

The U.S. National Science Foundation has extended funding of the Protein Data Bank for five years. Renewal of our NSF grant will provide core support of activities at Brookhaven through October 31, 1990. Naturally, we are extremely pleased that the Foundation has acted favorably on our request. Under the terms of the new grant we will be acquiring a dedicated computer system, which should help us to improve service to the Protein Data Bank users.

A new tape product, PDBPGMTP, which was announced in our April 1985 newsletter is now ready for distribution. This tape includes source codes for all PDB programs, both supported and unsupported. A notable recent addition is the Protein and Polypeptide Secondary Structure Calculation and Prediction Applied Program Package, ALB, by A. V. Finkelstein and O. B. Ptitsyn. PDBPGMTP also contains G. Gilliland's protein crystallization database CRYSTAL. Please note (Table 3) that ALB and CRYSTAL are only available on PDBPGMTP. Our order forms have been modified to include this new product.

We strongly recommend that all recipients of magnetic tapes from the Protein Data Bank make back-up copies of these tapes as soon as possible after they are received. We realize that magnetic tapes and tape drives are not perfectly reliable. Any difficulties in reading Protein Data Bank tapes should be reported to Brookhaven immediately. Tapes with unrecoverable read errors will be replaced free of charge if the problem is reported within 60 days of shipment. Beyond 60 days, replacements will be treated as normal orders. We strongly urge all users to report any errors in the contents of Protein Data Bank data entries. This allows us to continually improve the fidelity of the data.

Inquiries may be addressed to any of the persons listed below. The order form on pages 5-6 of this Newsletter may be used to order data from Brookhaven or Cambridge; users in Australia or Japan should contact their centers for detailed information.

<u>Area</u>	<u>Address of Center</u>	<u>Name</u>	
The Americas	Protein Data Bank	E. 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	O. Kennard	0223-66499
	Lensfield Road	S. Bellard	
	Cambridge CB2 1EW, England	G. Weber	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002, Australia	T. Graddon	03-418-7266
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, Osaka 565, Japan	Y. Katsube K. Yoshida	(06) 877-5111 ext. 3912

Supported by the U. S. National Science Foundation and U. S. National Institutes of Health.

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

CODE	ITEM	20-JAN-86			
		AVAILABILITY	US	UK	JA AUS
DATAPRTP	ALL CURRENT COORDINATE ENTRIES (TABLE B), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 10 - NO COORDINATES IN BIB ENTRIES)	X	X	X	X
YEARBSTP	*NEW OR REVISED COORDINATE ENTRIES FOR 1985	X	X		
PDBPGMTP	*COMPUTER PROGRAMS AND MISCELLANEOUS FILES (TABLE 3, PARTS A AND B)	X			
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	X	X	X	
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	X	X	X	
NONST3TP	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	X	X	X	
NONST4TP	STRUCTURE FACTOR HOLDINGS (PART 4 - TABLE 7)	X	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDK11TP	MODEL BUILDER'S KIT PLEASE INQUIRE AT US CENTER	X			
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGLOTPP	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHOLTP	COMPLETE TORSION ANGLES	X			
DSTNCTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FIS1PLTP	PHI/PSI PLOTS (LINE PRINTER)	X			
PHI5PTP	LISTS OF PHI/PSI/OMEGA VALUES	X			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	20-JAN-86			
		AVAILABILITY	US	UK	JA AUS
DATAPRFI	ALL CURRENT COORDINATE ENTRIES (TABLE B), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 10 - NO COORDINATES IN BIB ENTRIES)	X	X	X	
YEARBSFI	*NEW OR REVISED COORDINATE ENTRIES FOR 1985	X			
CORR1FI	*LIST OF CORRECTIONS NO. 17 (JUL/85 - JAN/86)	X	X	X	X
NONST1FI	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	X	X	X	
NONST2FI	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	X	X	X	
NONST3FI	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	X	X	X	
NONST4FI	STRUCTURE FACTOR HOLDINGS (PART 4 - TABLE 7)	X	X	X	
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDK11FI	MODEL BUILDER'S KIT PLEASE INQUIRE AT US CENTER	X			
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGLOTFI	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHOLFI	COMPLETE TORSION ANGLES	X			
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FIS1PLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHI5PFI	LISTS OF PHI/PSI/OMEGA VALUES	X			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, COMPUTER PROGRAMS AND MISCELLANEOUS FILES

NAME	PURPOSE	AUTHOR(S)	20-JAN-86	
			REV DATE/	SUPPORTED
PART A - AVAILABLE ON DATAPRTP, DATAPRFI, PDBPGMTP				
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E.ABOLA	2/84	YES
BRUKTP	MAKE VAX/VMS FILES FROM PDB TAPE	H.BOSSHARD	8/85	NO
CHIRAL	CHECK CHIRALITY	E.ABOLA	1/82	YES
CONNECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	8/82	YES
CONTACT	INTERMOLECULAR CONTACTS	L.ANDREWS	5/83	NO
DGLOTP	DIAGONAL PLOTS (LINE PRINTER)	E.SWANSON,F.BERNSTEIN	1/83	YES
DIHOLTP	COMPLETE TORSION ANGLES	E.ABOLA	3/80	YES
DRCTRY	DIRECTORY OF PDB DISTRIBUTION TAPE	E.ABOLA	5/84	YES
DSSP	SECONDARY STRUCTURE, SOLVENT EXPOSURE	R.KABSCH,C.SANDER	12/83	NO
DSTNCE	CALC DISTANCES FROM CONTACT RECORDS	F.BERNSTEIN	8/82	YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79	YES
L5M	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82	NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78	NO
PHI5PI	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79	YES
REFMTE	REFORMAT DATA FOR SUPERTAB, SUPERB	L.RELLICK,J.DUANE	12/83	NO
STEREO	EXTRACT X,Y,Z FROM STEREO DIAGRAMS	M.ROSSMANN	6/79	NO
TAPOIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	11/79	YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEBODA	1/82	NO
TORSRU	COMPLETE TORSION ANGLES	G.REEKE	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	3/82	YES
PART B - AVAILABLE ON PDBPGMTP				
ALB	*SECONDARY STRUCT. CALC., PREDICTION A.FINKELSTEIN,O.PTITSYN		10/85	NO
CRYSTAL	*DATA BASE - PROTEIN CRYSTALLIZATION G.GILLILAND		12/84	NO

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 NEWSLETTER  
SUPPORTED PROGRAMS ARE THOSE FOR WHICH STAFF OF THE PROTEIN DATA BANK WILL PROVIDE CORRECTIONS FOR DEMONSTRATED ERRORS.

