Number 29 THE PROTEIN DATA BANK NEWSLETTER July 1984

In our previous Newsletter (Number 28), many of you may have noticed the appearance of a new Table, listing atomic coordinate and structure factor entries that are in preparation. This separate listing should serve as an alert on new data sets that are expected to be available soon. Also, the other tables now list only items that actually are available.

At the IUCr Hamburg Congress in August, Thomas Koetzle looks forward to talking with Protein Data Bank users and depositors. The Data Bank will have a display in the commercial exhibition area. The Hamburg Congress should provide an excellent opportunity for producers and users of the various crystallographic data bases to discuss mutual concerns.

We would like to remind depositors that careful and complete preparation of our deposition form helps tremendously in our data entry processing. In addition, we appreciate receiving copies of all papers relevant to the structure, especially preprints and those published in books and the less readily available journals. With the large number of data sets we now receive, such assistance from our depositors is essential and greatly appreciated.

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.

Area	Address of Center	Name	
The Americas	Protein Data Bank Chemistry Department Brookhaven National Laboratory Upton, New York 11973, USA	E. E. Abola F. C. Bernstein T. F. Koetzle	516-282-4383 516-282-4382 516-282-4384
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard S. Bellard	0223-66499
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002, Australia	C. Garrow	03-418-7333
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, Osaka 565, Japan	N. Yasuoka	(06) 877-5111 ext. 3912

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

23-JUL-84

CODE	ITEM	NO.TAPES 800	1600	6250	AVAILABILITY US	UK	JA	AUS
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 7, 9)	2	2	1	X	X	X	X
YEAR83TP	NEW OR REVISED COORDINATE ENTRIES FOR 1983	1	1	1	X			
PART84TP	NEW OR REVISED COORD ENTRIES 1984(TO DATE)	1	1	1	X			
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	2	1	1	X	X	X	
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	2	1	1	X	X	X	
NONST3TP	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	1	1	1	X	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	1	X			
BLDKITTP	MODEL BUILDER*S KIT	PLEASE INQUIRE AT US CENTER						
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	1	X			
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	1	X			
DIHDRLTP	COMPLETE TORSION ANGLES	2	1	1	X			
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	1	X			
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	1	X			
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	1	X			

* NEW OR REPLACEMENT ENTRY SINCE APR-84 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

23-JUL-84

CODE	ITEM	AVAILABILITY US	UK	JA	AUS
DATAPRFI	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 7, 9)	X	X	X	
YEAR83FI	NEW OR REVISED COORDINATE ENTRIES FOR 1983	X			
PART84FI	NEW OR REVISED COORD ENTRIES 1984(TO DATE)	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	
CORR14FI	LIST OF CORRECTIONS NO. 14 (JAN/84 - JUL/84)	X	X	X	X
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDKITFI	MODEL BUILDER*S KIT	PLEASE INQUIRE AT US CENTER			
CONECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHDRLFI	COMPLETE TORSION ANGLES	X			
DSTNCEFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FISIPLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X			

* NEW OR REPLACEMENT ENTRY SINCE APR-84 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, AVAILABLE PROGRAMS

23-JUL-84

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	4/82 YES
BLDKIT	MODEL BUILDER*S KIT	E.ABOLA	2/84 YES
CHIRAL	CHECK CHIRALITY	E.ABOLA	1/82 YES
CONECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	8/82 YES
CONTCT	INTERMOLECULAR CONTACTS	L.ANDREWS	5/83 NO
DGPLOT	DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	1/83 YES
DIHDRL	COMPLETE TORSION ANGLES	E.ABOLA	3/80 YES
DRCTRY	DIRECTORY OF PDB DISTRIBUTION TAPE	E.ABOLA	5/84 YES
DSSP	SECONDARY STRUCTURE,SOLVENT EXPOSURE	W.KABSCH,C.SANDER	12/83 NO
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	8/82 YES
FISIPL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79 YES
LSM	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82 NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPSI	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
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	11/79 YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEBIODA	1/82 NO
TORSRU	COMPLETE TORSION ANGLES	G.REEKE	10/79 NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	3/82 YES

* NEW OR REPLACEMENT ENTRY SINCE APR-84 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)

23-JUL-84

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R1ACTSF	ACTINIDIN	E.BAKER	7/77 SF
CHYMOF	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 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*,CGCG,HIGH-SALT,SYNTHETIC)	H.DREW,R.DICKERSON	1/81 SF
R1BNASF	DNA(B,CGCGAATTCGCG,SYNTHETIC,290 DEG K)	H.DREW,R.DICKERSON	1/81 SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M.ROSSMANN	8/75 SF
R2GPDSF	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79 SF
R2MHBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER,HEIDNER,PERUTZ	6/80 SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	6/80 SF
RHUMDEH02	HEMOGLOBIN (HUMAN,DEOXY)	M.PERUTZ,G.FERMI	5/75 SF
LAMPRY1	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
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
RRUBY02	RUBREDOXIN	L.JENSEN	3/74 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)

