

## NEWSLETTER

We are pleased to announce that Dr. Wayne Hendrickson of the Naval Research Laboratory has accepted a three-year term on the Protein Data Bank Advisory Board. Also continuing on the board are Professors Harold Scheraga (Cornell) and Jane Richardson (Duke). At this time we would like to express our great appreciation to Professor Michael Rossmann of Purdue University for having served on the board for the past three years.

We are planning to include a new record type REVDAT (Revision Date) in our entries in the near future. REVDAT will contain the date of the latest revision for a given entry. We will classify our corrections in these records into two types: those which directly affect the atomic coordinates and those which do not do so. (The latter type are mostly of a typographical nature). The proposed record format will be:

Cols. 1-6	8-10	12	14-22	24-30	32	40-70
REVDAT	Modification Number	Serial Number	Date	IDENT Used	Modification Type	Comments

Further details will be provided shortly in our Atomic Coordinate Entry Format Description.

The Protein Data Bank has grown considerably over the years as shown in the following table.

Year	No. of entries distributed	No. of requests
1973	106	15
1974	99	16
1975	513	36
1976	1920	64
1977	5037	85
1978	4879	63
1979	7146	75
1980	9121	70
1981	18016	104

These distribution statistics represent activities only at Brookhaven. Copies of the files are maintained at the affiliated data centers listed below as well as being accessible through the PROPHET System.

Area	Address of Center	Name	
The Americas	Protein Data Bank	E. Abola	516-282-4383
	Chemistry Department	F. C. Bernstein	516-282-4382
	Brookhaven National Laboratory Upton, New York 11973 USA	T. F. Koetzle	516-282-4384
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard	0223-66499
		S. Bellard	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002 Australia	C. Garrow	03-419-1333
Japan	Institute for Protein Research Osaka University 5311, Yamada-Kami, Suita Osaka, Japan	M. Kakudo	(06) 877-5111 ext. 3836

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

CODE	ITEM	12-JAN-82		AVAILABILITY			
		NO. TAPES 800 1600		US	UK	JA	AUS
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	1	X	X	X	X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	X	X	X	X
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	1	1	X	X	X	X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	X			
BLDKITTP	MODEL BUILDER'S KIT						
CONNECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS						
DGPLOTP	DIAGONAL PLOTS (LINE PRINTER)	2	1	X			
DIHDLRTP	COMPLETE TORSION ANGLES	2	1	X			
DSTNCTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	X			
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X			
PHIPSTP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLE 6)

IDENT CODE	MOLECULE	DEPOSITOR	12-JAN-82	
			DATE/	CODE
RIACTSF	ACTINIDIN	E. BAKER	7/77	SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOH	4/73	SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/79	SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/79	SF
R2B5CSF	CYTOCHROME B5	F. S. MATHEWS	12/77	SF
R3CYTSF	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80	SF
R4CYTSF	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80	SF
RCYC5501	CYTOCHROME C550	R. TIMKOVICH	4/76	SF
R1ZNASF	DNA (Z, CCGG, HIGH-SALT, SYNTHETIC)	H. DREH, R. DICKERSON	1/81	SF
R1BNASF	DNA (B, CCGGAATTCGG, SYNTHETIC, 290 DEG K)	H. DREH, R. DICKERSON	1/81	SF
R0PD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	8/75	SF
R2G0DSF	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	SF
R1HMMSF	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81	SF
R2MHBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80	SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80	SF
RHMDEH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75	SF
LAMPRY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	5/73	SF
RLDH06	LACTATE DEHYDROGENASE	M. ROSSMANN	9/75	SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75	SF
R5LDHSF	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	1/81	SF
R1LZHSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	C. BLAKE, D. RICE	6/81	SF
R2LZHSF	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	C. BLAKE, D. RICE	6/81	SF
RMETMYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76	SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76	SF
R3RNASF	RIBONUCLEASE A	A. HLODANER	3/79	SF
R4RNASF	RIBONUCLEASE A	L. EISEN	3/79	SF
R4TNASF	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	6/80	SF

CODES  
SF STRUCTURE FACTORS

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	12-JAN-82		AVAILABILITY			
				US	UK	JA	AUS
DATAPRF1	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)			X	X	X	
NONST1F1	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)			X	X	X	
NONST2F1	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)			X	X	X	
CORROB1F1	*LIST OF CORRECTIONS NO. 9 (JUL/81 - JAN/82)			X	X	X	X
BENDERF1	PARAMETERS FOR BENT-WIRE MODELS			X			
BLDKITF1	MODEL BUILDER'S KIT						
CONNECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS						
DGPL0TF1	DIAGONAL PLOTS (LINE PRINTER)			X			
DIHDLRF1	COMPLETE TORSION ANGLES			X			
DSTNCF1	CONNECTIVITY SPECIFICATIONS WITH DISTANCES			X			
FIS1PLF1	PHI/PSI PLOTS (LINE PRINTER)			X			
PH1PS1F1	LISTS OF PHI/PSI/OMEGA VALUES			X			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLE 5)

