

# **Novel interactions of fluorinated nucleotide derivatives targeting orotidine-5'-monophosphate decarboxylase**

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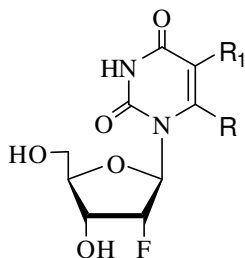
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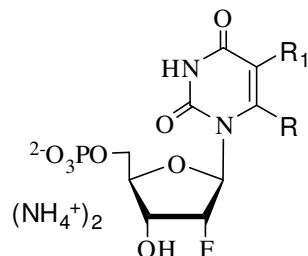
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### Purity Analyses.



- 27** R= I, R<sub>1</sub> = H  
**28** R= N<sub>3</sub>, R<sub>1</sub> = H  
**29** R= CN, R<sub>1</sub> = H  
**30** R= CONH<sub>2</sub>, R<sub>1</sub> = H  
**31** R= H, R<sub>1</sub> = CN  
**32** R= CO<sub>2</sub>Et, R<sub>1</sub> = H  
**38** R= NH<sub>2</sub>, R<sub>1</sub> = H



- 33** R= I, R<sub>1</sub> = H  
**34** R= N<sub>3</sub>, R<sub>1</sub> = H  
**35** R= CN, R<sub>1</sub> = H  
**36** R= CONH<sub>2</sub>, R<sub>1</sub> = H  
**37** R= H, R<sub>1</sub> = CN

Purity analysis for compounds **29-32** was evaluated on a Waters HPLC system equipped with a photodiode array detector using a Symmetry C18 5 $\mu$ m 4.6mm x 100 mm column. The methods used were of two types. Method A: 15% MeOH in H<sub>2</sub>O (1mL/min, isocratic) and Method B: 5% MeOH in CH<sub>3</sub>CN (0.5mL/min, isocratic). Purity analysis for compounds **27, 28, 33, 34,** and **38** was evaluated on a Waters<sup>TM</sup> LC/MS system equipped with a photodiode array detector using an XBridge C18 5 $\mu$ m 4.6mm x 150 mm column. The methods used were of three types. Method C: 10% MeOH in H<sub>2</sub>O (1mL/min, isocratic), Method D: 20% MeOH in H<sub>2</sub>O (1mL/min, isocratic), Method E: 3% AcOH in H<sub>2</sub>O (1mL/min, isocratic) and Method F: 20% CH<sub>3</sub>CN (with 0.05% TFA) in H<sub>2</sub>O (1mL/min, isocratic). Table 1 below shows the purity data obtained through HPLC.

Elemental analyses (C, H, and N) of compounds **35-37** were performed by the Analytical lab for Environmental Science Research and Training of the University of Toronto and Perkin Elmer Corporation. The results obtained were within 0.4% of the calculated values.

**Table 1.** Purity data for compounds **27-34** and **38**.

<b>Compounds</b>	<b>Methods</b>	<b>Average % purity</b>
<b>27</b>	C and F	96%
<b>28</b>	C and D	98%
<b>29</b>	A and B	98%
<b>30</b>	A and B	98%
<b>31</b>	A and B	98%
<b>32</b>	A and B	98%
<b>33</b>	C and F	93%
<b>34</b>	E and F	96%
<b>38</b>	E and D	98%

**Elemental analyses data for 35-37.**

**6-Cyano-2'-deoxy-2'-fluoro-β-D-uridine-5'-O-monophosphate (35).** Empirical formula: C<sub>10</sub>H<sub>11</sub>FN<sub>3</sub>O<sub>8</sub>P·2.7 NH<sub>3</sub>·3.85H<sub>2</sub>O: Calcd. C: 25.75, H: 5.79, N: 17.11. Found: C: 25.72, H: 5.76, N: 17.11

**6-Amido-2'-deoxy-2'-fluoro-β-D-uridine-5'-O-monophosphate (36).** Empirical formula: C<sub>10</sub>H<sub>13</sub>FN<sub>3</sub>O<sub>9</sub>P·1.95NH<sub>3</sub>·1.05H<sub>3</sub>PO<sub>4</sub>: Calcd: C: 23.77, H: 4.39, N: 13.72. Found: C: 23.72, H: 4.21, N: 13.90.

**5-Cyano-2'-deoxy-2'-fluoro-β-D-uridine-5'-O-monophosphate (37).** Empirical formula: C<sub>10</sub>H<sub>11</sub>FN<sub>3</sub>O<sub>8</sub>P·2.7NH<sub>3</sub>·3.85 H<sub>2</sub>O: Calcd: C: 25.75, H: 5.79, N: 17.11. Found: C: 25.72, H: 5.76, N: 17.11.