23-JUL-84

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R1ICBSF	CALCIUM-BINDING PROTEIN(INTESTINAL)	D.SZEBENYI,K.MOFFAT	7/83 SF
R1CCRSF	CYTOCHROME C (RICE)	H.OCHI,N.TANAKA	3/83 SF
R351CSF	CYTOCHROME C551 (OXIDIZED)	T.TAKANO,R.DICKERSON	9/81 SF
R451CSF	CYTOCHROME C551 (REDUCED)	T.TAKANO,R.DICKERSON	9/81 SF
R1ANASF	DNA(A,D-IODO-CCGG)SPACE GROUP P 43 21 2	B.CONNER,R.DICKERSON	6/82 SF
R1ANAP2	DNA(A,D-IODO-CCGG)SPACE GROUP P 21	B.CONNER,R.DICKERSON	6/82 SF
R2BNASF	DNA(B,CGCGAATTCGCG,SYNTHETIC,16 DEG K)	H.DREW,R.DICKERSON	11/81 SF
R3BNASF	DNA(B,9-BR-CGCGAATTCGCG,20 DEG C)	KOPKA,FRATINI,DICKERSON	2/82 SF
R4BNASF	DNA(B,9-BR-CGCGAATTCGCG, 7 DEG C)	KOPKA,FRATINI,DICKERSON	2/82 SF
R5BNASF	DNA(B,CGCGAATTCGCG,SYNTHETIC)/CISPLATIN	WING,PJURA,DREW,DCKRSN	8/83 SF
R1GAASF	GLUTAMINASE-ASPARAGINASE(ACINETOBACTER)	H.AMMON	12/82 SF
R1GASSF	GLUTAMINASE-ASPARAGINASE(PSEUDOMONAS 7A)	H.AMMON	12/82 SF
R1HMOSF	HEMERYTHRIN(MET)	STENKAMP,SIEKER,JENSEN	2/83 SF
R1HMZSF	HEMERYTHRIN(AZIDO,MET)	STENKAMP,SIEKER,JENSEN	2/83 SF
R2INSSF	INSULIN(BOVINE,2-ZINC)DES-PHE B1	C.REYNOLDS,G.DODSON	5/82 SF
R1LH1SF	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH1SF	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH2SF	LEGHEMOGLOBIN(AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH2SF	LEGHEMOGLOBIN(AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH3SF	LEGHEMOGLOBIN(CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH3SF	LEGHEMOGLOBIN(CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH4SF	LEGHEMOGLOBIN(DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH4SF	LEGHEMOGLOBIN(DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH5SF	LEGHEMOGLOBIN(FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH5SF	LEGHEMOGLOBIN(FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH6SF	LEGHEMOGLOBIN(NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH6SF	LEGHEMOGLOBIN(NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LH7SF	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R2LH7SF	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82 SF
R1LYMSF	LYSOZYME(HEN EGG-WHITE,MONOCLINIC)	HOGLE,RAO,SUNDARALINGAM	7/82 SF
R1MLTSF	MELITTIN	TERWILLIGER,EISENBERG	8/81 SF
R1OVOSF	OVOMUCOID FRAGMENT	E.PAPAMOKOS,R.HUBER	1/82 SF
R2BP2SF	PROPHOSPHOLIPASE A2 (BOVINE)	DIJKSTRA,HOL,DRENTH	9/81 SF
R1PYPSF	INORGANIC PYROPHOSPHATASE	E.HARUTYUNYAN ET AL.	2/83 SF
R1RN3SF	RIBONUCLEASE A	BORKAKOTI,MOSS,PALMER	6/82 SF
R4RSASFX	RIBONUCLEASE A (XRAY)	A.WLODAWER	6/82 SF
R4RSASFN	RIBONUCLEASE A (NEUTRON)	A.WLODAWER	6/82 SF
R3TLNSF	THERMOLYSIN(NATIVE)	B.MATTHEWS,M.HOLMES	2/82 SF
R2PTNSF	TRYPSIN(ORTHORHOMBIC,2.4M (NH4)2SO4)	J.WALTER,R.HUBER	10/81 SF
R1TPOSF	TRYPSIN(ORTHORHOMBIC)	BODE,WALTER,HUBER	9/82 SF
R3PTNSF	TRYPSIN(TRIGONAL,2.4M (NH4)2SO4)	J.WALTER,R.HUBER	10/81 SF
R3PTBSF	TRYPSIN(BENZAMIDINE INHIBITED)	BODE,SCHWAGER,WALTER	9/82 SF
R1TPPSF	TRYPSIN/P-AMIDINO-PHENYL-PHYRUVATE	WALTER,BODE,HUBER	9/82 SF
R4PTISF	TRYPSIN INHIBITOR(BOVINE,PANCREAS)	R.HUBER,J.DEISENHOFER	9/82 SF
R2PTCSF	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R.HUBER,J.DEISENHOFER	9/82 SF
R1TPASF	TRYPSIN(ANHYDRO)/TRYPSIN INHIBITOR	HUBER,BODE,DEISENHOFER	9/82 SF
R2TGASF	TRYPSINOGEN(2.4M MGSO4)	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
R2TGPSF	TRYPSINOGEN/TRYPSIN INHIBITOR	R.HUBER ET AL.	9/82 SF
R3TPISF	TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	R.HUBER ET AL.	9/82 SF
R2TPISF	TRYPSINOGEN/PTI/ILE-VAL (MERCURATED)	J.WALTER,R.HUBER	10/81 SF
R1TGSSF	TRYPSINOGEN/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)

23-JUL-84

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R2GCHSF	*GAMMA-CHYMOTRYPSIN	COHEN,DAVIES,SILVERTON	7/84 SF
R1CYPSF	CYTOCHROME C PEROXIDASE(YEAST)	FINZEL,POULOS,KRAUT	11/83 SF
R2C2CSF	CYTOCHROME C2(OXIDIZED)	BHATIA,FINZEL,KRAUT	11/83 SF
R3C2CSF	CYTOCHROME C2(REDUCED)	BHATIA,FINZEL,KRAUT	11/83 SF
R2HHBSF	*HEMOGLOBIN (HUMAN,DEOXY)	G.FERMI,M.PERUTZ	3/84 SF
R1HHOSF	HEMOGLOBIN(HUMAN,OXY)	B.SHAANAN	3/84 SF
R1MBOSF	MYOGLOBIN(SPERM WHALE,OXY)	S.PHILLIPS	3/84 SF

* NEW OR REPLACEMENT ENTRY SINCE APR-84 NEWSLETTER

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SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