IDENT CODE	MOLECULE	DEPOSITOR	12-JAN-82	
			DATE/	CODE
R351CSF	CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81	SF
R451CSF	CYTOCHROME C551 (REDUCED)	T. TAKANO, R. DICKERSON	9/81	SF
R2BNASF	*DNA (B, CCGGAATTCGG, SYNTHETIC, 16 DEG K)	H. DREH, R. DICKERSON	11/81	SF
R1MLTSF	MELITTIN	DIJKSTRA, HOL, DRENTH	9/81	SF
R2BP2SF	PROPHOSPHOLIPASE A2 (BOVINE)	J. WALTER, R. HUBER	10/81	SF
R2PTNSF	*TRYPSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R3PTNSF	*TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R2TGASF	*TRYPSINOGEN (2.4M MGS04)	J. WALTER, R. HUBER	10/81	SF
R1TGCSF	*TRYPSINOGEN (.5 CH3OH, .5 HOH)	J. WALTER, R. HUBER	10/81	SF
R1TGTSF	*TRYPSINOGEN (173 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TGTSF	*TRYPSINOGEN (103 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TPTSF	*TRYPSINOGEN/PT1/ILE-VAL (MERCURATED)	J. WALTER, R. HUBER	10/81	SF

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER  
CODES  
SF STRUCTURE FACTORS

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

NAME	PURPOSE	AUTHOR(S)	12-JAN-82	
			REV DATE/	SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G. WILLIAMS	1/79	YES
BLDKIT	MODEL BUILDER'S KIT	E. ABOLA	7/80	YES
CHIRAL	CHECK CHIRALITY	E. ABOLA	3/80	YES
CONNECT	GENERATE FULL CONNECTIVITY	F. BERNSTEIN	12/81	YES
CONCT	INTERMOLECULAR CONTACTS	L. ANDREWS	10/79	NO
DGPLOTP	DIAGONAL PLOTS ON PRINTER	E. SWANSON, F. BERNSTEIN	3/79	YES
DIHDLR	COMPLETE TORSION ANGLES	E. ABOLA	3/80	YES
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F. BERNSTEIN	3/79	YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F. BERNSTEIN	5/79	YES
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y. BEPPU	11/78	NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS, WILLIAMS, BERNSTEIN	2/79	YES
STEREO	EXTRACT X, Y, Z FROM STEREO DIAGRAMS	M. ROSSMANN	6/79	NO
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H. BERNSTEIN, F. BERNSTEIN	12/79	YES
TORSRU	COMPLETE TORSION ANGLES	G. REEKE	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L. ANDREWS, F. BERNSTEIN	5/78	YES