TABLE 4. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLES 5,6,7)

IDENT CODE	MOLECULE	DEPOSITOR	20-JAN-86	
			DATE/	CODE
RIACTSF	ACTINININ	E. BAKER	7/77	SF
CHYMCF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	4/73	SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74	SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74	SF
R2B5CSF	CYTOCHROME C (ALBACORE, OXIDIZED)	F. S. MATHEWS	12/77	SF
R3CYTSF	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO,R.DICKERSON	7/80	SF
RCYCS501	CYTOCHROME C550	R. TIMKOVICH	4/76	SF
R1ZNASF	DNA (Z', CGCG, HIGH-SALT, SYNTHETIC)	H. DREW,R.DICKERSON	1/81	SF
R1BNASF	DNA (B, CGCGAATTCGG, SYNTHETIC, 290 DEG K)	H. DREW,R.DICKERSON	1/81	SF
R6PD04	G-CERAMIDE-2-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	8/75	SF
R2GDSF	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	L. MADSSMANN	12/79	SF
R2MH6SF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80	SF
R1F0HSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FERRIER	6/80	SF
RHLMDEH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75	SF
LAMPFY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	5/73	SF
RLDH06	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75	SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75	SF
RL5LHSF	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	1/81	SF
RL2ZHSF	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
RME1MYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76	SF
ROE1MYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76	SF
R4TNASF	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	6/80	SF

CODES  
SF STRUCTURE FACTORS

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLES 4,6,7)

IDENT CODE	MOLECULE	DEPOSITOR	20-JAN-86	
			DATE/	CODE
R1CCRSF	CYTOCHROME C (RICE)	H. OCHI, N. TANAKA	3/83	SF
R351CSF	CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81	SF
RH51CSF	CYTOCHROME C551 (REDUCED)	T. TAKANO, R. DICKERSON	9/81	SF
R1ANASF	DNA (A, D-1000-CGCG) SPACE GROUP P 43 21 2	B. CONNER, R. DICKERSON	6/82	SF
R1ANAF2	DNA (A, D-1000-CGCG) SPACE GROUP P 21	B. CONNER, R. DICKERSON	6/82	SF
R2BNASF	DNA (B, CGCGAATTCGG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	SF
R2BNASF	DNA (B, 9-BR-CGCGAATTCGG, 20 DEG C)	KOPKA, FRATINI, DICKERSON/82	SF	
RHBNASF	DNA (B, 9-BR-CGCGAATTCGG, 7 DEG C)	KOPKA, FRATINI, DICKERSON/82	SF	
R5BNASF	DNA (B, CGCGAATTCGG, SYNTHETIC) / CISPLATIN	WING, PUJARA, DREW, DICKSON/83	SF	
R1GAASF	GLUTAMINASE-ASPARAGINASE (ACINETOBACTER)	H. AMMON	12/82	SF
R1GAS2F	GLUTAMINASE-ASPARAGINASE (PSEUDOMONAS 7A)	H. AMMON	12/82	SF
R1HM0SF	HEMERYTHRIN (MET)	STENKAMP, SIEKER, JENSEN	2/83	SF
R1HM2SF	HEMERYTHRIN (AZIDO, MET)	STENKAMP, SIEKER, JENSEN	2/83	SF
R2INSF	INSULIN (BOVINE, 2-ZINC) DES-PHE B1	C. REYNOLDS, G. DOOSON	5/82	SF
RL1HSF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LEGHEMOGLOBIN (FERRO) / NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	2/83	SF
RL1HSF	LEGHEMOGLOBIN (FERRO) / NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RL1HSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE, RAO, SUNDARALINGAM/78	SF	
R1MLTSF	MELITTIN	TERAHILLIGER, E. SEIBERG	8/81	SF
R10V0SF	OVOMUCOID (JAPANESE QUAIL)	E. PAPAIOGORGIS, R. HUBER	1/82	SF
R2P25SF	PROPHOSPHOLIPASE A2 (BOVINE)	D.JAKSTRA, H. ORENTH	9/81	SF
R1PYP5F	INORGANIC PYROPHOSPHATASE	E. HARUTYUNYAN ET AL.	2/83	SF
R1RN3SF	RIBONUCLEASE A	BORKAKOTI, MOSS, PALMER	6/82	SF
R3TLNSF	THERMOLYSIN (NATIVE)	B. MATTHEWS, M. HOLMES	2/82	SF
R2PTNSF	TRYP SIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R2PTNSF	TRYP SIN (ORTHORHOMBIC)	HOLBE, WALTER, HUBER	9/82	SF
R3PTNSF	TRYP SIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R3PTBSF	TRYP SIN (BENZAMIDINE INHIBITED)	BODE, SCHWAGER, WALTER	9/82	SF
R1PTPSF	TRYP SIN / P-AMIDINO-PHENYL-PYRUVATE	WALTER, BODE, HUBER	9/82	SF
R4PTISF	TRYP SIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	9/82	SF
R2PTCSF	TRYP SIN / TRYP SIN INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER	9/82	SF
R1PTASF	TRYP SIN (ANHYDRO) / TRYP SIN INHIBITOR	HUBER, BODE, DEISENHOFER	9/82	SF
R2TG6SF	TRYP SIN (2.4M MOSO4)	J. WALTER, R. HUBER	10/81	SF
R1TG6SF	TRYP SIN (0.5 CH3OH, .5 HOH)	J. WALTER, R. HUBER	10/81	SF
R1TG6SF	TRYP SIN (0.173 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TG6SF	TRYP SIN (0.103 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TG6SF	TRYP SIN / TRYP SIN INHIBITOR	R. HUBER ET AL.	9/82	SF
R3PTISF	TRYP SIN / TRYP SIN INHIBITOR / ILE-VAL	R. HUBER ET AL.	9/82	SF
R2PTISF	TRYP SIN / TRYP SIN INHIBITOR / ILE-VAL (MERCURATED)	J. WALTER, R. HUBER	10/81	SF
R1TG6SF	TRYP SIN / TRYP SIN INHIBITOR / PSTI	R. HUBER ET AL.	9/82	SF

CODES  
SF STRUCTURE FACTORS

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 3, SEE ALSO TABLES 4,5,7)