23-JUL-84

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/ STATUS
2APE	ACID PROTEINASE(ENDOTHIA PARASITICA)	T.BLUNDELL	9/81
2APP	ACID PROTEINASE(PENICILLIUMJANTHINELLUM)	A.SIELECKI,M.JAMES	1/83 R
1APR	ACID PROTEINASE(RHIZOPUS CHINENSIS)	D.DAVIES	8/79
2ACT	ACTINIDIN	E.BAKER	11/79
1ACX	ACTINOXANTHIN	V.PLETNEV,A.KUZIN	12/82
2ADK	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.-I.BRANDEN	8/79
5ADH	*ALCOHOL DEHYDROGENASE(APO)/ADP-RIBOSE	H.EKLUND,T.A.JONES	1/84
6ADH	*ALCOHOL DEHYDROGENASE(HOLO)/NADH/DMSO	H.EKLUND	1/84
7ADH	*ALCOHOL DEHYDRGNSE(ISONICOTINIMIDYLATED)	B.PLAPP,H.EKLUND	1/84
1ALP	ALPHA LYTIC PROTEASE	BRAYER,DELBAERE,JAMES	6/79
2TAA	TAKA-AMYLASE	KUSUNOKI,MATSUURA,KAKUDO	10/82
1ABP	L-ARABINOSE-BINDING PROTEIN	F.QUIOCHO,G.GILLILAND	5/80
1AAT	CYTOSOLIC ASPARTATE AMINOTRANSFERASE	HARUTYUNYAN,MALASHKEVICH	4/82 A
2ATC	ASPARTATE CARBAMOYLTRANSFERASE	W.LIPSCOMB	3/82
3ATC	ASPARTATE CARBAMOYLTRANSFERASE/CTP	W.LIPSCOMB	3/82 R
1AZA	*AZURIN(ALCALIGENES DENITRIFICANS)	E.BAKER,G.NORRIS	5/84
1AZU	AZURIN(PSEUDOMONAS AERUGINOSA)	E.ADMAN,L.SIEKER,L.JENSEN	8/80
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B.MATTHEWS	1/79 A
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
1ICB	CALCIUM-BINDING PROTEIN(INTESTINAL)	D.SZEBENYI,K.MOFFAT	7/83
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S.ARNOTT	5/78
2CAB	CARBONIC ANHYDRASE B (HUMAN)	K.KANNAN	10/83 R
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K.KANNAN	5/76
3CPA	CARBOXYPEPTIDASE A/GLYCYLTYROSINE	D.REES,W.LIPSCOMB	3/82 R
4CPA	CARBOXYPEPTIDASE A/POTATO INHIBITOR	D.REES,W.LIPSCOMB	3/82
5CPA	CARBOXYPEPTIDASE A/WATER (BOVINE)	D.REES,W.LIPSCOMB	5/82
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M.SCHMID,J.HERRIOTT	6/76 A
1CAR	CARRAGEENAN	S.ARNOTT	5/78
3CAT	CATALASE (BEEF LIVER)	M.ROSSMANN	7/82 R
4CAT	CATALASE(PENICILLIUM VITALE)	B.VAINSHTEIN ET AL.	2/83 B
1C4S	CHONDROITIN-4-SULFATE	S.ARNOTT	5/78
2C4S	CHONDROITIN-4-SULFATE (CA SALT)	S.ARNOTT	5/78
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D.BLOW	1/75
3CHA	ALPHA-CHYMOTRYPSIN	A.TULINSKY	8/76
2GCH	GAMMA-CHYMOTRYPSIN	COHEN,DAVIES,SILVERTON	5/80
1CHG	CHYMOTRYPSINOGEN	J.KRAUT,J.BIRKTOFT	3/75
1CTS	*CITRATE SYNTHASE(PIG)	REMINGTON,WIEGAND,HUBER	1/84
2CTS	*CITRATE SYNTHASE(PIG,COA,CITRATE CMPLX)	REMINGTON,WIEGAND,HUBER	1/84
3CTS	*CITRATE SYNTHASE(CHICKEN,COA,CITRATE)	REMINGTON,WIEGAND,HUBER	1/84
4CTS	*CITRATE SYNTHASE(PIG,OXALOACETATE CMPLX)	REMINGTON,WIEGAND,HUBER	1/84
1CTX	ALPHA COBRATOXIN	W.SAENGER,M.WALKINSHAW	3/82
2CNA	CONCANAVALIN A	G.REEKE,,J.BECKER,G.EDELMAN	4/75
3CNA	CONCANAVALIN A	K.HARDMAN	9/76
1CN1	CONCANAVALIN A (DEMETALLIZED)	M.SHOHAM	12/81
1CRN	CRAMBIN	W.HENDRICKSON,M.TEETER	5/81
2B5C	CYTOCHROME B5 (OXIDIZED)	F.S.MATHEWS	12/77
156B	CYTOCHROME B562 (E.COLI,OXIDIZED)	BETHGE,CZERWINSKI,MATHEWS	8/79
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	T.TAKANO,R.DICKERSON	7/80
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T.TAKANO,R.DICKERSON	7/80
1CYC	CYTOCHROME C (BONITO, HEART)	M.KAKUDO	8/76
1CCR	CYTOCHROME C (RICE)	H.OCHI,N.TANAKA	3/83
1CCY	CYTOCHROME C.PRIME	P.WEBER,R.SALEMME	8/81
1CYP	CYTOCHROME C PEROXIDASE(YEAST)	B.F.FINZEL,T.POULOS,J,KRAUT	11/83
2C2C	CYTOCHROME C2(OXIDIZED)	G.BHATIA,B.F.FINZEL,J,KRAUT	11/83 R
3C2C	CYTOCHROME C2(REDUCED)	G.BHATIA,B.F.FINZEL,J,KRAUT	11/83
2CDV	CYTOCHROME C3(DESULFOVIBRIO VULGARIS)	N.YASUOKA,M.KAKUDO	11/83 R
155C	CYTOCHROME C550	R.TIMKOVICH	8/76
351C	CYTOCHROME C551 (OXIDIZED)	MATSUURA,TAKANO,DICKERSON	7/81
451C	CYTOCHROME C551 (REDUCED)	MATSUURA,TAKANO,DICKERSON	7/81
3DFR	DIHYDROFOLATE REDUCTASE (L.CASEI)	J.BOLIN,D.MATTHEWS,J.KRAUT	6/82 R
4DFR	DIHYDROFOLATE REDUCTASE (E. COLI)	J.BOLIN,D.MATTHEWS,J.KRAUT	6/82 R
1ANA	DNA(A,5(PRIME)-D-IODO-CCGG-3(PRIME))	B.CONNER,R.DICKERSON	6/82
1BNA	DNA(B,CGCGAATTCGCG,SYNTHETIC,290 DEG K)	H.DREW,R.DICKERSON	1/81
2BNA	DNA(B,CGCGAATTCGCG,SYNTHETIC,16 DEG K)	H.DREW,R.DICKERSON	11/81
3BNA	DNA(B,9-BR-CGCGAATTCGCG,20 DEG C)	KOPKA,FRATINI,DICKERSON	2/82
4BNA	DNA(B,9-BR-CGCGAATTCGCG, 7 DEG C)	KOPKA,FRATINI,DICKERSON	2/82
5BNA	DNA(B,CGCGAATTCGCG,SYNTHETIC)/CISPLATIN	WING,PJURA,DREW,DICKERSON	8/83
1ZNA	DNA(Z',CGCG,HIGH-SALT,SYNTHETIC)	H.DREW,R.DICKERSON	1/81
1EST	ELASTASE (PORCINE, TOSYL)	H.WATSON	5/76
1ECD	ERYTHROCRUORIN (REDUCED, DEOXY)	W.STEIGEMANN,E.WEBER	3/79
1ECO	ERYTHROCRUORIN (CARBONMONOXY)	W.STEIGEMANN,E.WEBER	3/79
1ECA	ERYTHROCRUORIN (AQUO, MET)	W.STEIGEMANN,E.WEBER	3/79
1ECN	ERYTHROCRUORIN (CYANO, MET)	W.STEIGEMANN,E.WEBER	3/79
