

Steve Bryant has completed his Postdoctoral appointment with the Protein Data Bank. We want to wish Steve good luck in his new position with the New York State Department of Health.

As is usual with the start of a new fiscal year, Brookhaven has increased the charges for Protein Data Bank items, to cover rising costs. The new rates listed on the order form on pages 5-6 are effective October 1, 1988. Also, please note that because of the increased number of coordinate entries, DATAPRTP now requires three tapes at a density of 1600 cpi. The database still fits on a single tape at 6250 cpi.

Please mark any registered mail to BNL to the attention of Frances Bernstein. Registered mail not addressed to an individual cannot be delivered.

We are pleased to announce the inauguration of on-line access (BITNET fileserv) to DATAPRTP through the European Molecular Biology Laboratory, Heidelberg, FRG (Contact Peter Rice, telephone 0049-6221-387-241, electronic mail RICE@EMBL). EMBL joins the Canadian Scientific Numeric Data Base Service (CAN/SND) in Ottawa (contact Dr. Roger Gough, telephone 613-933-3294, electronic mail CANSND@NRCVM01) and the Pittsburgh Supercomputing Center (contact Dr. Hugh Nicholas, telephone 412-268-4960, electronic mail NICHOLAS@CPWPSCA) as on-line distributors.

The established Protein Data Bank centers continue to provide their full range of services. Inquiries may be addressed as shown below. The order form on pages 5-6 of this newsletter may be used to order data from Brookhaven. It is possible to place a standing order for each quarterly DATAPRTP release; anyone interested in placing such a standing order should contact Frances Bernstein. Please note that the order form on pages 5-6 should be used only for Brookhaven orders; users in Japan or Australia should contact their centers for detailed information.

Area	Address of Center	BITNET (BNL Only)	Name	Phone
Worldwide except Australia and Japan	Protein Data Bank	PDB@BNLCHM	Inquiries	516-282-4382
	Chemistry Department	ABOLA@BNLCHM	E. E. Abola	516-282-4383
	Brookhaven National Laboratory	BERNSTEIN@BNLCHM	F. C. Bernstein	516-282-4382
	Upton, NY 11973	KOETZLE@BNLCHM	P. A. Esposito	516-282-4382
	USA	WENG@BNLCHM	T. F. Koetzle	516-282-4384
			J. C. Weng	516-282-4382
Australia	CSIRO Division of Biotechnology 343 Royal Parade, Parkville Victoria 3052, Australia		P. Davis	03-342-4326
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2 Suita, Osaka 565, Japan		Y. Katsube	(06) 877-5111 ext. 3912

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TABLE 1. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE

09-OCT-88

CODE	ITEM	AVAILABILITY
USA	JAP	AUS
DATAPRTP	ALL CURRENT COORDINATE ENTRIES (TABLE 5), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 7 - NO COORDINATES IN BIB ENTRIES)	X X X
YEAR87TP	NEW OR REVISED COORDINATE ENTRIES FOR 1987	X
PART88TP	NEW OR REVISED COORDINATE ENTRIES FOR 1988 (TO DATE)	X
PDBPGMTP	COMPUTER PROGRAMS AND MISCELLANEOUS FILES (TABLE 3, PARTS A AND B)	X
NONST1TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 1)	X X
NONST2TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 2)	X X
NONST3TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 3)	X X
NONST4TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 4)	X X
NONST5TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 5)	X X
NONST6TP	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 6)	X X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	X
BLDKITTP	MODEL BUILDER'S KIT	X
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	PLEASE INQUIRE AT US CENTER
DGPLOTP	DIAGONAL PLOTS (LINE PRINTER)	X
D1HDRLTP	COMPLETE TORSION ANGLES	X
DSTNCTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X
FISIFLTP	PHI/PSI PLOTS (LINE PRINTER)	X
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES	X

\* NEW OR REPLACEMENT ENTRY SINCE JUL-88 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

09-OCT-88

CODE	ITEM	AVAILABILITY
USA	JAP	AUS
DATAPRFI	ALL CURRENT COORDINATE ENTRIES (TABLE 5), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 7 - NO COORDINATES IN BIB ENTRIES)	X X
YEAR87FI	NEW OR REVISED COORDINATE ENTRIES FOR 1987	X
PART88FI	NEW OR REVISED COORDINATE ENTRIES FOR 1988 (TO DATE)	X
CORR23FI	*LIST OF CORRECTIONS NO. 23 (JUL/88 - OCT/88)	X X X
NONST1FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 1)	X X X
NONST2FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 2)	X X X
NONST3FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 3)	X X X
NONST4FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 4)	X X X
NONST5FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 5)	X X X
NONST6FI	STRUCTURE FACTOR HOLDINGS (TABLE 4 - PART 6)	X X X
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X
BLDKITFI	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X
DGPIOTFI	DIAGONAL PLOTS (LINE PRINTER)	X
D1HDRLFI	COMPLETE TORSION ANGLES	X
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X
FISIFLFI	PHI/PSI PLOTS (LINE PRINTER)	X
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X

\* NEW OR REPLACEMENT ENTRY SINCE JUL-88 NEWSLETTER



Table listing protein entries with columns for accession number, protein name, and authors. The table is organized into two columns and contains numerous entries such as CYTOCHROME C550, CYTOCHROME C551, and various other enzymes and structural proteins.

Table with columns: ID, Name, Depositor, Date/Status. Includes entries like 2XIA \*D-XYLOSE ISOMERASE (S. RUBIGINOSUS) and MODEL STRUCTURES.

\* NEW OR REPLACEMENT ENTRY SINCE JUL-88 NEWSLETTER

STATUS CODES

BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
R RECENT (1986-1988) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 6. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION 09-OCT-88

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR(S), DATE/STATUS. Lists various protein entries like 5WGA AGGLUTININ (WHEAT GERM, ISOLECTIN 2) and 1FVB IMMUNOGLOBULIN FV B1912 MODEL.