IDENT CODE	MOLECULE	DEPOSITOR	20-JAN-86	
			DATE/	CODE
R1CATSF	CATALASE (BEEF LIVER)	M. ROSSMANN	11/81	SF
RHCHASF	ALPHA-CHYMOTRYPSIN (BOVINE)	H. TSUKADA, D. BLOW	11/84	SF
R2GCHSF	GAMMA-CHYMOTRYPSIN	COHEN, DANIELS, SILVERTON	7/84	SF
R3CYCSF	CYTOCHROME C2 (OXIDIZED)	BHATIA, FINZEL, KRAUT	11/83	SF
R3CC2SF	CYTOCHROME C2 (REDUCED)	BHATIA, FINZEL, KRAUT	11/83	SF
R2ANASF	DNA (A, GGGGCCCC, SYNTHETIC)	MCALL, BROWN, KENNARD	8/85	SF
R6BNASF	DNA (B, CGCGAATTCGG, SYNTHETIC) / NETROPSIN	M. KOPKA, R. DICKERSON	8/84	SF
R7BNASF	DNA (B, CGCGAATTCGG, ANISO TEMP FACTORS)	H. DREW, R. DICKERSON	11/85	SF
R7FYISF	FLAVODOXIN (D. VULGARIS, UNREFINED)	WATENPAUGH, SIEKER, JENSON/84	SF	
R1G1PSF	GLUTATHIONE PEROXIDASE (BOVINE)	O. EPP, R. LADENSTEIN	6/85	SF
R2HHSF	HEMOGLOBIN (HUMAN, DEOXY)	G. FERMI, M. PERUTZ	3/84	SF
R1HHSF	HEMOGLOBIN (HUMAN, OXY)	B. SHAANAN	3/84	SF
R1MCP5F	IGA FABI (KAPPA) / MCP603	G. COHEN ET AL.	7/84	SF
R2MCP5F	IGG PFC FRAGMENT	PAULAN, COHEN, DANIELS	10/84	SF
R1PFC5F	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	S. BRYANT ET AL.	4/85	SF
RL2ZTSF	MYOGLOBIN (SPERM WHALE, OXY)	HOSON, BRIAN, SIEKER, JENSON	4/85	SF
R1MBSF	MYOGLOBIN (SPERM WHALE, OXY)	S. PHILLIPS	3/84	SF
ROV0SF	OVOMUCOID THIRD DOMAIN (SILVER PHEASANT)	W. BODE, O. EPP	6/85	SF
R1P0SF	PAPAIN D	J. JANSONIUS	10/84	SF
R2PTISF	PROTEINASE II (RAT MAST CELL)	S. REMINGTON, B. MATTHEWS	9/84	SF
R2PTISF	PTI (X-RAY)	A. WLODAKER, R. HUBER	10/84	SF
R2PTISF	PTI (NEUTRON)	A. WLODAKER, R. HUBER	10/84	SF
R2RSASF	RIBONUCLEASE A (X-RAY)	A. WLODAKER	6/85	SF
R2RSASF	RIBONUCLEASE A (NEUTRON)	A. WLODAKER	6/85	SF
R2RSASF	RIBONUCLEASE A (PASTEURIANUM)	WATENPAUGH, SIEKER, JENSON/84	SF	
R2RSASF	VIRUS COAT PROTEIN (SBMV, T=1)	M. ROSSMANN	4/85	SF
R2RSASF	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M. ROSSMANN	4/85	SF

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TABLE 7. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 4, SEE ALSO TABLES 4,5,6)

IDENT CODE	MOLECULE	DEPOSITOR	20-JAN-86	
			DATE/	CODE
R2ICBSF	*CALCIUM-BINDING PROTEIN (INTESTINAL)	D. SZEKENYI, K. MOFFAT	12/85	SF
R2CCY5F	*CYTOCHROME C (PRIME)	F. FINZEL ET AL.	8/85	SF
R2CYP5F	*CYTOCHROME C PEROXIDASE (YEAST)	B. FINZEL, POULOS, KRAUT	8/85	SF
R1R5MF	*LYS 7-DNP-LYS 41 RIBONUCLEASE A	B. FINZEL ET AL.	8/85	SF

