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Stable Isotopes in Cell-Free Protein Synthesis

Structure Determination of Biomolecules by NMR

Modern multiple resonance and multi-dimensional Biomolecular NMR experiments require isotopic enrichment of the proteins, RNA and DNA, to achieve sufficient sensitivity and resolution. The biomolecules are typically enriched by biosynthesis. ISOTEC™ offers an extensive line of stable isotope labeled products for Biomolecular NMR applications.

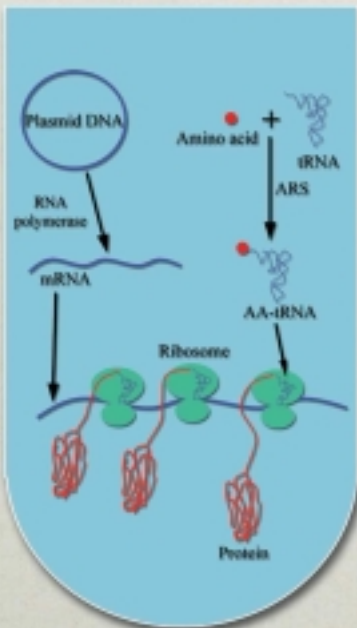
Stable Isotopes in Cell-Free Protein Synthesis

Munehiro Teshima-Scientist-ISOTEC™

Proteomics is an emerging field of post genome research, which examines the enormous amounts of information stored in the genomes of living organisms.¹ Biomolecular NMR and stable isotopes are important tools used to study the structure and function of proteins in structural genomics research. Most researchers use the protein expression systems of microorganisms or mammalian cells and stable isotope labeled (²H, ¹³C, ¹⁵N) D-glucose, ammonium salts, amino acids and / or complex growth media to produce proteins uniformly labeled with stable isotopes.

However, the protein expression system using living cells has limitations.

- Many expressed proteins are insoluble and aggregate in inclusion bodies.
- Intercellular proteases in the host cells may digest the proteins.
- Some proteins cannot be produced in living cells because of their toxicity.
- The amino acid metabolic system in the host cells can cause isotope dilution and diffusion for amino acids with selective stable isotope labeling.
- It may be difficult to grow organisms in deuterium labeled media.
- Prokaryote cannot glycosylate proteins.



These problems associated with living cells may be solved by the cell-free protein synthesis system. An additional benefit is that the cell-free protein synthesis system is suitable for automation and high throughput protein synthesis.

The basic idea of the cell-free protein synthesis system is to extract only the protein synthesis system (translation and / or transcription system) from living cells such as Escherichia Coli, rabbit reticulocyte or wheat germ, and allow the extract to synthesize the proteins in vitro from amino acids and specific DNA or mRNA used as a template.

The cell-free protein synthesis system is not a new technology, but the yield of the conventional batch type system used in the past was so low that radioisotopes were the only method sensitive enough for detection. In 1988, Dr. Spirin et al. developed a continuous flow cell-free protein synthesis system. They used an ultra-filtration system and succeeded in producing a couple of hundred µg of protein per ml of reaction mixture.²

Many ideas for the improvement of the continuous flow system such as using dialysis and condensation of the extract were incorporated by many researchers.³⁻⁷ In addition to these improvements, Dr. Yokoyama et al. optimized the reaction conditions and established a system to produce 6 mg of protein per ml of reaction mixture, and they applied this system to produce ¹³C, ¹⁵N-labeled proteins for Biomolecular NMR spectroscopy.⁸ Also, they succeeded in developing a site directed stable isotope labeling method for a protein by using a cell-free protein synthesis system.⁹

References: (1) <http://www.gsc.riken.go.jp/e/group/protgrE.html>. (2) Sprin, A. S., et al., *Science*, **1988**, 1162-1164, 242. (3) Kim, D. M., et al., *Biotechnol. Prog.*, **1996**, 645-649, 12. (4) Davis, J., et al., *Promega Notes Mag.* **1996**, 14-18, 56. (5) Nakano, H., et al., *Biosci. Biotechnol. Biochem.* **1994**, 631-634, 58. (6) Kim, D. M., et al., *Eur. J. Biochem.* **1996**, 881-886, 239. (7) Nakano, H., et al., *J. Biotechnol.* **1996**, 275-282, 46. (8) Yokoyama, S., et al., *FEBS Lett.* **1999**, 15-19, 442. (9) Yokoyama, S., et al., *J. Biomol. NMR* **1998**, 295-306, 11.