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER

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

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

12-JAN-82

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS		DATE/STATUS		
2APE	ACID PROTEINASE (ENDOTHA PARASITICA)	T. BLUNDELL	9/81 R	IKES	KERATAN SULFATE	S. ARNOTT	5/78
1APP	ACID PROTEINASE (PENICILLIUM JANTHINELLUM)	M. JAMES, J. HSU	12/79	1LXD	LACTATE DEHYDROGENASE (MOUSE TESTES)	W. MUSICK, M. ROSSMANN	9/78
2ACT	ACTINIDIN	D. DAVIES	8/79	4LDH	LACTATE DEHYDROGENASE (PIG)	W. EVENTOFF, M. ROSSMANN	4/77 R
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	E. BAKER	11/79 R	3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE (PIG)	M. ROSSMANN	11/79
1AGA	AGAROSE	G. SCHULZ	3/77 R	5LDH	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	10/80
2MGA	AGGLUTININ (WHEAT GERM)	S. ARNOTT	5/78	1HBL	LEGHEMOGLOBIN	VAINSHTEIN, HARUTYUNYAN	11/78
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C. WRIGHT	5/80 R	1LZH	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C. -I. BRANDEN	8/76	1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS	2/75
4ADH	ALCOHOL DEHYDROGENASE (APO)	C. -I. BRANDEN	8/79	2LYZ	LYSOZYME (HEN EGG-WHITE, SET R55D)	R. DIAMOND, D. PHILLIPS	2/75
1ALP	ALPHA LYTIC PROTEASE	BRAYER, DELBAERE, JAMES	6/79	3LYZ	LYSOZYME (HEN EGG-WHITE, SET R56A)	R. DIAMOND, D. PHILLIPS	2/75
1ABP	L-ARABINOSE-BINDING PROTEIN	F. QUICHO, G. GILLILAND	5/80	4LYZ	LYSOZYME (HEN EGG-WHITE, SET R59A)	R. DIAMOND, D. PHILLIPS	2/75
1ATC	ASPARTATE CARBAMOYLTRANSFERASE	CRAWFORD, MONACO, LIPSCOMB	8/79 A	5LYZ	LYSOZYME (HEN EGG-WHITE, SET R51A)	R. DIAMOND, D. PHILLIPS	2/75
1AZU	AZURIN	E. ADMAN, L. SIEKER, L. JENSEN	8/80	6LYZ	LYSOZYME (HEN EGG-WHITE, SET R51B)	R. DIAMOND, D. PHILLIPS	2/75
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 RA	7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH	5/77
1ABX	ALPHA-BUNGAROTOXIN	D. AGARD, S. SPENCER, R. STROUD	4/80 A	8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77
1CPV	CALCIUM-BINDING PARVALBUMIN SET 5A	R. KRETSINGER	8/74	9LYZ	LYSOZYME (HEN, NAM-NAG-NAM SUBSTRATE ONLY)	J. KELLY, M. JAMES	12/79
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74	1LZH	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	ARTYMIUK, BLAKE, RICE, WILSON	6/81 A
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74	2LZH	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	ARTYMIUK, BLAKE, RICE, WILSON	6/81 A
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M11)	R. KRETSINGER	8/74	1LZZ	LYSOZYME (TURKEY EGG-WHITE)	R. BOTT, R. SARMA	9/81 A
1CAB	CARBONIC ANHYDRASE B (HUMAN)	S. ARNOTT	5/78	1MOH	MALATE DEHYDROGENASE	L. BANASZAK	6/76 A
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76	1MLT	MELITTIN	TERHILLIGER, EISENBERG	8/81
1CPA	CARBOXYPEPTIDASE A (BOVINE)	H. L. LIPSCOMB	2/73	1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A. MCLACHLAN	8/78
1CPB	CARBOXYPEPTIDASE B (BOVINE)	H. L. LIPSCOMB	9/76 A	1MBS	MYOGLOBIN (SEAL, MET)	H. SCOULOUDI	3/79
1CAR	CARRAGEENAN	S. ARNOTT	5/78	1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	4/73
1CS	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78	2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76
2CS	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78	3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	S. PHILLIPS	8/81
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	S. ARNOTT	5/78	1MBD	MYOGLOBIN (SPERM WHALE, DEOXY)	S. PHILLIPS	8/81
3CHA	ALPHA-CHYMOTRYPSIN	S. ARNOTT	5/78	1MBO	MYOGLOBIN (SPERM WHALE, OXY)	S. PHILLIPS	8/81
2GCH	GAMMA-CHYMOTRYPSIN	D. BLOW	1/75 R	1MHR	MYOHEMERYTHRIN	W. HENDRICKSON	6/76 A