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 NEWSLETTER

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TABLE 8. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS
2APE	ACID PROTEIN INASE (ENDOTHIA PARASITICA)	T. BLUNDELL	9/81
2APP	ACID PROTEIN INASE (PENICILLIUM ANTHINELLUM)	SIELECKI, M. JAMES	1/83
1APR	ACID PROTEIN INASE (RHIZOPUS CHINENSIS)	D. DAVIES	8/79
2ACT	ACTININ	E. BAKER	1/79
1ACX	ACTINOXANTHIN	V. PLETNEV, A. KUZIN	12/82
1ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77
1AGA	AGAROSE	S. ARNOTT	5/78
2WGA	AGGLUTININ (WHEAT GERM)	C. WRIGHT	5/80
4ADH	ALCOHOL DEHYDROGENASE (APO)	C. -1. BRANDEN	8/79
5ADH	ALCOHOL DEHYDROGENASE (APO) /ADP-RIBOSE	H. EKUND, T. A. JONES	1/84
6ADH	ALCOHOL DEHYDROGENASE (BOJO) /NADH/DMSO	H. EKUND	1/84
7ADH	ALCOHOL DEHYDROGENASE (ISONICOTINIMIDYLATED)	B. PLAPP, H. EKUND	1/84
2ALP	ALPHA-LYTIC PROTEASE	M. FUJINAGA, M. JAMES	3/85 R
2TAA	TAKA-AMYLASE	KUSUNOKI, MATSUURA, KAKUDO	10/82
5AP1	ALPHA 1-ANTI TRYP SIN (MODIFIED, TETRAGONAL)	R. HUBER ET AL.	10/84
5AP1	ALPHA 1-ANTI TRYP SIN (MODIFIED, HEXAGONAL)	R. HUBER ET AL.	10/84
1ABP	L-ARABINOSIDE-BINDING PROTEIN	F. QUIJOCHO, G. GILLILAND	5/80
1AAT	CYTOSOLIC ASPARTATE AMINOTRANSFERASE	HARUTYUNYAN, MALASHKEVICH	4/82 A
2ATC	ASPARTATE CARBAMOYL TRANSFERASE	W. L. IPSOMB	3/82
4ATC	ASPARTATE CARBAMOYL TRANSFERASE	W. L. IPSOMB	4/84
5ATC	ASPARTATE CARBAMOYL TRANSFERASE /CTP	W. L. IPSOMB	4/84 R
1AZA	AZURIN (PSEUDOMONAS AERUGINOSA)	E. BAKER, G. NORRIS	5/84
1AZU	AZURIN (PSEUDOMONAS AERUGINOSA)	E. ADMAN, L. SIEKER, L. JENSEN	4/82 A
29CL	BACTERIOGLOBULOPHYLL A-PROTEIN	B. MATTHEWS	7/79
1ABX	ALPHA-BUNGAROTOXIN	D. AGARD, S. SPENCER, R. STROUD	4/80 A
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
21CB	"CALCIUM-BINDING PROTEIN (INTESTINAL)	D. SZEZENYI, K. MOFFAT	1/85 R
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S. ARNOTT	5/78
2CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	10/83
1CAG	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76
3CPA	CARBOXYPEPTIDASE A /GLUTAMYLTYROSINE	D. REES, W. L. IPSOMB	3/82
4CPA	CARBOXYPEPTIDASE A /POTATO INHIBITOR	D. REES, W. L. IPSOMB	3/82
5CPA	CARBOXYPEPTIDASE A /WATER (BOVINE)	D. REES, W. L. IPSOMB	5/82
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOT	6/76
1PTC	AD-ALPHAL-CARBOXYPEPTIDASE-TRANSEPTIDASE	J. KELLY, J. KNOX, P. MOEKS	10/85 A
1CAR	CARRAGEENAN	S. ARNOTT	5/78
7CAT	CATALASE (BEEF LIVER)	F. FITA, M. ROSSMANN	11/84 R
8CAT	CATALASE (BEEF LIVER)	F. FITA, M. ROSSMANN	11/84 R
4CAT	CATALASE (PENICILLIUM VITALE)	B. VAINSHTEIN ET AL.	2/83 B
1CHN	CHONDRITIN-4-SULFATE	S. ARNOTT	5/78
2CHS	CHONDRITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/84
4CHA	ALPHA-CHYMOTRYPSIN (BOVINE)	H. TSUKADA, D. BLOW	1/84
5CHA	ALPHA-CHYMOTRYPSIN (BOVINE)	R. BLEVINS, A. TULINSKY	1/85 R
2CGH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	5/80
1CHG	CHYMOTRYPSIN	J. KRAUT, J. BIRKTOFT	3/75
1CTS	CITRATE SYNTHASE (PIG)	REMINGTON, WIEGAND, HUBER	1/84
2CTS	CITRATE SYNTHASE (PIG, COA, CITRATE CMPLEX)	REMINGTON, WIEGAND, HUBER	1/84
3CTS	CITRATE SYNTHASE (CHICKEN, COA, CITRATE)	REMINGTON, WIEGAND, HUBER	1/84
4CTS	CITRATE SYNTHASE (PIG, OXALOACETATE CMPLEX)	REMINGTON, WIEGAND, HUBER	1/84
1CTA	ALPHA COBRATOXIN	W. SAENGER, M. WALKINGSHAW	3/82
2CNA	CONCAVANALIN A	G. REEKE, J. BECKER, G. EDELMAN	4/76
3CNA	CONCAVANALIN A	K. HARDMAN	9/76
1CN1	CONCAVANALIN A (DEMETALLIZED)	M. SHOHAM	12/81
1CRN	CRABIN	W. HENDRICKSON, M. TEETER	5/81
1OCR	GAMMA-I1 CRYSTALLIN (CALF)	T. BLUNDELL	8/85
25CC	CYTOCHROME B5 (OXIDIZED)	S. MATTHEWS	12/77
156B	CYTOCHROME B562 (E. COLI, OXIDIZED)	B. THIE, C. ZERWINSKI, MATTHEWS	6/79
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80
10CY	CYTOCHROME C (BONI TO, HEART)	M. KAKUDO	6/76
10CR	CYTOCHROME C (RIBONUCLEIC ACID)	H. OCHI, N. TANAKA	3/83
20CY	CYTOCHROME C (PRIME)	F. FINZEL ET AL.	8/85 R
20CY*	CYTOCHROME C PEROXIDASE (YEAST)	B. FINZEL, T. POULOS, J. KRAUT	3/85 R
20C2	CYTOCHROME C2 (OXIDIZED)	G. BHATIA, B. FINZEL, J. KRAUT	11/83
30C2	CYTOCHROME C2 (REDUCED)	G. BHATIA, B. FINZEL, J. KRAUT	11/83
10Y3	CYTOCHROME C3 (REDUCED)	R. HASER, M. FREY, F. PAYAN	6/85
20CV	CYTOCHROME C3 (DESOXYFOLIVIOBIL VULGARIS)	N. YASUOKA, M. KAKUDO	11/83
10C5	CYTOCHROME C5 (OXIDIZED, AZOTOBACTER VULG)	D. STOUT, D. CARTER	6/84
155C	CYTOCHROME C550	R. TIMKOVICH	8/76
351C	CYTOCHROME C551 (OXIDIZED)	MATSUURA, TAKANO, DICKERSON	7/81
1541C	CYTOCHROME C551 (REDUCED)	MATSUURA, TAKANO, DICKERSON	7/81
10CP	CYTOCHROME P450 (CAN, PSEUDOMONAS PUTIDA)	T. SCUDLOR ET AL.	11/85
30FR	DIPHOLYOLATE REDUCTASE (L. CASEI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82
40FR	DIPHOLYOLATE REDUCTASE (E. COLI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82
1ANA	DNA (A, S-PRIME) - D-10DD-CGG-3(PRIME)1	M. MCCALL, T. BROWN, O. KENNARD	8/85
2ANA	DNA (A, CCGCAATCCG, SYNTHETIC, 18 DEG K)	H. DREW, R. DICKERSON	11/81
18NA	DNA (B, CCGCAATCCG, SYNTHETIC, 18 DEG K)	H. DREW, R. DICKERSON	11/81
28NA	DNA (B, 9-BR-CGGCAATCCG, SYNTH, 20 DEG C)	KOPKA, FRATINI, DICKERSON	2/82
48NA	DNA (B, 9-BR-CGGCAATCCG, SYNTH, 7 DEG C)	KOPKA, FRATINI, DICKERSON	2/82
68NA	DNA (B, CCGCAATCCG, SYNTHETIC) / CISPLATIN	WING, PUJRA, DREW, DICKERSON	8/83
78NA	DNA (B, CCGCAATCCG, ANISO TEMP FACTORS)	KOPKA, R. DICKERSON	8/84
12NA	DNA (Z', CCGG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81
20N5	*GENE-5 DNA BINDING PROTEIN	G. BRAYER, A. MCPHERSON	1/86 R
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76
2EBK	*ERABUTOXIN (SEA SNAKE)	B. BLOW	9/85
1ECD	ERYTHROCUORIN (REDUCED, DEOXY)	W. STEIGEMANN, E. WEBER	3/79
1ECO	ERYTHROCUORIN (CARBONMONOXO)	W. STEIGEMANN, E. WEBER	3/79
1ECA	ERYTHROCUORIN (AQUO, MET)	W. STEIGEMANN, E. WEBER	3/79
1ECN	ERYTHROCUORIN (CYANO, MET)	W. STEIGEMANN, E. WEBER	3/79
2FD1	FERREDOXIN (AZOTOBACTER VINELANDII)	STOUT, GHOSH, FUREY, O'DONNELL	11/81
1FDX	FERREDOXIN (PHTOCOCUS AEROGENES)	E. ADMAN, L. SIEKER, L. JENSEN	8/76