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Labeled Products for Cell Free Synthesis

Fully labeled ^{15}N Amino Acids

		Atom %
33,212-7	L-Alanine- ^{15}N	98
60,011-3	L-Arginine- $^{15}\text{N}_4$ HCl	98
48,591-8	L-Asparagine- $^{15}\text{N}_2 \cdot \text{H}_2\text{O}$	98
33,213-5	L-Aspartic- ^{15}N Acid	98
60,912-9	L-Cysteine- ^{15}N	98
33,214-3	L-Glutamic- ^{15}N Acid	98
49,003-2	L-Glutamine- $^{15}\text{N}_2$	98
29,929-4	Glycine- ^{15}N	98
57,436-8	L-Histidine- $^{15}\text{N}_3$	95
33,215-1	L-4-Hydroxyphenylalanine- ^{15}N (L-Tyrosine)	98
60,901-3	L-Isoleucine- ^{15}N	98
34,096-0	L-Leucine- ^{15}N	98
60,902-1	L-Lysine- $^{15}\text{N}_2$ HCl	98
60,924-2	L-Methionine- ^{15}N	98
49,010-5	L-Phenylalanine- ^{15}N	98
60,899-8	L-Proline- ^{15}N	98
60,900-5	L-Serine- ^{15}N	98
60,909-9	L-Threonine- ^{15}N	98
57,460-0	L-Tryptophan- $^{15}\text{N}_2$	95
49,017-2	L-Valine- ^{15}N	98

Fully Labeled $^{13}\text{C},^{15}\text{N}$ Amino Acids

		Atom %
48,988-3	L-Alanine- $^{13}\text{C}_3,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,803-3	L-Arginine- $^{13}\text{C}_6,^{15}\text{N}_4$ HCl	98 ^{13}C ; 98 ^{15}N
60,815-7	L-Asparagine- $^{13}\text{C}_4,^{15}\text{N}_2 \cdot \text{H}_2\text{O}$	98 ^{13}C ; 98 ^{15}N
60,783-5	L-Aspartic Acid- $^{13}\text{C}_4,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,785-1	L-Glutamic Acid- $^{13}\text{C}_5,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,798-3	L-Glutamine- $^{13}\text{C}_5,^{15}\text{N}_2$	98 ^{13}C ; 98 ^{15}N
48,952-2	Glycine- $^{13}\text{C}_2,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,800-9	L-Histidine- $^{13}\text{C}_6,^{15}\text{N}_3$	97 ^{13}C ; 95 ^{15}N
60,799-1	L-4-Hydroxyphenylalanine- $^{13}\text{C}_9,^{15}\text{N}$ (L-Tyrosine)	99 ^{13}C ; 98 ^{15}N
60,809-2	L-Isoleucine- $^{13}\text{C}_6,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,806-8	L-Leucine- $^{13}\text{C}_6,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,804-1	L-Lysine- $^{13}\text{C}_6,^{15}\text{N}_2$ HCl	98 ^{13}C ; 98 ^{15}N
60,810-6	L-Methionine- $^{13}\text{C}_5,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,801-7	L-Phenylalanine- $^{13}\text{C}_9,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,811-4	L-Proline- $^{13}\text{C}_5,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,813-0	L-Serine- $^{13}\text{C}_3,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
60,777-0	L-Threonine- $^{13}\text{C}_4,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N
57,459-7	L-Tryptophan- $^{13}\text{C}_{11},^{15}\text{N}_2$	97 ^{13}C ; 95 ^{15}N
60,014-8	L-Valine- $^{13}\text{C}_5,^{15}\text{N}$	98 ^{13}C ; 98 ^{15}N

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Products for Peptide Synthesis

Products for Minimal Media

Products for Peptide Synthesis (N-FMOC and N-t-BOC Derivatives)