1CAT	CATALASE (BEEF LIVER)	A. TULINSKY	8/76	1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)	D. TERNONDELOU, G. PETSKO	8/80
1CHG	CHYMOTRYPSINOGEN	COHEN, DAVIES, SILVERTON	4/80 A	1PPT	AVIAN PANCREATIC POLYPEPTIDE	T. BLUNDELL	1/81
2CNA	CONCANAVALIN A	M. ROSSMANN	6/81 A	8PAP	PAPAINE (NATIVE)	J. DRENTH	11/76 R
3CNA	CONCANAVALIN A	J. KRAUT, J. BIRKTOFT	3/75	1PAD	PAPAINE (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
1CN1	*CONCANAVALIN A (DEMETALLIZED)	G. REEKE, J. BECKER, G. EDELMAN	4/75	3PAD	PAPAINE (OXIDIZED CYS-25)	J. DRENTH	11/76 R
1CRN	CRAMBIN	K. HARDMAN	9/76 R	4PAD	PAPAINE (TOS-LYS, CYS-25)	J. DRENTH	11/76 R
2BSC	CYTOCHROME B5 (OXIDIZED)	M. SHOAHAM	12/81 N	5PAD	PAPAINE (BOZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76 R
156B	CYTOCHROME B562 (E. COLI, OXIDIZED)	W. HENDRICKSON, M. TEETER	5/81	6PAD	PAPAINE (BOZOXY-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	F. S. MATHEWS	12/77 R	1PEP	PEPSIN (PORCINE)	N. ANDREVA ET AL.	7/78 A
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	BETHGE, CZERNIANSKI, MATHEWS	8/79	1PFC	*PFC FRAGMENT OF AN IGG	M. ANZEL	10/81
10CY	CYTOCHROME C (BONITO, HEART)	T. TAKANO, R. DICKERSON	7/80 R	2PCK	PHOSPHOKINASE (YEAST)	H. WATSON	5/76 A
10CY	CYTOCHROME C (PRIME)	T. TAKANO, R. DICKERSON	7/80 R	2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76 B
10CY	CYTOCHROME C2	M. KAKUDO	8/76	2PGM	PHOSPHOGLYCERATE MUTASE	H. WATSON	8/81 RN
155C	CYTOCHROME C550 (OXIDIZED)	P. WEBER, R. SALEMME	8/81	1BP2	PHOSPHOLIPASE A2 (BOVINE)	B. DIJKSTRA, J. DRENTH	4/81
351C	CYTOCHROME C551 (OXIDIZED)	J. KRAUT	3/73	2BP2	PHOSPHOLIPASE A2	B. DIJKSTRA, W. HOL, J. DRENTH	6/81
451C	CYTOCHROME C551 (REDUCED)	R. TIMKOVICH	8/76	1PCY	PLASTOCYANIN	J. GUSS, H. FREEMAN	8/80
1DFR	DIHYDROFOLATE REDUCTASE (L. CASEI)	MATSUURA, TAKANO, DICKERSON	7/81	2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE	9/77 R
2DFR	DIHYDROFOLATE REDUCTASE (E. COLI)	MATSUURA, TAKANO, DICKERSON	7/81	1PKY	PYRUVATE KINASE (CAT)	H. MUIRHEAD	1/80 A
1BNA	DNA (B, CGCGAATTCGCG, SYNTHETIC, 16 DEG K)	J. BOLIN, D. MATTHEWS, J. KRAUT	3/80	1RLX	RELAXIN (MODEL, CONFORMATION A, UNREFINED)	A. EVANS, A. NORTH	3/78
2BNA	*DNA (B, CGCGAATTCGCG, SYNTHETIC, 16 DEG K)	J. BOLIN, D. MATTHEWS, J. KRAUT	3/80	2RLX	RELAXIN (MODEL, CONFORMATION B, UNREFINED)	A. EVANS, A. NORTH	3/78
1ZNA	DNA (Z-I, CGCGCG, SYNTHETIC, MODEL)	H. DREW, R. DICKERSON	1/81	3RLX	RELAXIN (MODEL, CONFORMATION A, REFINED)	A. EVANS, A. NORTH	3/78
2ZNA	DNA (Z-II, CGCGCG, SYNTHETIC, MODEL)	H. DREW, R. DICKERSON	1/81	4RLX	RELAXIN (MODEL, CONFORMATION B, REFINED)	A. EVANS, A. NORTH	3/78
3ZNA	DNA (Z-III, CGCGCG, SYNTHETIC, MODEL)	H. DREW, R. DICKERSON	1/81	1RHD	RHODANASE	W. HOL	12/77
1EST	ELASTASE (PORCINE, TOSYL)	A. RICH	2/81	3RSA	RIBONUCLEASE A	A. WLODAWER	5/81 R
1ECD	ERYTHROCYRORIN (REDUCED, DEOXY)	H. WATSON	5/76	1RNS	RIBONUCLEASE-A	BORKAKOTI, MOSS, PALMER	10/81
1ECO	ERYTHROCYRORIN (CARBONMONOXY)	H. STEIGEMANN, E. WEBER	3/79	1RNS	RIBONUCLEASE-S	H. WICKOFF, F. RICHARDS	4/73
1ECA	ERYTHROCYRORIN (AQUO, MET)	H. STEIGEMANN, E. WEBER	3/79	2RXN	RUBREDOXIN (CLOSTRIDIUM PASTEURIANUM)	L. JENSEN	1/75
1ECN	ERYTHROCYRORIN (CYANO, MET)	H. STEIGEMANN, E. WEBER	3/79	3RXN	RUBREDOXIN (DESULFOVIBRIO VULGARIS)	E. ADMAN, L. SIEKER, L. JENSEN	9/80
1FDX	*FERREDOXIN (SPIROCOCCUS AEROGENES)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	1SNC	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73
3FXC	*FERREDOXIN (SPIRULINA PLATENSIS)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	1SGA	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER, DELBAERE, JAMES	6/78
2FDI	*FERREDOXIN (AZOTOBACTER VINELANDII)	TSUKIHARA, KATSUBE, KAKUDO	11/81 R	256B	STREPTOMYCES GRISEUS PROTEINASE B	DELBAERE, BRAYER, JAMES	6/79 R