3FXC	FERREDOXIN (SPIRULINA PLATENSIS)	TSUKIHARA, KATSUKE, KAKUDO	12/77
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M. LUDNIG	12/81
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LUDNIG	12/77
1FX1	FLAVODOXIN (VULGARIS, UNREFINED)	WATENPAUGH, SIEKER, JENSEN	10/84
168P	GALACTOSE-BINDING PROTEIN	S. MOWBRAY, G. PETSKO	8/83 A
16CN	GLUCAGON	T. BLUNDELL	10/77
1PG1	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77
1PG1	GLUTATHIONE PEROXIDASE (BOVINE)	O. EPP, R. LADENSTEIN	6/85
20RS	GLUTATHIONE REDUCTASE (HUMAN)	G. SCHULZ	11/81
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	7/75
2GPD	ALP-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79
3GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (HUMAN)	H. WATSON, J. CAMPBELL	6/83
1HRB	HEMERYTHRIN B	W. HENDRICKSON	6/76 A
1HRJ	HEMERYTHRIN (MET)	STENKAMP, SIEKER, JENSEN	2/83
1HRZ	HEMERYTHRIN (AZIDO, MET)	STENKAMP, SIEKER, JENSEN	2/83
1HR3	HEMERYTHRIN (AZIDO, MET, SIPHONOSOMA)	SMITH, HENDRICKSON, ADDISON	5/83
1HDS	HEMOGLOBIN (DEER, SICKLE CELL)	E. AMMA, G. GIRLINGS	10/79
2PHB	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, HEIDNER, PERUTZ	2/77
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73
3PHB	HEMOGLOBIN (HUMAN, DEOXY, SYMMETRY AVROD)	G. FERMI, M. PERUTZ	3/84 R
4PHB	HEMOGLOBIN (HUMAN, DEOXY, UNRESTRAINED)	G. FERMI, M. PERUTZ	3/84 R
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXO)	M. PERUTZ	3/84 R
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXO, NRG REFNO)	J. BALDWIN	8/79
1H40	HEMOGLOBIN (HUMAN, OXY)	B. SHAANAN	8/79
1FDH	HEMOGLOBIN (HUMAN, DEOXY)	J. FRIE	6/83
1H8S	HEMOGLOBIN S (HUMAN, SICKLE CELL)	E. PADLAN, W. LOVE	8/76
2LHB	HEMOGLOBIN (CYANO, MET, SEA LAMPREY)	HONZATKO, HENDRICKSON, LOVE	9/85 R
2LHX	HEXOKINASE (YEAST) FORM B111	STEITZ, ANDERSON, STENKAMP	3/82
1HKG	HEXOKINASE (E. COLI, GLUCOSE COMPLEX (YEAST))	W. BENNETT JR., T. STEITZ	12/80
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
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78
1MCP	IGA FAB (KAPPA)MCP603		
2MCP	IGA FAB (KAPPA)MCP603/PHOSPHOCHOLINE		
1FB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL		
3FAB	IMMUNOGLOBULIN FAB, PRIME, NEW		
1PFC	IMMUNOGLOBULIN B-J FRAGMENT (V-DIMER) REI		
1REI	IMMUNOGLOBULIN B-J FRAGMENT (V-DIMER) REI		
2RHE	IMMUNOGLOBULIN B-J FRAGMENT (V-MER) RHE		
1FC1	IMMUNOGLOBULIN FC (HUMAN)		
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX		
1G6	IGG PFC		
11G2	IMMUNOGLOBULIN G1 (LAMBDA) KOL		
11NS	INSULIN (PORCINE, 2-ZINC)		
21NS	INSULIN (BOVINE, 2-ZINC) DES-PHE B1		
2PKA	KALLIKREIN A (PORCINE)		
2KAI	KALLIKREIN A (PORCINE) /PTI (BOVINE)		
1KGA	KDPG ALDOLASE		
1KES	KERATAN SULFATE		
4LDH	LACTATE DEHYDROGENASE (DOGFISH)		
3LDH	LACTATE DEHYDROGENASE /NAD/PYRUVATE (DOGF)		
5LDH	LACTATE DEHYDROGENASE /5-LAC/NAD (PIG)		
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)		
1LH1	LEGHEMOGLOBIN (ACETATE MET)		
2LH1	LEGHEMOGLOBIN (ACETATE MET)		
1LH2	LEGHEMOGLOBIN (AQUO MET)		
2LH2	LEGHEMOGLOBIN (AQUO MET)		
1LH3	LEGHEMOGLOBIN (AQUO MET)		
2LH3	LEGHEMOGLOBIN (CYANO MET)		
1LH4	LEGHEMOGLOBIN (DEOXY)		
2LH4	LEGHEMOGLOBIN (DEOXY)		
1LH5	LEGHEMOGLOBIN (FLUORO MET)		
2LH5	LEGHEMOGLOBIN (FLUORO MET)		
1LH6	LEGHEMOGLOBIN (NICOTINATE MET)		
2LH6	LEGHEMOGLOBIN (NICOTINATE MET)		
1LH7	LEGHEMOGLOBIN (FERRO) /NITROBENZENE		
2LH7	LEGHEMOGLOBIN (FERRO) /NITROBENZENE		
1LH8	LYSOZYME (BACTERIOPHAGE T4)		
1LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
2LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
3LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
4LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
5LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
6LH9	LYSOZYME (HEN EGG-WHITE, SET R52)		
7LH9	LYSOZYME (HEN EGG-WHITE, TRICLINIC)		
1LZ1	LYSOZYME (HEN EGG-WHITE, TRICLINIC)		
8LZ1	LYSOZYME (HEN EGG-WHITE, INACTIVATED)		
9LZ1	LYSOZYME (HEN, NAM-NAG-NAM SUBSTRATE ONLY, J. KELLY, M. JAMES)		
1LZ2	LYSOZYME (HEN, NAM-NAG-NAM SUBSTRATE ONLY, J. KELLY, M. JAMES)		
2LZ2	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)		
1LYM	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)		
1LZ1	LYSOZYME (HUMAN)		
1LZ2	LYSOZYME (TURKEY EGG-WHITE)		
2M8H	MALATE DEHYDROGENASE		
1MLT	MELITTIN		
2MT2	*CD, ZN METALLOTHIONEIN (ISOFORM I)		
1MBS	MYOGLOBIN (SEAL, MET)		
1MBN	MYOGLOBIN (SPERM WHALE, MET)		
2MBN	MYOGLOBIN (SPERM WHALE, MET)		
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)		
1MB0	MYOGLOBIN (SPERM WHALE, DEOXY)		
1MB1	MYOGLOBIN (SPERM WHALE, OXY)		
1MB5	MYOGLOBIN (SPERM WHALE, CO, NEUTRON)		
1MHR	MYOHEMERITRIN		
1MUR	MURICIN B (L. ATICAUDA SEMIFASCIATA)		
1NS3	SCORPION NEUROTOXIN (VARIANT 3)		
10V0	OVUMUCOID THIRD DOMAIN (JAPANESE QUIL)		
20V0	OVUMUCOID THIRD DOMAIN (SILVER PHEASANT)		
1PPT	AVIAN PANCREATIC POLYPEPTIDE		
2PAP	PAPAIN (NAIVE)		
1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)		
2PAD	PAPAIN (CYS DERIV OF CYS-25)		
3PAD	PAPAIN (OXIDIZED CYS-25)		
4PAD	PAPAIN (TOS-LYS, CYS-25)		
5PAD	PAPAIN (ZOOXY-GLY-PHE-GLY, CYS-25)		
6PAD	PAPAIN (ZOOXY-PHE-ALA, CYS-25)		
1PPD	PAPAIN D		
1PEP	PEPSIN (PORCINE)		
3PGK	PHOSPHOGLYCERATE KINASE (YEAST)		
2PHK	PHOSPHOGLYCERATE KINASE (HORSE)		
3PHK	PHOSPHOGLYCERATE KINASE (HORSE)		
1BP2	PHOSPHOLIPASE A2 (BOVINE)		
2BP2	PHOSPHOLIPASE A2 (BOVINE)		
3BP2	PHOSPHOLIPASE A2 (BOVINE) TRANSAMINATED		
1PAP	PHOSPHOLIPASE A2 (PORCINE)		
1PCY	PLASTOCYANIN (C24)		
2PCY	PLASTOCYANIN (POPLAR, APO)		
3PCY	*PLASTOCYANIN (HG2+ SUBSTITUTED)		
2PRE	PREALBUMIN (HUMAN, PLASMA)		
2SGA	PROTEININASE A (STREPTOMYCES GRISEUS)		
3PRF	PROTEININASE B (STREPTOMYCES GRISEUS) /OMTKY3		
3PR2	PROTEININASE II (RAT MAEL CELL)		
1PYF	INORGANIC PYROPHOSPHATASE		
1PYK	PYRUVATE KINASE (CAT)		
1RHD	RIBONUCLEASE		
1R2S	RIBONUCLEASE A (X-RAY-NEUTRON)		
1RN3	RIBONUCLEASE A (X-RAY, OXIDIZED)		
1RSM	*LYS 7-DNP-LYS 4 RIBONUCLEASE A		
1RNS	RIBONUCLEASE H		
4RXN	RUBREDOXIN (C. PASTEURIANUM, UNCONSTR REF)		

