is formed by: charging a flask under nitrogen with 1,3,5-trichloro-1,3,5-triazinane-2,4,6-trione and MeCN;

adding diethyl hydrogen phosphate and Et_3N to the flask;

cooling the flask to 0 °C and adding 1H-benzo[d]imidazol-2-amine dissolved in THF; and

warming the reaction mixture to 15 – 25 °C for 1 hour.

15. The compound of claim 1, having a deuterium enrichment factor of 4,000 or greater at each deuterium atom.

16. The compound of claim 3, having a deuterium enrichment factor of 4,000 or greater at each deuterium atom.

17. The method of claim 5, further comprising radio-labeling the compound of formula (I) by replacing the tosylate group with an ^{18}F atom.

18. The method of claim 5, wherein the removing the benzoate group from compound (I-P1) occurs in the presence of NaOEt and EtOH.

19. The method of claim 18, wherein the removing takes place in a reactor under nitrogen.

20. The method of claim 5, wherein the replacing the hydroxyl group in compound (I-P2) with a tosyl group additionally includes basification after reacting (I-P2) with tosylate.

21. The method of claim 20, wherein:
the reacting with tosylate occurs in a reactor under nitrogen in a solvent mixture comprising MeCN and NMP; and

the basification is carried out with K_3PO_4.

22. The method of claim 5, wherein the coupling of the compound of formula (II) with the compound of formula (III) comprises:
charging a reactor under nitrogen with MeCN followed by compound (II) and compound (III);

adding MeTHF and Et_3N to the reactor;

cooling the reactor to between –10 and 10 °C;

adding $POCl_3$ to the reactor;

heating the contents of the reactor to 65 – 95 °C over a minimum of 2 hours;

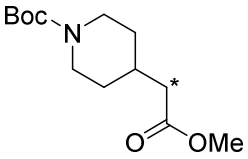
maintaining the contents of the reactor at 80 °C for at least 1.5 hours;

cooling the contents to 15 – 25 °C and adding 25 w/w% solution of K_2CO_3.

23. The method of claim 5, wherein the carbon atom labeled (*) is doubly deuterated, and wherein removing the benzoate group from d_4-(I-P1) comprises:
adding NaOH to a solution of d_4-(I-P1).

24. The method of claim 5, wherein the carbon atom labeled (*) is doubly deuterated, and wherein the replacing the hydroxyl group in d_4-(I-P2) by a tosyl group to give compound d_4-(I), comprises:
adding 4-methylbenzenesulfonic anhydride to a solution of d_4-(I-P2) and $TsOH \cdot H_2O$ in MeCN; and

heating the mixture to 40 °C.

25. The method of claim 6, wherein the compound  is purified by a method comprising passing the compound over charcoal, filtering and drying the resulting oil.

26. The method of claim 6, wherein the introducing a benzoyl group to the hydroxyl group of (II-P1) comprises:
charging compound (II-P1) to a reactor under nitrogen, with toluene, Et_3N, DMAP, and benzoyl chloride at a temperature between –5 and 5 °C.

27. The method of claim 6, wherein the removing the Boc protecting group from (II-P2) comprises:
charging a reactor under nitrogen at 0 – 5 °C with AcCl and 1-PrOH, compound (II-P2) in toluene solution; and

heating the mixture to 50 °C for 1 hour.

28. The method of claim 6, wherein the reacting (II-P3) with (IV) comprises:
charging a reactor under nitrogen at 20 – 30 °C with compound (II-P3), (*E*)-3-ethoxyacrylic acid (IV), and Et_3N; and

heating the mixture to 40 °C for 1 hour.

29. The method of claim 6, wherein the compound of formula (II) is formed by reacting (II-P3) with (IVa), and (IVa) is formed by reacting (IV) with $SOCl_2$ in DCM.

30. The method of claim 6, wherein the carbon atom labeled (*) is doubly deuterated, and wherein compound (II-P2) is created by:
adding BzCl to a solution of II-P1 in Et_3N and THF at 0 – 10 °C for 1 hour.

31. The method of claim 6, wherein the carbon atom labeled (*) is doubly deuterated, and wherein the removing the Boc protecting group from compound (II-P2) comprises:
adding HCl in EtOAc to a solution of (II-P2) in EtOAc.

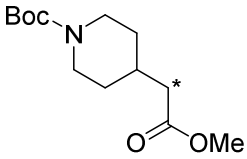
32. The method of claim 6, wherein the carbon atom labeled (*) is doubly deuterated and the reacting d_4-(II-P3) with (IVa) comprises:
adding (IVa) to d_4-(II-P3) in ET_3N and THF at 0 – 10 °C for 1 hour.

33. The method of claim 6, wherein the carbon atom labeled (*) is doubly deuterated and the coupling of the compound of formula (II) with the compound of formula (III) comprises:
forming a solution of compound (III) and d_4-(II) in 2-MeTHF and MeCN;

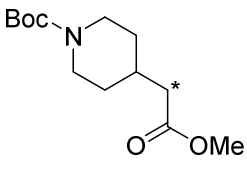
adding Et_3N followed by $POCl_3$ to the solution;

heating the solution to 80 °C for 4 hours; and

adding $NaHCO_3$ to the solution.

34. The method of claim 7, wherein a reactor under nitrogen was charged with anhydrous THF, the compound 

, and $LiAlD_4$ at 0 – 5 °C for 1 hour.

35. The method of claim 8, wherein the deuterium gas was applied to a pressure reactor containing compound 

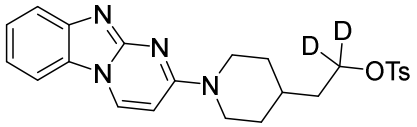
, NaOMe,

Carbonylchlorohydrido{bis[2-(diphenylphosphinomethyl)ethyl]amino}ethyl]amino}ruthenium(II), and PhMe, at a temperature of 100 °C, and a pressure of 20 atmospheres for 24 hours.

36. The method of claim 10, wherein the second deuterating agent is CD_3ONa in CD_3OD, and the reacting with the second deuterating agent takes place at 80 °C for 12 hours.

37. The method of claim 10, wherein the first deuterating agent is $LiAlD_4$ in THF, and the reacting takes place at –10 °C.

38. A composition comprising a compound of formula (I), wherein the di-deuterated compound is present at an isotopic purity of > 95% relative to non-deuterated and mono-deuterated forms.



(I)