

THE PROTEIN DATA BANK  
NEWSLETTER

Number 8

April 1979

This brief Newsletter gives up-to-date holdings and ordering information (Tables 1-4). The 13 new or replacement atomic coordinate entries since the last Newsletter (December 1978) are flagged with asterisks in Table 3. Available programs are listed in Table 4. The list of structure factors and other non-standard entries has not been increased and so is not reprinted here.

To order data, please fill out the request form (last two sides).

A full Newsletter, with general items of interest and a listing of corrections, will be distributed in July. The persons listed below will also be happy to answer inquiries.

<u>Area</u>	<u>Address of Center</u>	<u>Name</u>	<u>Telephone</u>
The Americas	Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	F. C. Bernstein	516-345-4382
		T. F. Koetzle	516-345-4384
		G.J.B. Williams	516-345-4383
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, ENGLAND	O. Kennard S. Bellard	0223-66499
Australia	C.S.I.R.O. Division of Applied Organic Chemistry Box 4331 G.P.O. Melbourne, Victoria 3001 AUSTRALIA	B. J. Poppleton	640251
Japan	Department of Chemistry Faculty of Sciences The University of Tokyo Bunkyo-ku, Tokyo, JAPAN	M. Tasumi	(03)812-2111

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

27-MAR-79

CODE	ITEM
DATAPRTP	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)
NONSTDTP	ALL NON-STANDARD ENTRIES
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)
DSTNCETP	*CONNECTIVITY SPECIFICATIONS WITH DISTANCES
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES

ITEM DSTNCETP REQUIRES TWO TAPES AT 800CPI, OTHER ITEMS COMPRISE ONE TAPE EACH

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

27-MAR-79

CODE	ITEM	NO. OF FICHE	PRICE
DATAPRFI	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)	11	\$38.70
NONSTDFI	ALL NON-STANDARD ENTRIES	11	\$38.70
CORR03FI	LIST OF CORRECTIONS #3 (MAY-NOV 1978)	1	FREE
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	2	\$26.90
CONECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	9	\$36.30
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	4	\$30.30
DSTNCFI	*CONNECTIVITY SPECIFICATIONS WITH DISTANCES	18	\$41.70
FISIFLFI	PHI/PSI PLOTS (LINE PRINTER)	1	\$26.70
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	4	\$30.30

PRICES QUOTED ARE IN U.S. DOLLARS FOR DISTRIBUTIONS FROM BROOKHAVEN. REQUESTORS FROM OTHER CENTERS SHOULD INQUIRE FOR AVAILABILITY AND PRICES.

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

27-MAR-79

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS
1ACT	ACTINIDIN	E. BAKER	7/77
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R
1AGA	AGAROSE	S. ARNOTT	5/78 P
1WGA	AGGLUTININ (WHEAT GERM)	C. S. WRIGHT	2/78 A
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I. BRANDEN	8/76
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C.-I. BRANDEN	8/76
2BCL	*BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 RA
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S. ARNOTT	5/78 P
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/76
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A (BOVINE)	W. LIPSCOMB	2/73
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOTT	9/76 A
1CAR	CARRAGEENAN	S. ARNOTT	5/78 P
1C4S	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78 P
2C4S	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78 P