Table with columns: ID, Name, Depositor, Date/Status. Continuation of protein entries like 1FVB IMMUNOGLOBULIN FV B1912 MODEL.

Table with columns: ID, Name, Depositor, Date/Status. Lists entries like 5CYT CYTOCHROME C (ALBACORE, REDUCED) and 1R1P PHOSPHOFUCTOKINASE (E. COLI) - F6P-ADP/MG.

\* NEW OR REPLACEMENT ENTRY SINCE JUL-88 NEWSLETTER

STATUS CODES

A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P IN PREPARATION
R REPLACEMENT FOR ENTRY IN TABLE 5
SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES (NO COORDINATES)

Table with columns: ID, Name, Depositor, Date/Status. Lists numerous protein entries like 0EAP ACID PROTEINASE (ENDOTHRIA PARASITICA) and 0WGI AGGLUTININ (WHEAT GERM, ISOLECTIN 1).

\* NEW OR REPLACEMENT ENTRY SINCE JUL-88 NEWSLETTER

TABLE 8. CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS 09-OCT-88

CORRECTIONS TO ENTRIES MAY BE OBTAINED IN ONE OF TWO WAYS -

A. ORDER CORR23FI. THERE IS NO CHARGE FOR THIS MICROFICHE WHICH CONTAINS A LISTING OF ALL CORRECTIONS APPLIED IN THE LAST THREE MONTHS.

B. ORDER A NEW COPY OF DATAPRTP.

THE FOLLOWING DATA SETS HAVE HAD CORRECTIONS APPLIED. PLEASE CONSULT A COPY OF THE PROTEIN DATA BANK ATOMIC COORDINATE AND BIBLIOGRAPHIC ENTRY FORMAT DESCRIPTION FOR A FULL DESCRIPTION OF RVDAT RECORDS.

Table with columns: RVDAT ID, Date, Entry Name, Count, Remark. Lists corrections for entries like 09-OCT-88 8BNAC, 09-OCT-88 3CTSB, etc.

THE FOLLOWING DATA SETS HAVE BEEN REPLACED

Table with columns: OBSLTE, Old Entry, New Entry. Lists replaced entries like 07-SEP-88 1C12, 07-SEP-88 15EC, etc.

## BROOKHAVEN ORDER FORM (Please include a self-addressed label)

1. Name \_\_\_\_\_ Date \_\_\_\_\_  
 Address \_\_\_\_\_ Telephone \_\_\_\_\_  
 \_\_\_\_\_ Electronic Mail \_\_\_\_\_  
 \_\_\_\_\_

## 2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (April 1988)  
 Latest Newsletter  
 Atomic Coordinate and Bibliographic Entry Format Description  
 for DATAPRTP and DATAPRFI (January 1985)  
 Current DATAPRTP Directory  
 Sources of Visual Aids for Macromolecular Structure (February 1988)  
 Non-Standard Entries (Structure Factors) Format Description  
 Data Deposition Form

## 3. Please send the following magnetic tape items (from Table 1).

	6250 cpi	1600 cpi	TK50
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$288	<input type="checkbox"/> \$367	<input type="checkbox"/> \$312
VAX/VMS COPY	<input type="checkbox"/> \$288	<input type="checkbox"/> \$367	<input type="checkbox"/> \$312
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$367	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$367	
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	<input type="checkbox"/> \$312
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
NONST5TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
NONST6TP			
Unlabelled ASCII	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	
Unlabelled EBCDIC	<input type="checkbox"/> \$288	<input type="checkbox"/> \$288	

Cost: \_\_\_\_\_

Special order items (described in Table 1): Please inquire at Brookhaven for availability and price.

YEAR87TP	CONECTTP	DSTNCETP
PART88TP	DGPLOTP	FISIPLTP
BENDERTP	DIHDRLTP	PHIPSITP

(Continued)

4. Foreign air mail postage for tape items listed in 3 above mailed from Brookhaven to destinations outside the U.S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19 = \_\_\_\_\_

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$310, postage included. Correction fiche are free.

Items: \_\_\_\_\_ Cost: \_\_\_\_\_

6. Please send the following printed listings. Each listing costs \$82, postage included.

Ident Code(s) (From Table 5): \_\_\_\_\_ Cost: \_\_\_\_\_

7. **Total charges** - All prices are expected to be valid through September 30, 1989. After that date please confirm prices.

Magnetic tape charges (3 above) \_\_\_\_\_

Foreign air mail postage charges (4 above) \_\_\_\_\_

Microfiche charges (5 above) \_\_\_\_\_

Printed listing charges (6 above) \_\_\_\_\_

Bank charge \_\_\_\_\_

No charge for checks drawn in U.S. dollars on  
U.S. bank, otherwise \$10 \_\_\_\_\_

TOTAL COST : \_\_\_\_\_

**METHOD OF PAYMENT:**

Brookhaven requires that either a written purchase order or check payable to

**BROOKHAVEN NATIONAL LABORATORY**

be received before service is provided. Order forms and purchase orders maybe sent by facsimile to (United States) 516-282-5815. The original order forms and purchase orders should also be sent to Brookhaven by mail.

( ) check \_\_\_\_\_ is ( ) enclosed  
( ) purchase order number \_\_\_\_\_ ( ) sent separately

Please return **ORDER FORM** to

**BROOKHAVEN NATIONAL LABORATORY**  
Chemistry Department - Bldg. 555  
Ms. F. C. Bernstein  
Upton, New York 11973 USA  
(516-282-4382)

It is advisable to send a photocopy of this order form directly to Brookhaven; experience shows that purchasing departments often do not forward this form with the order.