		Atom %
48,583-7	L-Alanine- ¹³ C ₃ , ¹⁵ N,N-t-BOC	98 ¹³ C; 98 ¹⁵ N
48,990-5	L-Alanine- ¹⁵ N,N-FMOC	98
48,991-3	L-Alanine- ¹⁵ N,N-t-BOC	98
57,989-0	L-Asparagine- ¹⁵ N ₂ ,α-N-FMOC	98
49,290-6	L-Aspartic- ¹⁵ N Acid,N-FMOC	98
57,795-2	L-Aspartic- ¹⁵ N Acid,N-FMOC,α-O-t-butyl	98
58,879-2	L-Aspartic- ¹⁵ N Acid,N-t-BOC	98
58,840-7	L-Glutamic Acid- ¹³ C ₅ , ¹⁵ N,N-t-BOC,α-O-Benzyl Ester (97%CP)	98 ¹³ C; 98 ¹⁵ N
49,000-8	L-Glutamic- ¹⁵ N Acid,N-FMOC	98
60,915-3	L-Glutamic- ¹⁵ N Acid,N-FMOC,γ-O-t-Butyl Ester	98
58,769-9	L-Glutamic- ¹⁵ N Acid,N-t-BOC	98
58,770-2	L-Glutamine- ¹⁵ N ₂ ,α-N-t-BOC	98
48,953-0	Glycine- ¹³ C ₂ , ¹⁵ N,N-FMOC	98 ¹³ C; 98 ¹⁵ N
58,773-7	Glycine- ¹³ C ₂ , ¹⁵ N,N-t-BOC	98 ¹³ C; 98 ¹⁵ N
48,575-6	Glycine- ¹⁵ N,N-FMOC	98
48,670-1	Glycine- ¹⁵ N,N-t-BOC	98
59,109-2	L-4-Hydroxyphenylalanine- ¹⁵ N,N-t-BOC(L-Tyrosine)	98
59,722-8	L-Isoleucine- ¹³ C ₆ , ¹⁵ N,N-FMOC	98 ¹³ C; 98 ¹⁵ N
57,862-2	L-Isoleucine- ¹⁵ N,N-FMOC	98
48,595-0	L-Leucine- ¹⁵ N,N-FMOC	98
49,293-0	L-Leucine- ¹⁵ N,N-t-BOC · H ₂ O	98
57,796-0	L-Lysine- ¹⁵ N ₂ ,α-N-FMOC,ε-N-t-BOC	98
60,919-6	L-Methionine- ¹⁵ N,N-FMOC	98
60,907-2	L-Phenylalanine- ¹⁵ N,N-FMOC	98
48,683-3	L-Phenylalanine- ¹⁵ N,N-t-BOC	98
58,951-9	L-Proline- ¹⁵ N,N-FMOC	98
60,914-5	L-Serine- ¹⁵ N,N-FMOC,O-t-Butyl	98
48,600-0	L-Valine- ¹⁵ N,N-FMOC	98
48,601-9	L-Valine- ¹⁵ N,N-t-BOC	98

For a complete list of amino acids and protected amino acids please contact us at
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Products for Minimal Media

Sugars

		Atom %
38,937-4	D-Glucose- ¹³ C ₆	99
55,215-1	D-Glucose- ¹³ C ₆ ,C-d ₇	99 ¹³ C; 97-99 D
55,200-3	D-Glucose-C-d ₇	97-99
61,633-8	D-Glucose-d ₁₂	97-99

¹⁵N Salts

29,925-1	Ammonium- ¹⁵ N Chloride	98
36,650-1	Ammonium- ¹⁵ N, d ₄ Chloride	98 ¹⁵ N; 98 D
48,801-1	Ammonium- ¹⁵ N Hydroxide (~3N aqueous soln.)	98
29,928-6	Ammonium- ¹⁵ N ₂ Sulfate	98
59,399-0	Ammonium- ¹⁵ N ₂ , d ₈ Sulfate	99 ¹⁵ N; 98 D

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Labeled Complex Growth Media