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	STOUT, GHOSH, FUREY, ODONNELL	11/81 R	255I	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y. MITSUI ET AL.	4/80 R
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LUDWIG	12/77 R	1SBT	SUBTILISIN BPN*	J. KRAUT	9/76
1GCG	GLUCAGON	M. LUDWIG	10/77	25BT	SUBTILISIN NOVO	J. DRENTH	9/76
1PG1	GLUCOSE-6-PHOSPHATE ISOMERASE	T. BLUNDELL	7/77	250D	SUPEROXIDE DISMUTASE	J. RICHARDSON, D. RICHARDSON	3/80 R
2ORS	*GLUTATHIONE REDUCTASE (HUMAN)	H. MUIRHEAD	11/81 RN	1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	4/75
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRIM)	G. SCHULZ	7/75	2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS	4/75
2GPD	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B. -O. SODERBERG	5/76 A
1HRB	HEMERYTHRIN B	W. HENDRICKSON	6/76 A	4TNA	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	4/78 R
1HMM	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 R	6TNA	TRANSFER RNA (YEAST, PHE)	S. -H. KIM ET AL.	11/78 R
1HDS	HEMOGLOBIN (DEER, SICKLE CELL)	E. AMMA, R. GIRLING	10/79	8TNA	TRANSFER RNA (YEAST, PHE)	I. WILSON, D. PHILLIPS	9/76
2HMB	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, HEIDNER, PERUTZ	2/77 R	1T1M	TRIOSE PHOSPHATE ISOMERASE	R. KRETSINGER, C. BARRY	6/80 A
20HB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73	2PTN	*TRYPSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 RP
1HMB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	8/79	3PTN	*TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 P
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY)	J. BALDWIN	8/79	2PTB	TRYPSIN (BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	1/77 R
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY, NRG REFND)	J. BALDWIN	8/76	3PTP	TRYPSIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	12/77 R
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76	3PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76 R
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73	2TGA	TRYPSINOGEN (2.4M MO50H)	R. HUBER, W. BODE	11/76
1HKG	HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	W. BENNETT JR., T. STEITZ	12/80	1TGC	*TRYPSINOGEN (5 CH3OH, .5 HOH)	J. WALTER, R. HUBER	10/81 P
2YHX	HEXOKINASE (YEAST) FORM BIII	STEITZ, ANDERSON, STENKAMP	3/78 R	1TGT	*TRYPSINOGEN (173 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81 P
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	12/77	2TGT	*TRYPSINOGEN (103 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81 P
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78	1TGB	TRYPSINOGEN (WITH CA, FROM PEG)	BODE, FEHLHAMMER, HUBER	3/79
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78	1TGN	TRYPSINOGEN	A. KOSSIAKOFF, R. STROUD	9/79
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78	1TGP	TRYPSINOGEN/TRYPsin INHIBITOR	W. BODE, P. SCHWAGER, R. HUBER	3/79
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78	1TPI	TRYPSINOGEN/TRYPsin INHIBITOR/ILE-VAL	W. BODE, P. SCHWAGER, R. HUBER	3/79
3FAB	IMMUNOGLOBULIN FAB*	R. POLJAK	9/81 R	2TPI	*TRYPSINOGEN/PTI/ILE-VAL (MERCURATED)	J. WALTER, R. HUBER	10/81 P
1MCG	IMMUNOGLOBULIN B-J INTACT MCG	SCHIFFER, EDMUNDSON ET AL.	5/78 A	15BV	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M. ROSSMANN	12/79 B
1RE1	IMMUNOGLOBULIN B-J FRAGMENT (V-DIMER) RE1	O. EPP, R. HUBER	3/76				
1RHE	IMMUNOGLOBULIN B-J FRAGMENT (V-MNMR) RHE	B. WANG, C. YOO, M. SAX	12/77 A				
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J. DEISENHOFER	5/81				
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J. DEISENHOFER	5/81				
1INS	INSULIN (PORCINE, 2-ZINC)	G. DODSON, D. HODGKIN	7/80				
1KGA	KDPG ALDOLASE	A. TULINSKY	8/78 A				