2FD1	FERREDOXIN (AZOTOBACTER VINELANDII)	STOUT,GHOSH,FUREY,ODONNELL	11/81
1FDX	FERREDOXIN (PEPTOCOCCUS AEROGENES)	E.ADMAN,L.SIEKER,L.JENSEN	8/76
3FXC	FERREDOXIN (SPIRULINA PLATENSIS)	TSUKIHARA,KATSUBE,KAKUDO	12/81
3FXN	FLAVODOXIN (CLOSTRIDIUM MP,OXIDIZED)	M.LUDWIG	12/77
4FXN	FLAVODOXIN (CLOSTRIDIUM MP,SEMIQUINONE)	M.LUDWIG	12/77
1GBP	GALACTOSE-BINDING PROTEIN	S.MOWBRAY,G.PETSKO	8/83 A
1GCN	GLUCAGON	T.BLUNDELL	10/77
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H.MUIRHEAD	7/77 A
2GRS	GLUTATHIONE REDUCTASE (HUMAN)	G.SCHULZ	11/81
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M.ROSSMANN	7/75
2GPD	APO-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
1HMQ	HEMERYTHRIN(MET)	STENKAMP,SIEKER,JENSEN	2/83 R
1HMZ	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,R.GIRLING	10/79
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	R.LADNER,HEIDNER,PERUTZ	2/77
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M.PERUTZ,G.FERMI	11/73
2HHB	*HEMOGLOBIN(HUMAN,DEOXY)	G.FERMI,M.PERUTZ	3/84 R
3HHB	*HEMOGLOBIN(HUMAN,DEOXY,SYMMETRY AVRGD)	G.FERMI,M.PERUTZ	3/84 R
4HHB	*HEMOGLOBIN(HUMAN,DEOXY,UNRESTRAINED)	G.FERMI,M.PERUTZ	3/84 R
1HCO	HEMOGLOBIN(HUMAN,CARBONMONOXY)	J.BALDWIN	8/79
2HCO	HEMOGLOBIN(HUMAN,CARBONMONOXY,NRG REFND)	J.BALDWIN	8/79
1HHO	HEMOGLOBIN (HUMAN, OXY)	B.SHAANAN	6/83
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	8/76
1HBS	HEMOGLOBIN S (HUMAN,SICKLE CELL)	E.PADLAN,W.LOVE	6/82
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	3/73
2YHX	HEXOKINASE (YEAST) FORM BIII	STEITZ,ANDERSON,STENKAMP	3/78
1HKG	HEXOKINASE A - 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
1FB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL	M.MARQUART,R.HUBER	5/83
3FAB	IMMUNOGLOBULIN FAB.PRIME. NEW	R.POLJAK	9/81
1MCG	IMMUNOGLOBULIN B-J INTACT MCG	SCHIFFER,EDMUNDSON ET AL.	5/78 A
1RE1	IMMUNOGLOBULIN B-J FRAGMENT(V-DIMER)REI	D.EPP,R.HUBER	3/76
2RHE	IMMUNOGLOBULIN B-J FRAGMENT(V-MNMER)RHE	FUREY,WANG,YOO,SAX	6/83 R
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J.DEISENHOFER	5/81
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J.DEISENHOFER	5/81
1IG2	IMMUNOGLOBULIN G1 (LAMBDA) KOL	M.MARQUART,R.HUBER	5/83
1INS	INSULIN(PORCINE,2-ZINC)	G.DODSON,D.HODGKIN	7/80
2INS	INSULIN(BOVINE,2-ZINC) DES-PHE B1	C.REYNOLDS,G.DODSON	5/82
2PKA	*KALLIKREIN A(PORCINE)	W.BODE,Z.CHEN	5/84
2KAI	*KALLIKREIN A(PORCINE)/PTI(BOVINE)	W.BODE,Z.CHEN	5/84
1KGA	KDPG ALDOLASE	A.TULINSKY	8/78 A
1KES	KERATAN SULFATE	S.ARNOTT	5/78
4LDH	LACTATE DEHYDROGENASE (DOGFISH)	W.EVENTOFF,M.ROSSMANN	4/77
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE(DOGF)	M.ROSSMANN	11/74
5LDH	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U.GRAU,M.ROSSMANN	10/80
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W.MUSICK,M.ROSSMANN	9/78
1LH1	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82 R
2LH1	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH2	LEGHEMOGLOBIN(AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
2LH2	LEGHEMOGLOBIN(AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH3	LEGHEMOGLOBIN(CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
2LH3	LEGHEMOGLOBIN(CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH4	LEGHEMOGLOBIN(DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82
2LH4	LEGHEMOGLOBIN(DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH5	LEGHEMOGLOBIN(FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
2LH5	LEGHEMOGLOBIN(FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH6	LEGHEMOGLOBIN(NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82
2LH6	LEGHEMOGLOBIN(NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82
1LH7	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82
2LH7	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82
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 RS16)	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
9LYZ	LYSOZYME(HEN,NAM-NAG-NAM SUBSTRATE ONLY)	J.KELLY,M.JAMES	12/79
1LZH	LYSOZYME (HEN EGG-WHITE,MONOCLINIC)	ARTYMIUK,BLAKE,RICE,WILSON	6/81 A
2LZH	LYSOZYME (HEN EGG-WHITE,ORTHORHOMBIC)	ARTYMIUK,BLAKE,RICE,WILSON	6/81 A
1LYM	LYSOZYME(HEN EGG-WHITE,MONOCLINIC)	HOGLE,RAO,SUNDARALINGAM	7/82
1LZ2	LYSOZYME (TURKEY EGG-WHITE)	R.BOTT,R.SARMA	9/81 A
2MDH	MALATE DEHYDROGENASE	J.BIRKTOFT,L.BANASZAK	3/83 R
1MLT	MELITTIN	TERWILLIGER,EISENBERG	8/81
1MBS	MYOGLOBIN (SEAL, MET)	H.SCOULOUDI	3/79
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
1MBD	MYOGLOBIN (SPERM WHALE, DEOXY)	S.PHILLIPS	8/81