1T51	TYROSYL TRANSFER RNA SYNTHETASE	BHAT,BLOW,BRICK,NYBORG	7/82 A
1RHV	*RHINOVIRUS 14(HUMAN)	M.ROSSMANN	10/85 A
25TV	VIRUS (SATELLITE TOBACCO NECROSIS)	T.A.JONES,L.LILJAS	6/84
45BV	VIRUS COAT PROTEIN(SOUTHERN BEAN MOSAIC)	M.ROSSMANN	4/85 R
2T8V	VIRUS (TOMATO BUSHY STUNT)	S.HARRISON	6/84

TABLE 11. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

20-JAN-86

MODEL STRUCTURES

2ZNA	DNA(2-11,CGCGCG,SYNTHETIC,MODEL)	A.RICH	2/81
3ZIG	DNA(2-11,CGCGCG,SYNTHETIC,MODEL)	A.RICH	2/81
1DNX	DNA(ATCGGCTAAG...MODEL)	J.SUSSMAN,E.TRIFONOV	11/82
11GE	IMMUNOGLOBULIN E(FRAGMENT)MODEL	E.PADLAN,D.DAVIES	1/85
1GF1	INSULIN-LIKE GROWTH FACTOR I (MODEL)	BLUNDELL,BEDARKAR,HUMBEL	12/82
1GF2	INSULIN-LIKE GROWTH FACTOR II (MODEL)	BLUNDELL,BEDARKAR,HUMBEL	12/82
1MLP	MUREIN LIPOPROTEIN (MODEL)	A.MCLAHLAN	8/79
1RLX	RELAXIN(MODEL,CONFORMATION A,UNREFINED)	A.EVANS,A.NORTH	3/78
2RLX	RELAXIN(MODEL,CONFORMATION B,UNREFINED)	A.EVANS,A.NORTH	3/78
3RLX	RELAXIN(MODEL,CONFORMATION A,REFINED)	A.EVANS,A.NORTH	3/78
4RLX	RELAXIN(MODEL,CONFORMATION B,REFINED)	A.EVANS,A.NORTH	3/78
1TNC	TROPONIN (CA-BINDING COMPONENT,MODEL)	R.KRETSINGER,C.D.BARRY	6/80 A

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 NEWSLETTER

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
R	RECENT (1984-1985) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 9. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION

20-JAN-86

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS
NONE			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 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 9
SF	STRUCTURE FACTORS

TABLE 10. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES (NO COORDINATES)