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER

STATUS CODES

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

TABLE 8. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

12-JAN-82

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

12-JAN-82

DEAP	ACID PROTEINASE (ENDOTHRAS PARASITICA)
DAOC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX
DAF1	APOFERRITIN (HORSE)
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
OICB	*CALCIUM-BINDING PROTEIN (MINOR A FORM,BOVINE)
OC22	CARBOXYPEPTIDASE A-INHIBITOR COMPLEX
UCT5	CITRATE SYNTHASE (PIG)
OCTX	ALPHA COBRATOXIN
OCN2	CONCANAVALIN A (DEMETALLIZED)
OCRO	CRO REPRESSOR
OGCR	*GAMMA-CRYSTALLIN II (CALF)
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)
OCVY	*CYTOCHROME C3 (DESULFOVIBRIO VULGARIS MIYAZAKI)
O5C1	CYTOCHROME C555 (CHLOROBIUM THIOSULFATOPHILUM)
OC3A	DES-ARG77-C3A ANAPHYLATOXIN
DES2	ELASTASE COMPLEX (PIG)
DETU	ELONGATION FACTOR TU COMPLEX (E. COLI)
DEBX	ERABUTOXIN B
OFX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
DGAP	CATABOLITE GENE ACTIVATOR PROTEIN
OGP1	GLUTATHIONE PEROXIDASE (BOVINE)
OGD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
OHHG	HAEMAGGLUTININ
OHBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)
OPHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)
OAU1	IMMUNOGLOBULIN, BENGE-JONES FRAGMENT (KAPPA) AU
OROY	IMMUNOGLOBULIN, BENGE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY
OMCP	IMMUNOGLOBULIN FAB (KAPPA) MCP503
OFB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL
OIG1	IMMUNOGLOBULIN G1 (KAPPA) DOB
OIG2	IMMUNOGLOBULIN G1 (LAMBDA) KOL
OIN1	*INSULIN (PORCINE)
OIN2	INSULIN (PORCINE)
OGF1	INSULIN-LIKE GROWTH FACTOR I (HUMAN)
OGF2	INSULIN-LIKE GROWTH FACTOR II (HUMAN)
OLZ1	LYSOZYME (HUMAN)
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)
OLZ6	*LYSOZYME (STREPTOMYCES ERYTHRAEUS)
OCTF	L7/L12 (E. COLI, C-TERMINUS)
OMB5	MYOGLOBIN (SPERM WHALE, CARBON MONOXIDE, NEUTRON STUDY)
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)
OSN3	SCORPION NEUROTOXIN VARIANT-3
OOVO	OVOMUCOID FRAGMENT
DPFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)
OBP1	PHOSPHOLIPASE A2 (PORCINE)
OPR2	*PHOSPHOLIPASE A2 (RATTLESNAKE)
OPPA	PHOSPHORYLASE A (RABBIT)
OPB1	PHOSPHORYLASE B (RABBIT)
ORX5	RELAXIN (PORCINE, MODEL)
ORSA	RIBONUCLEASE A (BOVINE)
ORS3	*RIBONUCLEASE A (BOVINE, NEUTRON STUDY)
FMIT	INITIATOR TRANSFER RNA (E. COLI, F/MET)
OTA1	TRANSFER RNA (YEAST, ASP, A FORM)
OTA2	TRANSFER RNA (YEAST, ASP, B FORM)
OTR1	TRANSFER RNA (YEAST, PHE)
OMTS	*METHIONYL TRANSFER RNA SYNTHETASE
OTS1	TYROSYL TRANSFER RNA SYNTHETASE (BACILLUS STEAROTHERMOPHILUS)
OGN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)
OUTG	UTEROGLOBIN (RABBIT)
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)
OTBV	VIRUS (TOMATO BUSHY STUNT)

\* NEW OR REPLACEMENT ENTRY SINCE OCT-81 NEWSLETTER

THE CORRECTIONS IN THIS TABLE ARE GIVEN IN THE FORM OF 'UPDATE' MODIFICATIONS AND CONSIST OF 'UPDATE' DIRECTIVES PLUS NEW DATA RECORDS THAT ARE TO BE INSERTED OR THAT REPLACE ERRONEOUS RECORDS IN CERTAIN DATA BANK ENTRIES. 'UPDATE' IS THE CDC LIBRARY-FILE MANAGEMENT SYSTEM UNDER WHICH THE MASTER PROTEIN DATA BANK FILE IS MAINTAINED. FOR A DESCRIPTION OF 'UPDATE' USERS ARE REFERRED TO THE 'UPDATE REFERENCE MANUAL' PUBLICATION NUMBER 60342500, CONTROL DATA CORPORATION, ARDEN HILLS, MN, 1974. BRIEFLY, EACH DATA ENTRY IS GIVEN AN IDENTIFICATION CODE WHICH ALSO SERVES AS THE 'UPDATE 'DECK' NAME. EACH RECORD IN THE FILE IS IDENTIFIED WITH TWO TAGS. THE FIRST TAG IS SIMPLY THE 'DECK' NAME (OR AN 'IDENT' NAME -SEE BELOW) AND THE SECOND IS A SEQUENCE NUMBER WITHIN THE 'DECK' (OR 'IDENT'). THESE TAGS ARE INCLUDED IN CHARACTERS 73-80 OF THE RECORDS IN EACH DATA ENTRY AS DISTRIBUTED.