1MBO	MYOGLOBIN (SPERM WHALE, OXY)	S.PHILLIPS	8/81
1MBS	MYOGLOBIN(SPERM WHALE,CO,NEUTRON)	HANSON,NORVELL,SCHOENBORN	11/82
1MHR	MYOHEMERYTHRIN	W.HENDRICKSON	6/76 A
1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)	D.TSERNOGLOU,G.PETSKO	8/80
1SN3	SCORPION NEUROTOXIN(VARIANT 3)	C.BUGG ET AL.	12/82
1OVO	OVOMUCOID THIRD DOMAIN(JAPANESE QUAIL)	E.PAPAMOKOS,R.HUBER	1/82
1PPT	AVIAN PANCREATIC POLYPEPTIDE	T.BLUNDELL	1/81
8PAP	PAPAIN (NATIVE)	J.DRENTH	11/76
1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J.DRENTH	11/76
2PAD	PAPAIN (CYS DERIV OF CYS-25)	J.DRENTH	11/76
3PAD	PAPAIN (OXIDIZED CYS-25)	J.DRENTH	11/76
4PAD	PAPAIN (TOS-LYS, CYS-25)	J.DRENTH	11/76
5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J.DRENTH	11/76
6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J.DRENTH	11/76
1PEP	PEPSIN (PORCINE)	N.ANDREEVA ET AL.	7/78 A
1PFC	PFC FRAGMENT OF AN IGG	L.M.AMZEL	10/81
3PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H.WATSON	7/82 R
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P.EVANS,C.BLAKE	9/76 B
3PGM	PHOSPHOGLYCERATE MUTASE	H.WATSON	4/82 R
1BP2	PHOSPHOLIPASE A2 (BOVINE)	B.DIJKSTRA,J.DRENTH	4/81
2BP2	PROPHOSPHOLIPASE A2 (BOVINE)	B.DIJKSTRA,W.HOL,J.DRENTH	6/81
3BP2	PHOSPHOLIPASE A2 (BOVINE) TRANSAMINATED	B.DIJKSTRA,J.DRENTH	6/83
1P2P	PHOSPHOLIPASE A2 (PORCINE)	B.DIJKSTRA ET AL.	6/83
1PCY	PLASTOCYANIN	J.GUSS,H.FREEMAN	8/80
2PCY	PLASTOCYANIN(POPLAR)	GARRETT,GUSS,FREEMAN	11/83
2PAB	PREALBUMIN (HUMAN, PLASMA)	S.OATLEY,C.BLAKE	9/77
2SGA	PROTEINASE A(STREPTOMYCES GRISEUS)	M.JAMES,A.SIELECKI	1/83 R
3SGB	PROTEINASE B(STREP. GRISEUS)/OMTKY3	A.SIELECKI ET AL.	1/83
1PYP	INORGANIC PYROPHOSPHATASE	E.HARUTYUNYAN ET AL.	2/83
1PYK	PYRUVATE KINASE (CAT)	H.MUIRHEAD	11/83 A
1RHD	RHODANESE	W.HOL	12/77
4RSA	RIBONUCLEASE A (XRAY+NEUTRON)	A.WLODAWER	6/82 R
1RN3	RIBONUCLEASE A	BORKAKOTI,MOSS,PALMER	10/81
1RNS	RIBONUCLEASE S	H.WYCKOFF,F.RICHARDS	4/73
2RXN	RUBREDOXIN(CLOSTRIDIUM PASTEURIANUM)	L.JENSEN	1/75
3RXN	RUBREDOXIN(DESULFOVIBRIO VULGARIS)	E.ADMAN,L.SIEKER,L.JENSEN	9/80
2SNS	STAPHYLOCOCCAL NUCLEASE	M.LEGG,F.A.COTTON,E.HAZEN	5/82 R
2SSI	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y.MITSUI ET AL.	4/80
1SBT	SUBTILISIN BPN.PRIME.	J.KRAUT	8/72
2SBT	SUBTILISIN NOVO	J.DRENTH	9/76
1SIC	SUBTILISIN BPN(PRIME)/SSI COMPLEX	Y.MITSUI ET AL.	4/84 A
2SOD	SUPEROXIDE DISMUTASE	J.RICHARDSON,D.RICHARDSON	3/80
3TLN	THERMOLYSIN(NATIVE)	B.MATTHEWS,M.HOLMES	2/82 R
4TLN	THERMOLYSIN(L-LEU-NHOH)	B.MATTHEWS,M.HOLMES	2/82
5TLN	THERMOLYSIN(HONH-BZMALONYL-A-G-NTROANLD)	B.MATTHEWS,M.HOLMES	2/82
7TLN	THERMOLYSIN(CH2CO(N-OH)LEUOCH3)	B.MATTHEWS,M.HOLMES	1/83 R
1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B.-O.SODERBERG	5/76 A
4TNA	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	4/78
6TNA	TRANSFER RNA (YEAST, PHE)	S.-H.KIM ET AL.	11/78
8TNA	TRANSFER RNA (YEAST, PHE)	M.SUNDARALINGAM	2/79
1TIM	TRIOSE PHOSPHATE ISOMERASE	I.WILSON,D.PHILLIPS	9/76
2PTN	TRYPSIN(ORTHORHOMBIC,2.4M (NH4)2SO4)	J.WALTER,R.HUBER,W.BODE	10/81
1TPO	TRYPSIN(ORTHORHOMBIC)	W.BODE,J.WALTER,R.HUBER	9/82
3PTN	TRYPSIN(TRIGONAL,2.4M (NH4)2SO4)	J.WALTER,R.HUBER,W.BODE	10/81
3PTB	TRYPSIN(BENZAMIDINE INHIBITED)	W.BODE,P.SCHWAGER,J.WALTER	9/82 R
1TPP	TRYPSIN/P-AMIDINO-PHENYL-PYRUVATE	J.WALTER,W.BODE,R.HUBER	9/82
3PTP	TRYPSIN (DIP INHIBITED)	J.CHAMBERS,R.STROUD	12/77
4PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R.HUBER,J.DEISENHOFER	9/82 R
2PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R.HUBER,J.DEISENHOFER	9/82 R
1TPA	TRYPSIN(ANHYDRO)/TRYPSIN INHIBITOR	HUBER,BODE,DEISENHOFER	9/82
1TGN	TRYPSINOGEN	A.KOSSIAKOFF,R.STROUD	9/79
2TGA	TRYPSINOGEN(2.4M MGSO4)	J.WALTER,R.HUBER,W.BODE	10/81
1TGC	TRYPSINOGEN(.5 CH3OH,.5 HOH)	J.WALTER,R.HUBER,W.BODE	10/81
1TGT	TRYPSINOGEN(173 DEG K,.7 CH3OH,.3 HOH)	J.WALTER,R.HUBER,W.BODE	10/81
2TGT	TRYPSINOGEN(103 DEG K,.7 CH3OH,.3 HOH)	J.WALTER,R.HUBER,W.BODE	10/81
1TGB	TRYPSINOGEN (WITH CA, FROM PEG)	BODE,FEHLHAMMER,HUBER	3/79
2TGP	TRYPSINOGEN/TRYPSIN INHIBITOR	R.HUBER ET AL.	9/82 R
3TPI	TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	R.HUBER ET AL.	9/82 R
2TPI	TRYPSINOGEN/PTI/ILE-VAL (MERCURATED)	J.WALTER,R.HUBER,W.BODE	10/81
1TGS	TRYPSINOGEN/PSTI	R.HUBER ET AL.	9/82
1TSI	TYROSYL TRANSFER RNA SYNTHETASE	BHAT,BLOW,BRICK,NYBORG	7/82 A
2STV	*VIRUS (SATELLITE TOBACCO NECROSIS)	T.A.JONES,L.LILJAS	6/84
2SBV	VIRUS COAT PROTEIN(SOUTHERN BEAN MOSAIC)	M.ROSSMANN	5/82 R
2TBV	*VIRUS (TOMATO BUSHY STUNT)	S.HARRISON	6/84