Fermentation with ISOGRO™-¹³C Powder Supplementation

Andrew Clark University of Alabama Huntsville

E. coli (Rosetta™(DE3)pLysS, Novagen®) was grown in a fermentor (BioFlo 3000®, New Brunswick) with a 2-liter vessel containing minimal media with ISOGRO™-¹³C as a supplement in a quantity which is 5 % of its recommended usage. The composition of the minimal media, as adapted from Molecular Cloning (Maniatis et al.), is as follows: Na₂HPO₄ (12.8 g/L), KH₂PO₄ (3 g/L), NaCl (0.5 g/L), MgSO₄ (0.001 M), CaCl₂ (5E-5 M), glucose (2 g/L), NH₄Cl (1 g/L), and ampicillin (60 mg/ml).

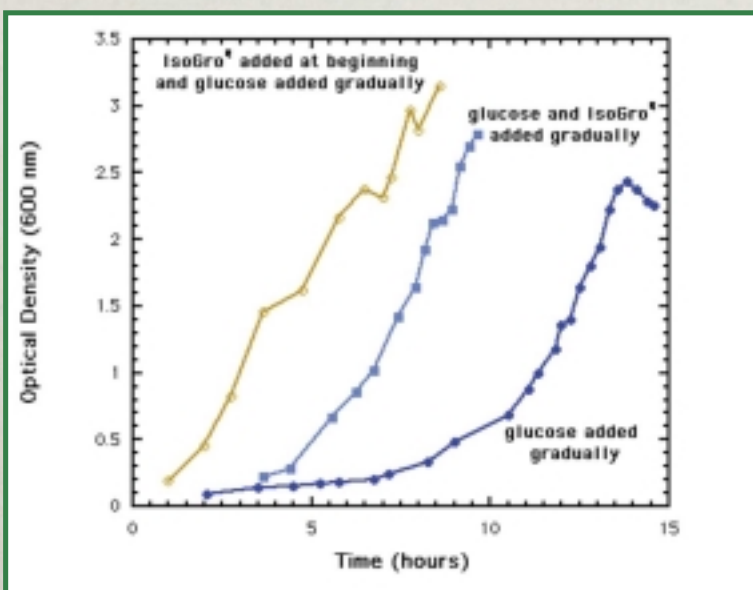
First of all, a 200-ml minimal media culture was grown in a shaker flask with and without 0.1 g of ISOGRO™-¹³C (5 % of its recommended usage) to assess its effectiveness as a supplement in the shaker flask before implementing it into fermentation. The culture with the ISOGRO™ absent grew to a maximal optical density at 600 nm (OD) of 1.4, whereas the culture with the ISOGRO™ present grew to a maximal OD of 2.5.

With this information in hand, I set out to assess the effectiveness of using ISOGRO™ as a supplement in the fermentor. The recombinant protein I am working with is encoded by the pET-3b vector (Novagen®) which contains the T7 promoter, and so its expression is induced by the addition of IPTG (Sigma # I 6758). It had already been previously established that there was a direct correlation between the maximal OD reached in the fermentor and the quantity of protein rendered upon preparation of the cells and purification.

It had also been established that the maximal OD could be increased by adding the glucose gradually instead of all at the beginning. This led me to speculate as to whether the maximal OD could be increased by adding the ISOGRO™ gradually. The results of all of my fermentation runs involving ISOGRO™ and one control experiment are presented in the following table:

OD	Experiment
2.4	5 ml of 20 % glucose (m/v) added at beginning and 15 ml of 20 % glucose added gradually in 5-ml increments. ISOGRO™ was absent (control).
3.2	5 ml of 20 % glucose and 0.9 g ISOGRO™- ¹³ C added at beginning and 15 ml of 20 % glucose added gradually in 5-ml increments.
2.8	5 ml of 20 % glucose and 12.5 ml of ISOGRO™- ¹³ C (1 g/50 ml) added at beginning and 15 ml of 20 % glucose and 37.5 ml of ISOGRO™- ¹³ C added gradually in 5- and 12.5-ml increments, respectively.
3.0	5 ml of 20 % glucose and 50 ml of ISOGRO™- ¹³ C (1 g/50 ml) added at beginning and 15 ml of 20 % glucose added gradually in 5-ml increments.