CORRECTIONS MAY BE MADE USING 'UPDATE' DIRECTIVES TO 'INSERT' NEW RECORDS OR 'DELETE' OLD ONES. EACH CORRECTION SET BEGINS WITH A 'IDENT' DIRECTIVE. THIS IDENTIFIES THE CORRECTION SET, E.G. AS '1MBN1' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK '1MBN1' FOR SPERM-WHALE MYOGLOBIN, '1MBN2' FOR THE SECOND CORRECTION, ETC. 'DELETE' DIRECTIVES SPECIFY A RECORD OR INCLUSIVE RUN OF RECORDS TO BE DELETED. IF DATA RECORDS OCCUR IMMEDIATELY FOLLOWING 'DELETE', THESE ARE TO BE INSERTED IN PLACE OF THE RECORDS DELETED. 'INSERT' DIRECTIVES ARE USED TO SPECIFY A PARTICULAR RECORD AFTER WHICH INFORMATION IS TO BE INSERTED. THE RECORDS TO BE INSERTED FOLLOW IMMEDIATELY AFTER 'INSERT' IN THE CORRECTION SET. WITHIN EACH CORRECTION NEW RECORDS PLACED IN THE FILE ARE GIVEN THE 'IDENT' NAME AND NUMBERED SEQUENTIALLY.

```

*IDENT,1SRX1
*INSERT,1SRXH.5
REMARK 16
REMARK 16 CORRECTION. CONVERT ATOMIC COORDINATES TO ANGSTROM UNITS BY
REMARK 16 DIVIDING ALL X, Y, Z BY 2.0. MODIFY REMARK 11 TO REFLECT
REMARK 16 THIS CHANGE. INSERT SSBOND RECORD. 14-SEP-81.
*INSERT,1SRXE.1
REMARK 11 (THIS REMARK IS NO LONGER APPLICABLE - SEE REMARK 16).
*INSERT,1SRX.52
SSBOND 1 CYS 32 CYS 35
*DELETE,1SRX.58,165
ATOM 2 CA SER 1 15.200 .850 39.750 1.00 0.00
ATOM 6 CA ASP 2 15.850 4.400 39.000 1.00 0.00
ATOM 16 CA LYS 3 18.450 6.700 38.250 1.00 0.00
ATOM 25 CA ILE 4 17.850 9.350 35.850 1.00 0.00
.
ATOM 802 CA ALA 105 18.800 -5.500 17.800 1.00 0.00
ATOM 807 CA ASN 106 21.400 -3.250 19.250 1.00 0.00
ATOM 815 CA LEU 107 21.650 -4.300 23.100 1.00 0.00
ATOM 823 CA ALA 108 21.700 -7.800 24.700 1.00 0.00
TER 829 ALA 108 0.000 0.000 0.000
*DELETE,1SRXH.6
MASTER 74 0 0 4 5 5 1 3 108 2 0 9

*IDENT,1HCOB
*INSERT,1HCOA.5
REMARK 7
REMARK 7 CORRECTION. CHANGE SIGN OF (3,3) ELEMENT OF SCALE
REMARK 7 TRANSFORMATION. 13-OCT-81.
*DELETE,1HCO.100
SCALE3 .004389 0.000000 -.002753 0.000000
*DELETE,1HCOA.6
MASTER 46 0 2 16 0 0 0 6 2282 2 94 23

*IDENT,2HCOB
*INSERT,2HCOA.5
REMARK 7
REMARK 7 CORRECTION. CHANGE SIGN OF (3,3) ELEMENT OF SCALE
REMARK 7 TRANSFORMATION. 13-OCT-81.
*DELETE,2HCO.101
SCALE3 .004389 0.000000 -.002753 0.000000
*DELETE,2HCOA.6
MASTER 47 0 2 16 0 0 0 6 2282 2 94 23

*IDENT,1CPAK
*INSERT,1CPAJ.18
REMARK 19
REMARK 19 CORRECTION. CORRECT SCALE TRANSFORMATION. 06-JAN-82.
*DELETE,1CPA.107,109
SCALE1 .019451 0.000000 .002588 0.000000
SCALE2 0.000000 .016697 0.000000 0.000000
SCALE3 0.000000 0.000000 .021379 0.000000
*DELETE,1CPAJ.19
MASTER 122 6 1 8 8 32 0 6 2453 2 6 25

*IDENT,1CYCH
*INSERT,1CYCG.5
REMARK 12
REMARK 12 CORRECTION. CORRECT (2,2) ELEMENT OF SCALE TRANSFORMATION.
REMARK 12 06-JAN-82.
*DELETE,1CYC.44
SCALE2 0.000000 .011823 0.000000 0.000000
*DELETE,1CYCG.6
MASTER 60 0 1 5 0 3 0 9 839 1 48 8

*IDENT,4HYAB
*INSERT,4HYAA.3
REMARK 6
REMARK 6 CORRECTION. CORRECT ORIGX AND SCALE TRANSFORMATIONS.
REMARK 6 REVISE COORDINATES ACCORDINGLY. 06-JAN-82.
*DELETE,4HYA.57,62
ORIGX1 .047778 .027585 0.000000 0.000000
ORIGX2 0.000000 .055170 0.000000 0.000000
ORIGX3 0.000000 0.000000 .035336 0.000000
SCALE1 .047778 .027585 0.000000 0.000000
SCALE2 0.000000 .055170 0.000000 0.000000
SCALE3 0.000000 0.000000 .035336 0.000000
*DELETE,4HYA.64,201
HETATM 1 C1 NAG 1 6.180 12.208 15.186 1.00 0.00
HETATM 2 C2 NAG 1 6.510 13.259 16.239 1.00 0.00
HETATM 3 C3 NAG 1 6.253 12.715 17.637 1.00 0.00
HETATM 4 C4 NAG 1 4.834 12.172 17.736 1.00 0.00

HETATM 135 O HOH 9 8.272 10.038 -9.735 1.00 0.00
HETATM 136 O HOH 10 8.455 13.179 8.691 1.00 0.00
HETATM 137 O HOH 11 4.681 15.340 1.189 1.00 0.00
HETATM 138 O HOH 12 6.694 7.314 -7.095 1.00 0.00
*DELETE,4HYAA.4
MASTER 39 0 3 0 0 0 0 6 138 0 126 1

*IDENT,1SGAE
*INSERT,1SGAD.3
REMARK 10
REMARK 10 CORRECTION. CORRECT (1,1) ELEMENT OF SCALE TRANSFORMATION.
REMARK 10 06-JAN-82.
*DELETE,1SGA.84
SCALE1 .018136 0.000000 0.000000 0.000000
*DELETE,1SGAD.4
MASTER 65 0 0 0 0 0 0 6 1265 1 2 14
    
```