MODEL STRUCTURES

2ZNA	DNA(Z-I,CGCGCG,SYNTHETIC,MODEL)	A.RICH	2/81
3ZNA	DNA(Z-II,CGCGCG,SYNTHETIC,MODEL)	A.RICH	2/81
1DNN	DNA(ATCGGCTAAG...,MODEL)	J.SUSSMAN,E.TRIFONOV	11/82
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.MCLACHLAN	8/78
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 APR-84 NEWSLETTER

STATUS CODES

BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
R RECENT (1982-1984) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 8. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION

23-JUL-84

1AP1	*ALPHA 1-ANTITRYPSIN(MODIFIED,TETRAGONAL)	R.HUBER ET AL.	6/84	P
2AP1	*ALPHA 1-ANTITRYPSIN(MODIFIED,HEXAGONAL)	R.HUBER ET AL.	6/84	P
4ATC	*ASPARTATE CARBAMOYLTRANSFERASE	W.LIPSCOMB	4/84	P
5ATC	*ASPARTATE CARBAMOYLTRANSFERASE/CTP	W.LIPSCOMB	4/84	RP
1MCP	*IMMUNOGLOBULIN FAB (KAPPA) MCP603	SATOW,COHEN,PADLAN,DAVIES	7/84	P
R1MCPSF	*IMMUNOGLOBULIN FAB (KAPPA) MCP603	G.COHEN ET AL.	7/84	SF