20-JAN-86

0EAP	ACID PROTEINASE (ENDOTHA PARASITICA)
0AF1	APOFERRITIN (HORSE)
0MAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
0RNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)
0CLN	CALMODULIN(CHICKEN)
0CD1	CALOTROPIN D1 (CALOTROPIS GIGANTEA)
0ZGP	D-ALANYL-D-ALANINE PEPTIDASE (Zn <sup>2+</sup> G PEPTIDASE)
0GCI	GAMMA-CHYMOTRYPSIN - INACTIVATOR COMPLEX
0CN2	CONCAVALIN A (DEMETALLIZED)
0CRO	CRO REPRESSOR
05C1	CYTOCHROME C555 (CHLOROBIDIUM THIOSULFATOPHILUM)
0C3A	DES-ARG77-C3A ANAPHYLATOXIN
0CCF	DIIHYDROGLUTATE REDUCTASE (CHICKEN LIVER)
0ANB	DNA(GGTATACC)
0ANB	DNA(GGUAUJACC)
0GTC	DNA (A,GGGCTCC,SYNTHETIC)
0DP1	DNA POLYMERASE I
0ESZ	ELASTASE COMPLEX (PIG)
0ETU	ELONGATION FACTOR TU COMPLEX (E. COLI)
0FX1	FERRDOXIN I (APHANOTHECE SACRUM)
0FX3	FLAVODOXIN(OXIDIZED,ANACYSTIS NIDULANS)
0FX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
0GSP	D-GALACTOSE-BINDING PROTEIN(ESCHERICHIA COLI)
0GAP	CATABOLITE GENE ACTIVATOR PROTEIN
0GD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
0HM6	HEMAGGLUTININ
0HP1	HEMOCYANIN(PANULIRUS INTERRUPTUS)
0DCH	HEMOGLOBIN (COBALT,DEOXY)
0HB3	HEMOGLOBIN (GLYCERA DIBRANCHIATA)
0PH4	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLOUESCENS)
0AUI	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU
0ROY	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY
01G1	IMMUNOGLOBULIN G1 (KAPPA) DOB
01N4	INSULIN (HUMAN)
01N1	INSULIN (PORCINE)
01N2	INSULIN (PORCINE)
01N3	DESPENTAPEPTIDE INSULIN(BEEF)
0LRP	N-TERMINAL DOMAIN OF LAMBDA REPRESSOR
0GLH	LYSOZYME (EMBON GOOSE)
0LZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)
0LZT	LYSOZYME (HEN EGG-WHITE,HIGH-TEMPERATURE)
0LZ6	LYSOZYME (STREPTOMYCES ERYTHRAEUS)
0TEL	LYSOZYME (TORTOISE EGG-WHITE)
0CTF	L7/L12 (E. COLI, C-TERMINUS)
0B2M	BETA2-MICROGLOBULIN
0MBA	MYOGLOBIN (APLYSIA LIMACINA)
0M81	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
0M83	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)
0PFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)
0PR2	PHOSPHORASE A2 (RATTLESNAKE)
0PPA	PHOSPHORYLASE A (RABBIT)
0PBI	PHOSPHORYLASE B (RABBIT)
05GC	COMPLEX (PROTEINASE A - CHYMOSTATIN)
0RX5	RELAXIN (PORCINE, MODEL)
0R5A	RIBONUCLEASE A (BOVINE)
0R5B	RIBONUCLEASE (BOVINE SEMINAL)
0RBI	RIBONUCLEASE BI(BINASE)
0RST	RIBONUCLEASE ST (STREPTOMYCES ERYTHREUS)
0RNT	RIBONUCLEASE T1-2(PRIME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)
05SP	SULFATE-BINDING PROTEIN
0SDP	FE-SUPEROXIDE DISMUTASE (ESCHERICHIA COLI)
0SDP	FE-SUPEROXIDE DISMUTASE (PSEUDOMONAS OVALIS)
0TH1	THAUMATIN
0TT4	THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)
0FMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)
0TA1	TRANSFER RNA (YEAST, ASP, A FORM)
0TRI	TRANSFER RNA (YEAST, PHE)
0MT5	METHIONYL TRANSFER RNA SYNTHETASE
0YPI	TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)
0UBQ	UBIQUITIN(HUMAN)
0UT3	UTEROGLOBIN (RABBIT)
0TMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)

\* NEW OR REPLACEMENT ENTRY SINCE OCT-85 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 COORDINATE 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 'IMBN' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN, 'IMBNB' 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,3SBVB  
\*INSERT,3SBVA.6  
REMARK 7  
REMARK 7 THIS ENTRY IS OBSOLETE. 17-JUL-85.  
\*INSERT,3SBV.3  
OBSLTE 17-JUL-85 3SBV 4SBV  
\*INSERT,3SBV.6  
REVDAT 3 17-JUL-85 3SBVB 3 OBSLTE  
\*DELETE,3SBVA.7  
MASTER 146 0 3 0 0 0 0 6 4723 3 0 63

\*IDENT,1ALPC  
\*INSERT,1ALPB.5  
REMARK 8  
REMARK 8 CORRECTION. THIS ENTRY IS OBSOLETE. 17-JUL-85.  
\*INSERT,1ALP.3  
OBSLTE 17-JUL-85 1ALP 2ALP  
\*INSERT,1ALP.9  
REVDAT 4 17-JUL-85 1ALPC 3 OBSLTE  
\*DELETE,1ALPB.6  
MASTER 43 0 0 0 0 0 0 6 1391 1 6 16

\*IDENT,4RSAD  
\*INSERT,4RSA.5  
REMARK 11  
REMARK 11 CORRECTION. THIS ENTRY IS OBSOLETE. 17-JUL-85.  
\*INSERT,4RSA.3  
OBSLTE 17-JUL-85 4RSA 5RSA  
\*INSERT,4RSA.6  
REVDAT 5 17-JUL-85 4RSAD 3 OBSLTE  
\*DELETE,4RSA.6  
MASTER 90 2 2 3 14 0 3 6 2249 1 13 10

\*IDENT,1MT2A  
\*INSERT,1MT2.46  
REMARK 7  
REMARK 7 CORRECTION. THIS ENTRY IS OBSOLETE. 14-NOV-85.  
\*INSERT,1MT2.7  
REVDAT 2 14-NOV-85 1MT2A 3 OBSLTE  
\*INSERT,1MT2.3  
OBSLTE 14-NOV-85 1MT2 2MT2  
\*DELETE,1MT2.514  
MASTER 40 2 2 0 0 0 0 7 6 414 1 27 5

\*IDENT,2YHXF  
\*INSERT,2YHXE.9  
REMARK 13  
REMARK 13 CORRECTION. REPLACE ALL OCCURRENCES OF RESIDUES GAM, DEL,  
REMARK 13 EPS WITH UNK. 15-JAN-86.  
\*INSERT,2YHX.7  
REVDAT 7 15-JAN-86 2YHXF 3 REMARK SEQRES FTNOTE HET  
FORMUL ATOM HETATH  
\*DELETE,2YHX.93,97  
REMARK 5 RESIDUES OF UNCERTAIN IDENTITY FOR WHICH ATOMS IN THE SIDE  
REMARK 5 CHAIN WERE LOCATED UP TO THE GAMMA, DELTA, AND EPSILON  
REMARK 5 POSITIONS WERE ORIGINALLY DESIGNATED GAM, DEL AND EPS,  
REMARK 5 RESPECTIVELY. BY THE DEPOSITOR. IN THIS ENTRY THESE  
REMARK 5 RESIDUES ALL HAVE BEEN RENAMED UNK AND FLAGGED BY  
REMARK 5 APPROPRIATE FOOTNOTES.