It appears that whereas the OD increased when the glucose was added gradually, the OD actually increased when the ISOGRO™ was added all at once at the beginning. There was a significant increase in the maximal OD reached due to the addition of the ISOGRO™ as a supplement instead of as the sole source of nutrients. This optimization of high-density *E. coli* fermentation will definitely lead to an increase in the yield of protein from the cultures grown and improve our laboratory's capability to produce large quantities of isotope labeled proteins for Biomolecular NMR studies.



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Labeled Complex Growth Media *continued*

Buffers & Reagents

Typical Procedure for Growing E. coli Using ISOGRO™ Powder

To prepare 100mL ISOGRO™ medium:

1. Dissolve 1.0g of ISOGRO™ powder in about 90mL of Millipore® water.
2. Make stock solutions of the following salts and use the quantities indicated in the medium preparation:

Salt	Conc. of Stock Soln.	Qty./100mL medium
K ₂ HPO ₄	100g/L	1.8mL
KH ₂ PO ₄	50g/L	2.8mL
MgSO ₄	50g/L	2.0mL
CaCl ₂ ·H ₂ O	37g/L	30μL

3. Adjust pH to 7.0 with NaOH and bring solution up to 100mL with Millipore® water.
4. Pass the solution through a 0.22μm filter and transfer the filtrate to an autoclaved shaker flask (for example: 50mL medium in a 500mL flask).
5. The culture is inoculated with a loop of E. coli which has been maintained on a nutrient agar slant.
6. Shake the culture flask in a 37°C water bath.
7. The absorbance of the culture is measured at 600nm with a 1:3 dilution into water.

Note: Researcher's specific expression applications do vary; so our preparation should serve as a guideline.

		Atom %
60,686-3	ISOGRO™- ¹³ C Powder - Growth Medium	99
61,672-9	ISOGRO™-D Powder - Growth Medium	97-99
60,687-1	ISOGRO™- ¹⁵ N Powder - Growth Medium	98
60,683-9	ISOGRO™- ¹³ C, ¹⁵ N Powder - Growth Medium	99 ¹³ C; 98 ¹⁵ N
60,830-0	ISOGRO™- ¹⁵ N,D Powder - Growth Medium	98 ¹⁵ N; 97-99 D
60,829-7	ISOGRO™- ¹³ C, ¹⁵ N,D Powder - Growth Medium	99 ¹³ C; 98 ¹⁵ N; 97-99 D

Buffers and Reagents

		Atom %
15,178-5	Acetic Acid-d ₄	99.5
17,657-5	Ammonium-d ₄ Bromide	98
17,567-6	Ammonium-d ₄ Chloride	98
17,670-2	Ammonium-d ₄ Deuterioxide (25% in D ₂ O)	99
48,835-6	Butanedioic Acid-d ₆	98
48,553-5	DL-1,4-Dithiothreitol-d ₁₀	98
48,561-6	Dodecylphosphorylcholine-d ₃₈	98
48,937-9	Ethylenediaminetetraacetic-d ₁₂ Acid	98
42,622-9	Formic Acid-d ₂ (95% in D ₂ O)	98
17,583-8	Glycine-d ₅	98
36,602-1	Imidazole-d ₄	98
61,522-6	2-Mercaptoethanol-d ₆	96
37,384-2	Sodium Formate-d	99
45,185-1	Sodium Lauryl-d ₂₅ Sulfate	98
44,910-5	TRIS-d ₁₁ (crystalline) [Tris(hydroxymethyl)aminomethane]	99
48,624-8	TRIS-d ₁₁ (~1M solution in D ₂ O)	99
44,749-8	Glycerol-d ₈	98
45,452-4	Glycerol-1,1,2,3,3-d ₅	98
48,947-6	Glycerol- ¹³ C ₃	99
27,717-7	Methyl- ¹³ C Alcohol (< 5% ¹⁸ O) (Methanol)	99
28,201-4	Sodium Acetate- ¹³ C ₂	99
17,607-9	Sodium Acetate-d ₃	99
29,911-1	Sodium Acetate- ¹³ C ₂ , d ₃	99 ¹³ C; 99 D

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References: R. Ishima, J.M. Louis, D. Torchia. *Journal of Biomolecular NMR* 21:167-171, 2001 N.K. Goto, K.H. Gardner, G.A. Mueller, R.C. Willis, L.E. Kay. *Journal of Biomolecular NMR* 13:369-374, 1999.