* NEW OR REPLACEMENT ENTRY SINCE APR-84 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 3
SF	STRUCTURE FACTORS

TABLE 9. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

23-JUL-84

0EAP	ACID PROTEINASE (ENDOTHIA PARASITICA)
0ADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX
0AF1	APOFERRITIN (HORSE)
0MAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
0AZA	AZURIN(ALCALIGENES DENITRIFICANS)
0RNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)
0CD1	CALOTROPIN DI (CALOTROPIS GIGANTEA)
0PTE	D-ALANYL-CARBOXYPEPTIDASE-TRANSPEPTIDASE
0ZGP	D-ALANYL-D-ALANINE PEPTIDASE (ZN2+ G PEPTIDASE)
0CTS	CITRATE SYNTHASE (PIG)
0CN2	CONCANAVALIN A (DEMETALLIZED)
0CR0	CRO REPRESSOR
0GCR	GAMMA-CRYSTALLIN II (CALF)
0CY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)
05C1	CYTOCHROME C555 (CHLOROBIUM THIOSULFATOPHILUM)
0C3A	DES-ARG77-C3A ANAPHYLATOXIN
0CDF	DIHYDROFOLATE REDUCTASE (CHICKEN LIVER)
0AN8	DNA(GGTATACC)
0AN8	DNA(GG+UA+UACC)
0ESZ	ELASTASE COMPLEX (PIG)
0ETU	ELONGATION FACTOR TU COMPLEX (E. COLI)
0EBX	ERABUTOXIN B
0FX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)
0FX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
0GBP	D-GALACTOSE-BINDING PROTEIN(ESCHERICHIA COLI)
0GAP	CATABOLITE GENE ACTIVATOR PROTEIN
0GP1	GLUTATHIONE PEROXIDASE (BOVINE)
0GD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
0HMG	HEMAGGLUTININ
0DCH	HEMOGLOBIN (COBALT,DEOXY)
0HBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)
0PHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)
0AUI	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU
0ROY	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY
0MCP	IMMUNOGLOBULIN FAB (KAPPA) MCP603
0IG1	IMMUNOGLOBULIN G1 (KAPPA) DOB
0IN1	INSULIN (PORCINE)
0IN2	INSULIN (PORCINE)
0PKA	KALLIKREIN A(PORCINE)
0KAI	KALLIKREIN A/BOVINE PANCREATIC INHIBITOR
0LRP	N-TERMINAL DOMAIN OF LAMBDA REPRESSOR
0GLM	LYSOZYME(EMBDEN GOOSE)
0LZ1	LYSOZYME (HUMAN)
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)
0MBA	MYOGLOBIN (APLYSIA LIMACINA)
0MBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
0MB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)
0PFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)
0PP2	PHOSPHOLIPASE A2 (RATTLESNAKE)
0PPA	PHOSPHORYLASE A (RABBIT)
0PB1	PHOSPHORYLASE B (RABBIT)
0RX5	RELAXIN (PORCINE, MODEL)
0RSA	RIBONUCLEASE A (BOVINE)
0RST	RIBONUCLEASE ST (STREPTOMYCES ERYTHREUS)
0RNT	RIBONUCLEASE T1-2(PRIME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)
0SDE	FE-SUPEROXIDE DISMUTASE(ESCHERICHIA COLI)
0SDP	FE-SUPEROXIDE DISMUTASE(PSEUDOMONAS OVALIS)
0TT4	THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)
0FMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)
0TA1	TRANSFER RNA (YEAST, ASP, A FORM)
0TA2	TRANSFER RNA (YEAST, ASP, B FORM)
0TR1	TRANSFER RNA (YEAST, PHE)
0MTS	METHIONYL TRANSFER RNA SYNTHETASE
0YP1	TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)
0GN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)
0UTG	UTEROGLOBIN (RABBIT)
0STV	VIRUS (SATELLITE TOBACCO NECROSIS)
0TMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)
0TBV	VIRUS (TOMATO BUSHY STUNT)

* NEW OR REPLACEMENT ENTRY SINCE APR-84 NEWSLETTER

TABLE 10. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

23-JUL-84

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 '1MBNA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK '1MBN' FOR SPERM-WHALE MYOGLOBIN, '1MBNB' 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,1PYPA
*INSERT,1PYP.114
REMARK   8
REMARK   8 THE TRANSFORMATION PRESENTED ON THE.*MTRIX* RECORDS BELOW
REMARK   8 WILL YIELD COORDINATES FOR THE OTHER MOLECULE IN THE
REMARK   8 ASYMMETRIC UNIT WHEN APPLIED TO THE COORDINATES IN THIS
REMARK   8 ENTRY.
REMARK   9
REMARK   9 CORRECTION. REVISE SECONDARY STRUCTURE SPECIFICATIONS
REMARK   9  ACCORDING TO DEPOSITORS INSTRUCTIONS.  CORRECT SCALE
REMARK   9  TRANSFORMATION.  ADD MTRIX TRANSFORMATION AND REMARK 8
REMARK   9  TO EXPLAIN IT.  CORRECT REVDAT RECORD.  31-MAY-84.
*INSERT,1PYP.6
REVDAT   2   31-MAY-84 1PYPA   3       REVDAT REMARK HELIX  SHEET
REVDAT   2 2                   3       TURN   SCALE  MTRIX
*DELETE,1PYP.7
REVDAT   1   27-OCT-83 1PYP    0
*DELETE,1PYP.137,172
HELIX    1  H1 ASP    169  PHE    177  1
HELIX    2  H2 GLY    179  ILE    193  1
HELIX    3  H3 ASN    210  ALA    230  1
HELIX    4  H4 SER    253  ILE    260  1 FIRST 3 RSDS IN 3/10 CONFIG
SHEET    1   I 3 TYR     2  GLY      8  0
SHEET    2   I 3 LEU    13  ASP     22 -1
SHEET    3   I 3 GLY    23  PRO     25 -1
SHEET    1  II 4 LEU    65  GLN     70  0
SHEET    2  II 4 ASN    54  ILE     59 -1
SHEET    3  II 4 ARG    77  PRO     84 -1
SHEET    4  II 4 TRP   278  ILE    281  1
SHEET    1 III 4 GLY   148  VAL    154  0
SHEET    2 III 4 LEU   139  GLU    147 -1
SHEET    3 III 4 GLU   199  ALA    203 -1
SHEET    4 III 4 ALA   208  ASN    210  1
SHEET    1 BAR 6 ASN    41  ILE     49  0
SHEET    2 BAR 6 HIS    90  PRO     96 -1
SHEET    3 BAR 6 ASN   115  GLU    125 -1
SHEET    4 BAR 6 VAL   154  ASP    158  1
SHEET    5 BAR 6 GLN   132  LEU    139 -1
SHEET    6 BAR 6 ASN    41  ILE     49 -1
TURN     1  T1 ALA    28  ASP    31
TURN     2  T2 PRO    33  ALA    36
TURN     3  T3 ALA    36  GLU    39
TURN     4  T4 PRO    50  THR    53
TURN     5  T5 THR    53  ALA    55
TURN     6  T6 GLU    62  LEU    65
TURN     7  T7 PHE    95  THR    98
TURN     8  T8 HIS   106  THR   109
TURN     9  T9 THR   109  VAL   112
TURN    10 T10 TYR   129  GLN   132
TURN    11 T11 ASP   146  GLU   149
TURN    12 T12 ASP   158  ASP   161
TURN    13 T13 LEU   163  LYS   166
TURN    14 T14 ALA   164  LEU   167
TURN    15 T15 ILE   193  GLY   196
TURN    16 T16 PHE   204  GLU   207
TURN    17 T17 ALA   230  SER   233
TURN    18 T18 SER   234  LYS   237
TURN    19 T19 ASN   243  LEU   246
TURN    20 T20 LEU   246  THR   249
TURN    21 T21 THR   249  TYR   252
TURN    22 T22 ASP   272  ILE   275
*DELETE,1PYP.178
SCALE2      -.011176  -.003123  -.008575        1.14388
*INSERT,1PYP.179
MTRIX1   1 -1.000000  0.000000  0.000000        0.00000
MTRIX2   1  0.000000 -1.000000  0.000000        0.00000
MTRIX3   1  0.000000  0.000000  1.000000        0.00000
*DELETE,1PYP.2416
MASTER      117    0    0    4   17   22    0    9 2236    0    0   22