\*IDENT,1PYPD  
\*INSERT,1PYPC.15  
REMARK 13  
REMARK 13 CORRECTION. REVISE ALL ATOMIC COORDINATES. IT WAS FOUND  
REMARK 13 THAT THE COORDINATES IN THIS ENTRY WERE NOT IN AN  
REMARK 13 ORTHOGONAL FRAME, CONTRARY TO PROTEIN DATA BANK  
REMARK 13 SPECIFICATIONS. REPLACE ORIGX, SCALE, AND MTRIX  
REMARK 13 TRANSFORMATIONS. 15-JAN-86.  
\*INSERT,1PYP.6  
REVDAT 5 15-JAN-86 1PYPD 3 ORIGX SCALE MTRIX ATOM  
\*DELETE,1PYP.174,1PYPA.60  
ORIGX1 1.000000 .168958 0.000000 0.00000  
ORIGX2 0.000000 1.014173 0.000000 0.00000  
ORIGX3 0.000000 0.000000 1.000000 0.00000  
SCALE1 0.019146 .003235 0.000000 0.00000  
SCALE2 0.000000 .014428 0.000000 0.00000  
SCALE3 0.000000 0.000000 .010474 0.00000  
MTRIX1 1 -.956279 -.209069 60.39569  
MTRIX2 1 -.156818 -.233943 .943029 92.63294  
MTRIX3 1 -.209064 .943029 258821 -59.36417  
\*DELETE,1PYP.180,2415  
ATOM 1 N THR 1 19.390 30.869 -12.049 1.00 0.00  
ATOM 2 CA THR 1 18.725 30.216 -13.185 1.00 0.00  
ATOM 3 C THR 1 19.773 29.573 -14.036 1.00 0.00  
ATOM 4 O THR 1 19.638 28.409 -14.501 1.00 0.00  
ATOM 5 CB THR 1 17.889 31.291 -13.906 1.00 0.00

ATOM 2232 CD2 PHE 280 21.786 70.916 -13.301 1.00 0.00  
ATOM 2233 CE1 PHE 280 22.802 69.559 -15.490 1.00 0.00  
ATOM 2234 CE2 PHE 280 23.195 70.706 -13.492 1.00 0.00  
ATOM 2235 CZ PHE 280 23.665 70.015 -14.548 1.00 0.00  
ATOM 2236 N ILE 281 16.798 68.951 -12.426 1.00 0.00  
\*DELETE,1PYPC.15  
MASTER 136 0 0 4 19 22 0 9 2236 0 0 22

ORDER 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 (August 1985)
  - Sources of Visual Aids for Macromolecular Structure (October 1985)
  - Atomic Coordinate and Bibliographic Entry Format Description for DATAPRTP and DATAPRFI (January 1985)
  - Current DATAPRTP Directory
  - Non-Standard Entries (Structure Factors) Format Description
    - NONST1TP and NONST1FI (April 1985)
    - NONST2TP and NONST2FI (January 1986)
    - NONST3TP and NONST3FI (January 1986)
    - NONST4TP and NONST4FI (January 1986)
  - Data Deposition form

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

DATAPRTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$260(200)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$260(200)
	<input type="checkbox"/> 800 cpi, ASCII, \$300(231)	<input type="checkbox"/> 800 cpi, EBCDIC, \$300(231)
YEAR85TP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)
PDBPGMTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	This product is available only in VAX/VMS ANSI labelled magnetic tape format based on Level 3 of the ANSI Standard.
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	
NONST1TP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$260(200)	<input type="checkbox"/> 800 cpi, EBCDIC, \$260(200)
NONST2TP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$260(200)	<input type="checkbox"/> 800 cpi, EBCDIC, \$260(200)
NONST3TP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$260(200)	<input type="checkbox"/> 800 cpi, EBCDIC, \$260(200)
NONST4TP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)
RENDERTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)
CONNECTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$260(200)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$260(200)
	<input type="checkbox"/> 800 cpi, ASCII, \$300(231)	<input type="checkbox"/> 800 cpi, EBCDIC, \$300(231)
DGPLOTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)
DIHDLTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$260(200)	<input type="checkbox"/> 800 cpi, EBCDIC, \$260(200)
DSTNCETP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$260(200)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$260(200)
	<input type="checkbox"/> 800 cpi, ASCII, \$300(231)	<input type="checkbox"/> 800 cpi, EBCDIC, \$300(231)
FISIPLTP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)
PHIPSITP	<input type="checkbox"/> 6250 cpi, ASCII, \$220(169)	<input type="checkbox"/> 6250 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 1600 cpi, ASCII, \$220(169)	<input type="checkbox"/> 1600 cpi, EBCDIC, \$220(169)
	<input type="checkbox"/> 800 cpi, ASCII, \$220(169)	<input type="checkbox"/> 800 cpi, EBCDIC, \$220(169)

Special Instructions (to be completed for Brookhaven requests only).

( ) We are especially interested in the pending entries with the following Ident Codes: \_\_\_\_\_ . Please delay shipment until the date \_\_\_\_\_ if any of these entries are expected to be available by that date.

( ) Normal order-will be processed as soon as possible.

4. Please send the following microfiche items (from Table 2). Each microfiche item costs \$182 (£140), postage included. Correction fiche are free.

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

5. Please send the following printed listings. Each listing costs \$74 (£57), postage included.

Ident Code(s) (From Table 7): \_\_\_\_\_ Total Cost: \_\_\_\_\_

6. Foreign air mail postage for tapes from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the U. K. A postage surcharge of \$16 (£17) is required per item.

Number of items x \$16.00 (£17) = \_\_\_\_\_

7. Total charges

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

Microfiche charges (4 above) \_\_\_\_\_

Printed listing charges (5 above) \_\_\_\_\_

Foreign air mail postage charges (6 above) \_\_\_\_\_

Total \_\_\_\_\_

**Method of Payment:**

Cambridge: Cambridge prefers that no check is sent with order. Inclusion of purchase order is desirable but not mandatory.

Brookhaven: Brookhaven requires that either a check or written purchase order payable to Brookhaven National Laboratory be received before service is provided.

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

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**Please return to**

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

or

Dr. G. Weber  
University Chemical Laboratory  
Lensfield Road  
Cambridge CB2 1EW, England

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