2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75	R
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76	
1GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	2/77	
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFT	3/75	
2CNA	CONCAVALIN A	REEKE, BECKER, EDELMAN	4/75	
3CNA	CONCAVALIN A	K. HARDMAN	9/76	R
2B5C	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77	R
1CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	9/76	
2CYT	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	9/76	
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76	
1C2C	CYTOCHROME C2	J. KRAUT	3/73	
155C	CYTOCHROME C550	R. TIMKOVICH	8/76	
251C	CYTOCHROME C551	R. DICKERSON	8/78	R
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76	
1ECD	*ERYTHROCRUORIN (REDUCED, DEOXY)	STEIGEMANN, WEBER	3/79	P
1ECO	*ERYTHROCRUORIN (CARBONMONOXY)	STEIGEMANN, WEBER	3/79	P
1ECA	*ERYTHROCRUORIN (AQUO, MET)	STEIGEMANN, WEBER	3/79	P
1ECN	*ERYTHROCRUORIN (CYANO, MET)	STEIGEMANN, WEBER	3/79	P
1FDX	FERREDOXIN	ADMAN, SIEKER, JENSEN	8/76	
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M. LUDWIG	12/77	R
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LUDWIG	12/77	
1GCN	GLUCAGON	T. BLUNDELL	10/77	
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77	
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	7/75	
1HRG	HEMERYTHRIN B	W. HENDRICKSON	6/76	A
1HMN	*HEMERYTHRIN (MET, AQUO)	R. STENKAMP ET AL.	1/79	A
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	LADNER, HEIDNER, PERUTZ	2/77	R
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73	
1HHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75	
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76	
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73	
2VHX	HEXOKINASE (YEAST) FORM BIII	STEITZ, ANDERSON, STENKAMP	3/78	R
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75	
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	11/77	
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78	P
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78	P
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78	P
1FAB	IMMUNOGLOBULIN FAB (NEW)	R. POLJAK	8/76	
1MCG	IMMUNOGLOBULIN B-J MCG	SCHIFFER, EDMUNDSON ET AL.	5/78	A
1REI	IMMUNOGLOBULIN B-J FRAGMENT REI	O. EPP, R. HUBER	3/76	
1RHE	IMMUNOGLOBULIN B-J FRAGMENT RHE	WANG, YOO, SAX	12/77	A
1KGA	KDPG ALDOLASE	A. TULINSKY	8/78	A
1KES	KERATAN SULFATE	S. ARNOTT	5/78	P
4LDH	LACTATE DEHYDROGENASE	W. EVENTOFF, M. ROSSMANN	4/77	R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	11/74	
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W. NUSICK, M. ROSSMANN	9/73	
1HBL	LEGHEMOGLOIN	VAINSHTEIN, HARUTYUNYAN	11/78	
1LZM	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77	
1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS	2/75	
2LYZ	LYSOZYME (HEN EGG-WHITE, SET RS5D)	R. DIAMOND, D. PHILLIPS	2/75	
3LYZ	LYSOZYME (HEN EGG-WHITE, SET RS6A)	R. DIAMOND, D. PHILLIPS	2/75	
4LYZ	LYSOZYME (HEN EGG-WHITE, SET RS9A)	R. DIAMOND, D. PHILLIPS	2/75	
5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS	2/75	
6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS13)	R. DIAMOND, D. PHILLIPS	2/75	
7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH	5/77	
8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77	
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	6/76	A
1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A. MCLACHLAN	8/78	
1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	4/73	
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76	
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76	
1MBS	*MYOGLOBIN (SEAL, MET)	H. SCOULUDI	2/79	N
1MHR	MYOHEMERYTHRIN	W. HENDRICKSON	6/76	A
8PAP	PAPAIN (NATIVE)	J. DRENTH	11/76	R
1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	11/76	R
2PAD	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH	11/76	R
3PAD	PAPAIN (OXIDIZED CYS-25)	J. DRENTH	11/76	R
4PAD	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH	11/76	R
5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76	R
6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH	11/76	R

1PEP	PEPSIN (PORCINE)	N. ANDREEVA ET AL.	7/78	A
1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76	A
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76	B
1PGM	PHOSPHOGLYCERATE MUTASE	CAMPBELL, WATSON, HODGSON	8/75	A
2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE	9/77	R
1RLX	RELAXIN(MODEL, CONFORMATION A, UNREFINED)	A. EVANS, A.C.T. NORTH	3/78	
2RLX	RELAXIN(MODEL, CONFORMATION B, UNREFINED)	A. EVANS, A.C.T. NORTH	3/78	
3RLX	RELAXIN(MODEL, CONFORMATION A, REFINED)	A. EVANS, A.C.T. NORTH	3/78	
4RLX	RELAXIN(MODEL, CONFORMATION B, REFINED)	A. EVANS, A.C.T. NORTH	3/78	
1RHD	RHODANESE	W. HOL	12/77	
1RNS	RIBONUCLEASE S	H. WYCKOFF, F. RICHARDS	4/73	
2RXN	RUBREDOXIN	L. JENSEN	1/75	
1SNS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73	
1SGA	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER, DELBAERE, JAMES	6/78	
1SGB	STREPTOMYCES GRISEUS PROTEINASE B	M. JAMES	5/76	A
1SBT	SUBTILISIN BPN'	J. KRAUT	8/72	
2SBT	SUBTILISIN NOVO	J. DRENTH	9/76	
1SSI	*SUBTILISIN INHIBITOR (STREPTOMYCES)	Y. MITSUI ET AL.	1/79	A
1SOD	SUPEROXIDE DISMUTASE	J. AND D. RICHARDSON	8/75	A
1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	4/75	
2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS	4/75	
1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B.-O. SODERBERG	5/76	A
4TNA	TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUG	4/78	R
6TNA	TRANSFER RNA (YEAST, PHE)	S.-H. KIM ET AL.	11/78	R
8TNA	*TRANSFER RNA (YEAST, PHE)	M. SUNDARALINGAM	2/79	R
1TIM	TRIOSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS	9/76	
1PTN	TRYPSIN (NATIVE, PH8)	FEHLHAMMER, BODE, SCHWAGER	1/77	
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	1/77	R
1PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R. HUBER, W. BODE	11/76	
3PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76	R
3PTP	TRYPSIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	12/77	R
1TGP	*TRYPSINOGEN/TRYPSIN INHIBITOR	BODE, SCHWAGER, HUBER	3/79	P
1TPI	*TRYPSINOGEN/TRYPSIN INHIBTR/ILE-VAL	BODE, SCHWAGER, HUBER	3/79	P
1TGA	*TRYPSINOGEN (MGSO4, WITHOUT CA)	BODE, FEHLHAMMER, HUBER	3/79	P
1TGB	*TRYPSINOGEN (WITH CA, FROM PEG)	BODE, FEHLHAMMER, HUBER	3/79	P

\* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (DEC/78)

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
N	NEW ENTRY WITH DEPOSITOR FOR APPROVAL
P	IN PREPARATION
R	REPLACES AN OUT-OF-DATE PARAMETER SET

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

27-MAR-79

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	1/79 YES
CONECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	3/79 YES
DGLOT	DIAGONAL PLOTS ON PRINTER	E.SWANSON, F.BERNSTEIN	3/79 YES
DSTNCE	*CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	3/79 YES
FISIPL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	11/78 YES
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS, WILLIAMS, BERNSTEIN	11/78 YES
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS, F.BERNSTEIN	5/78 YES

\* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER

SUPPORTED PROGRAMS ARE THOSE FOR WHICH STAFF OF THE PROTEIN DATA BANK WILL PROVIDE CORRECTIONS FOR DEMONSTRATED ERRORS.

REQUEST FORM

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

2. Send the following information (please check):

( ) description of atomic coordinate entries (no charge)

( ) the magnetic tape items listed below (from Table 1)

\_\_\_\_\_  
(Item "DATAPRTP" comprises all atomic coordinate sets and programs)

( ) the microfiche items listed below (from Table 2)

\_\_\_\_\_

3. Tape: I am sending a new 2400 foot reel of magnetic tape ( ) yes ( ) no

4. Tape format desired:

- |             |              |                         |                              |
|-------------|--------------|-------------------------|------------------------------|
| ( ) 7 track | ( ) 556 cpi  | ( ) BCD-7 track only    | ( ) Unlabelled (preferred)   |
| ( ) 9 track | ( ) 800 cpi  | ( ) ASCII-9 track only  | ( ) Labelled, - User's label |
|             | ( ) 1600 cpi | ( ) EBCDIC-9 track only | _____ Retained               |

NOTE: All current coordinate entries and programs can be written to one 2400' reel of magnetic tape for one unit charge (see over) if some space economies are achieved by blocking the records. Please indicate here the maximum block size permitted if this is less than 5120 characters (bytes) \_\_\_\_\_.

(Please complete reverse side)

## REQUEST FORM

## 5. Charges

(i) For requests to Brookhaven

- A. Data preparation (unit charge per magnetic tape) \$ \_\_\_\_\_
- |                                       |         |     |
|---------------------------------------|---------|-----|
| Employee of U.S. Department of Energy | \$40.25 | ( ) |
| Employee of other U.S. Federal Agency | \$47.45 | ( ) |
| All others                            | \$51.00 | ( ) |
- B. Magnetic Tape (charge per tape) \$ 8.85 \$ \_\_\_\_\_  
(please check if answer to 3 above was NO)
- C. Postage (per magnetic tape) \$ \_\_\_\_\_
- |                             |         |     |
|-----------------------------|---------|-----|
| U.S. and Canada             | \$ 2.00 | ( ) |
| Air Mail to Other Countries | \$17.00 | ( ) |
- D. Microfiche items (Price from Table 2) \$ \_\_\_\_\_
- E. Total Charge \$ \_\_\_\_\_
- F. Payment to the order of Brookhaven National Laboratory  
by ( ) check is ( ) enclosed  
( ) purchase order number \_\_\_\_\_ ( ) sent separately to  
the Protein Data Bank

Brookhaven requires that either a check or actual purchase order be received before data are shipped. Inclusion of check with order will expedite processing.

(ii) For requests to Cambridge

- A. Data preparation and postage (per user-supplied tape) £ \_\_\_\_\_
- |                       |        |     |
|-----------------------|--------|-----|
| Within United Kingdom | £27.50 | ( ) |
| Elsewhere             | £35.00 | ( ) |
- B. Magnetic tape £ 8.00 ( )  
(Please check if NO was checked on 3 above) £ \_\_\_\_\_
- C. Microfiche (please inquire for prices) £ \_\_\_\_\_
- D. Total £ \_\_\_\_\_

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. We would appreciate receiving reprints of any such publications.