*IDENT,DRCTRY1
*DELETE,DRCTRY.6
C                              LAST REVISION.  5/84
*INSERT,DRCTRY.120
C
C     CORRECTION TO PROPERLY OPEN AND CLOSE *FOREIGN* TAPE FILES
C     31-MAY-84
*DELETE,DRCTRY.235
 1016 FORMAT('$ENTER A TAPE LABEL TO BE USED IN THE TITLE (8-CHAR.)-')
*INSERT,DRCTRY.237
      CALL OPEN(' ',1,IRTN)
*INSERT,DRCTRY.316
      CALL CLOSE(IRTN)
C
C     POSITION THE TAPE TO THE NEXT FILE
C
      CALL OPEN(' ',-1,IRTN)
*INSERT,DRCTRY.959
      CALL CLRBFS
      CALL CLRFLS
*INSERT,DRCTRY.1109
C
C     RESET I/O BUFFER STATUS
C
      ENTRY CLRBFS
      INPBFS=.FALSE.
      RETURN
*INSERT,DRCTRY.1128
      LOGICAL FLSTAT
      DATA FLSTAT/.FALSE./
*INSERT,DRCTRY.1140
C
      IF(FLSTAT) THEN
       WRITE(5,1030)
 1030  FORMAT('LAST FILE WAS NOT CLOSED')
       STOP
      ENDIF
*INSERT,DRCTRY.1146
      IF(FILNUM.GT.0) THEN
*INSERT,DRCTRY.1156
      ENDIF
      FLSTAT=.TRUE.

*IDENT,2CABA
*INSERT,2CAB.77
REMARK   7
REMARK   7 RESIDUE 74 IN THIS ENTRY IS IDENTIFIED AS GLN.  HOWEVER,
REMARK   7 CHEMICAL SEQUENCE AND RECENT DIFFRACTION STUDIES ON AN
REMARK   7 INHIBITOR COMPLEX INDICATE THAT IT SHOULD BE ASP.
REMARK   8
REMARK   8 CORRECTION. ADD REMARK 7 AND FTNOTE 5.  ADD FTNOTE NUMBER
REMARK   8  TO RESIDUE 74.  30-MAY-84.
*INSERT,2CAB.7
REVDAT   2   30-MAY-84 2CABA   3       REMARK FTNOTE ATOM
*INSERT,2CAB.106
FTNOTE   5
FTNOTE   5 SEE REMARK 7.
*DELETE,2CAB.692,700
ATOM    578  N   GLN    74      25.568   -.779 -21.834  1.00 24.93    5
ATOM    579  CA  GLN    74      24.576  -1.451 -20.948  1.00 24.77    5
ATOM    580  C   GLN    74      24.593   -.767 -19.562  1.00 22.33    5
ATOM    581  O   GLN    74      25.422    .114 -19.295  1.00 21.19    5
ATOM    582  CB  GLN    74      24.658  -2.955 -20.908  1.00 26.49    5
ATOM    583  CG  GLN    74      23.237  -3.600 -20.690  1.00 28.64    5
ATOM    584  CD  GLN    74      23.305  -4.342 -19.349  1.00 28.74    5
ATOM    585  OE1 GLN    74      28.874  -5.429 -19.275  1.00 30.46    5
ATOM    586  NE2 GLN    74      22.747  -3.757 -18.307  1.00 28.44    5
*DELETE,2CAB.2159
MASTER       75   10    1    7   10   11    0    6 2010    1    4   21
```

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 (January 1984)
   - ( ) Sources of Visual Aids for Macromolecular Structure (April 1984)
   - ( ) Atomic Coordinate Entry Format Description for DATAPRTP and DATAPRFI (June 1984)
   - ( ) Current DATAPRTP Directory
   - ( ) Non-Standard Entries (Structure Factors) Format Description
     - ( ) NONST1TP and NONST1FI (April 1983)
     - ( ) NONST2TP and NONST2FI (January 1984)
     - ( ) NONST3TP and NONST3FI (April 1984)
   - ( ) Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs $184 (£123 from Cambridge); each 2-tape item costs $225 (£150). Domestic postage is included.

Item	Number of Tapes	Cost

Total _____

Special Instructions (to be completed for Brookhaven requests only). Please check the appropriate box.

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

		Availability US	Availability UK
( )	9 track, 6250 cpi, EBCDIC	yes	yes
( )	9 track, 1600 cpi, EBCDIC	yes	yes
( )	9 track, 800 cpi, EBCDIC	yes	yes
( )	9 track, 6250 cpi, ASCII	yes	yes
( )	9 track, 1600 cpi, ASCII	yes	yes
( )	9 track, 800 cpi, ASCII	yes	yes

All tapes are distributed in blocked form with fixed record length and block size. Brookhaven normally uses a block size of 4800 characters. Please indicate here any difficulties this might cause.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs $122 (£81), postage included. Correction fiche are free.

Item	Cost

Total _____

6. Please send the following printed listings. Each listing costs $71, (£47), postage included.

Ident Code (From Table 3)	Cost

Total _____

7. Foreign 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 (£10) is required per magnetic tape (not per item).

Number of tapes x $15.00 (£10) = _____

8. Total charges

Magnetic tape charges (3 above) _____
Microfiche charges (5 above) _____
Printed listing charges (6 above) _____
Foreign air mail postage charges (7 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
( ) purchase order number _____

is ( ) enclosed
( ) sent separately

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

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.