α -Keto Acids

		Atom %
57,134-2	2-Ketobutyric-4- ^{13}C Acid, Sodium Salt•xH ₂ O (97% CP)	99
58,927-6	2-Ketobutyric-4- $^{13}C,3,3-d_2$ Acid, Sodium Salt•H ₂ O(98% CP)	99 ^{13}C ; 98 D
60,754-1	2-Ketobutyric Acid- $^{13}C_4,3,3-d_2$, Sodium Salt•xH ₂ O (98% CP)	99 ^{13}C ; 97-98 D
60,753-3	2-Ketobutyric-4- $^{13}C,3,3,4,4,4-d_5$ Acid, Sodium Salt•xH ₂ O (98% CP)	99 ^{13}C ; 98 CD ₂ ; 50-70 CD ₃
57,133-4	2-Keto-3-methyl- ^{13}C -butyric-4- ^{13}C Acid, Sodium Salt	99
58,906-3	2-Keto-3-methyl- ^{13}C -butyric-4- $^{13}C,3-d_1$ Acid, Sodium Salt	99 ^{13}C ; 98 D
58,490-3	2-Keto-3-methyl- d_3 -butyric-4- ^{13}C Acid, Sodium Salt	99 ^{13}C ; 98 D
59,641-8	2-Keto-3-methyl- d_3 -butyric Acid-1,2,3,4- $^{13}C_4$, Sodium Salt	99 ^{13}C ; 98 D
60,756-8	2-Keto-3-methylbutyric Acid- $^{13}C_5$, 3- d_1 , Sodium Salt	99 ^{13}C ; 98 D
49,073-3	Sodium Pyruvate-3- ^{13}C	99
60,848-3	Sodium Pyruvate-3- ^{13}C -3,3,3- d_3	99 ^{13}C ; 50-60 D

Labeled Nucleotides

$^{13}C,^{15}N$ -Ribonucleotides (minimum 90% chemical purity), supplied as sodium salts

		Atom %
60,835-1	Adenosine- $^{13}C_{10},^{15}N_5$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,837-8	Cytidine- $^{13}C_9,^{15}N_3$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,838-6	Guanosine- $^{13}C_{10},^{15}N_5$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,839-4	Uridine- $^{13}C_9,^{15}N_2$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N

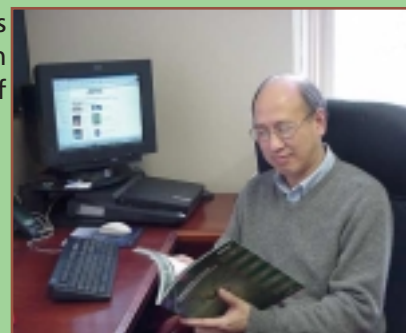
$^{13}C,^{15}N$ - Deoxyribonucleotides, supplied as sodium salts

		Atom %
60,840-8	2'-Deoxyadenosine- $^{13}C_{10},^{15}N_5$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,841-6	2'-Deoxycytidine- $^{13}C_9,^{15}N_3$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,842-4	2'-Deoxyguanosine- $^{13}C_{10},^{15}N_5$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N
60,843-2	2'-Deoxythymidine- $^{13}C_{10},^{15}N_2$ 5'-triphosphate	99 ^{13}C ; 98 ^{15}N

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Version	Cat. No.	Cat. No.	Cat. No.
Single user, commercial	Z54,016-1	Z54,126-5	Z53,808-6
Single user, academic	Z54,028-5	Z54,138-9	Z53,818-3
Network	Z54,039-0	Z54,149-4	Z53,797-7
Demo program	Z54,159-1		

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