## REQUEST FORM

(Please include a self-addressed label)

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

## 2. Documentation desired (no charge).

- ( ) Latest Newsletter  
 ( ) Introduction to The Protein Data Bank (June 1981)  
 ( ) Sources of Visual Aids for Macromolecular Structure (June 1981)  
 ( ) Atomic Coordinate Entry Format Description for DATAPRTP and  
 DATAPRFI (December 1981)  
 ( ) Non-Standard Entries (Structure Factors) format description for  
 NONST1TP and NONST1FI (September 1981)  
 ( ) Non-Standard Entries (Structure Factors) format description for  
 NONST2TP and NONST2FI (January 1982)  
 ( ) Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each  
 1-tape item costs \$122 (¥68); each 2-tape item costs \$147 (¥82).  
 Domestic postage is included.

<u>Item</u>	<u>Number of Tapes</u>	<u>Cost</u>
-------------	------------------------	-------------

Total \_\_\_\_\_

## 4. Tape format desired (all tapes are unlabelled)

- ( ) 9 track, 1600 cpi, EBCDIC  
 ( ) 9 track, 800 cpi, EBCDIC  
 ( ) 9 track, 1600 cpi, ASCII  
 ( ) 9 track, 800 cpi, ASCII  
 ( ) 7 track, 800 cpi, BCD

Only the first two formats are normally prepared at Cambridge; please  
 inquire for availability of other formats.

All tapes are distributed in blocked form with fixed record length and  
 block size. Brookhaven normally uses a block size close to, but less  
 than, 5120 characters. Please indicate here any difficulties this might  
 cause.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$84 (£ 47 from Cambridge). Correction fiche are free.

ItemCost

Total \_\_\_\_\_

6. Air mail postage from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of \$15 (£ 8) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£ 8) = \_\_\_\_\_

7. Total charges

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

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

Air mail postage charges (6 above). \_\_\_\_\_

Total \_\_\_\_\_

For Brookhaven only:

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

Payment to the order of Brookhaven National Laboratory

by ( ) check \_\_\_\_\_ is ( ) enclosed  
 ( ) purchase order number \_\_\_\_\_ ( ) sent separately to the  
 Protein Data Bank

Please return to

Ms. F. C. Bernstein  
 Chemistry Department  
 Brookhaven National Laboratory  
 Upton, New York 11973 USA

or

Dr. S. Bellard  
 University Chemical Laboratory  
 Lensfield Road  
 Cambridge CB2 1EW, England