

PROMISE: a database of bioinorganic motifs

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ABSTRACT

The PROMISE (prosthetic centres and metal ions in protein active sites) database aims to present comprehensive sequence, structural, functional and bibliographic information on metalloproteins and other complex proteins, with an emphasis on active site structure and function. The database is available on the WorldWide Web at <http://bioinf.leeds.ac.uk/promise/>

PROMISE aims to be a comprehensive information source on bioinorganic motifs in proteins. Its focus is on protein active site structure and on the relationships between polypeptide and prosthetic centre, combining the relevant sequence, 3-D structural and physico-chemical information (1,2). Bioinorganic motifs provide a basis for classification of complex proteins, alternative and complementary to those employed in other 'secondary' protein databases (see ref. 1 for comparison of PROMISE with other databases).

As of 15 September 1998, PROMISE version 2.0 contained six major groups (diiron-carboxylate proteins, haem proteins, iron-sulphur proteins, molybdopterin-containing proteins, mononuclear iron proteins and chlorophyll-containing proteins) comprising nine intermediate class entries and 56 protein family entries, each with an associated bibliographic entry (a total of 5403 references). Table 1 presents a full list of entries in PROMISE.

A number of novel bioinorganic motifs and prosthetic groups reported during the last few years have been included in PROMISE 2.0 (Fig. 1). Many entries have been revised, sometimes radically, to reflect the new data. For example, the recent X-ray structure of 'prismane' protein has revealed that it does not contain an [Fe₆S₆] (prismane) cluster (Fig. 2a); instead, it contains an [Fe₄S₄] cubane cluster and a novel 'hybrid' cluster with an unusual mixture of bridging ligands and coordinations (Fig. 2b) (5). Similarly, an [Fe₈S₈] model for the P-cluster of nitrogenase molybdenum-iron (MoFe) protein (Fig. 2c) was discarded when it was found that the P-cluster exists as an [Fe₈S₇] cluster in both oxidised and reduced states (Fig. 2d and e) (7). The [Fe₈S₈] model appears to have resulted from the inappropriate modelling of a mixture of the two P-cluster redox states by a single structure.

PROMISE is available on the WorldWide Web from URL: <http://bioinf.leeds.ac.uk/promise/> or <http://metallo.scripps.edu/PROMISE/>. Use of Netscape version 2.0 or higher is recommended. The SRS browser (3) provides simple and fast textual search through the whole PROMISE database. Any feedback and corrections will be gratefully received.

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Table 1. Contents of PROMISE version 2.0

PROMISE groups, classes and families	Bibliography files		3-D example
	Structural studies †	Reviews †	
Chlorophyll-containing proteins		99	
Bacteriochlorophyll <i>a</i> protein	23		3BCL
Light-harvesting complex II of purple bacteria	51	18	1LGH
Photosynthetic reaction centre of purple bacteria	166	24	1PRC
Diiron-carboxylate proteins		15	
Class I: Ribonucleotide reductase R2-type proteins	107	54	1RIB
Class II: Ferroxidase			
Bacterioferritin (cytochrome <i>b</i> ₁ ; cytochrome <i>b</i> ₅₅₇)	14	} 61	1BCF, 1BFR
Ferritin	60		
Rubrerythrin	9		
Class III: Haemerythrin family	43		1HMO
Class IV: Purple acid phosphatase	41	11	1KBP
Haem proteins		103	
Catalases	46	14	1CAF
Cytochrome <i>c</i> oxidase	294	105	1OCC
Cytochrome <i>bc</i> ₁ complex *	50	43	
Cytochromes			
Cytochromes <i>b</i>			
Cytochrome <i>b/b</i> ₆ *	17		
Cytochrome <i>b</i> ₅ family	64	14	3B5C
Soluble cytochrome <i>b</i> ₅₆₂	21		256B
Cytochromes <i>c</i>		79	
Class I cytochromes <i>c</i>	287		1CRY
Class II cytochromes <i>c</i>	37		1BBH
Class III cytochromes <i>c</i>	80		2CY3
Class IV cytochromes <i>c</i>	20		1PRCC
Cytochrome <i>c</i> ₁	10		
Cytochrome <i>f</i>	6		1CTM
Cytochrome <i>cd</i> ₁ nitrite reductase *	50		
Hydroxylamine oxidoreductase *	21		
Globins	757	119	1BBB, 1MBO
Haem peroxidases			
Animal haem peroxidases	27	26	1MHL
Fungal, plant and bacterial haem peroxidases	219	46	2CYP
Haem-thiolate proteins			
Chloroperoxidase	39		1CPO
Nitric oxide synthases *	50	414	
P450 proteins	105	148	3CPP

Iron-sulphur proteins		45	
Fe(Cys) ₄ proteins			
Desulforedoxin-type Fe(Cys) ₄ proteins	8		1DXG
Desulfoferrodoxin *	6		
Rubredoxin-type Fe(Cys) ₄ proteins	42		1CAD
Fe ₂ S ₂ proteins			
Adrenodoxin-type ferredoxins	26		1PUT
Plant-type ferredoxins	64	13	1FRR
Rieske iron-sulphur proteins	56		1RIE
Fe ₄ S ₄ / Fe ₃ S ₄ proteins			
Aconitase family	37	29	7ACN
Bacterial-type mono-, di- and polycluster ferredoxins	131	7	1FXR
Endonuclease III family	6		2ABK
Glutamine PRPP amidotransferase *	13		1A00
High potential iron proteins (HiPIPs)	47		1ISU
Nickel-iron hydrogenase	53		1FRV
Nitrogenase component I (MoFe protein)	75	} 39	2MIN
Nitrogenase component II (Fe protein)	29		1NIP
"Prismane" proteins	12		
Sirohaem-Fe ₄ S ₄ enzymes	44		1GEP
Trimethylamine dehydrogenase	14		2TMD
Molybdopterin-containing proteins *		34	
Aldehyde ferredoxin oxidoreductase family *	8		1AOR
DMSO reductase family *	71		1FDO
Sulphite oxidase family *	42		
Xanthine oxidase family *	108		1ALO
Mononuclear iron proteins		11	
Aromatic amino acid hydroxylases *	51	62	
Aromatic-ring-hydroxylating dioxygenases *	22		
Extradiol aromatic-ring cleavage monooxygenases	20	} 11	1HAN
Intradiol aromatic-ring cleavage monooxygenases	30		2PCD
Isopenicillin N synthase	14	11	1IPS
Lipoxygenases	65	24	2SBL
Nitrile hydratase *	21	5	
Total	3652	1750	

†The numbers in the columns correspond to the numbers of literature references in the associated bibliographic entries.

*Entries added in the last year.

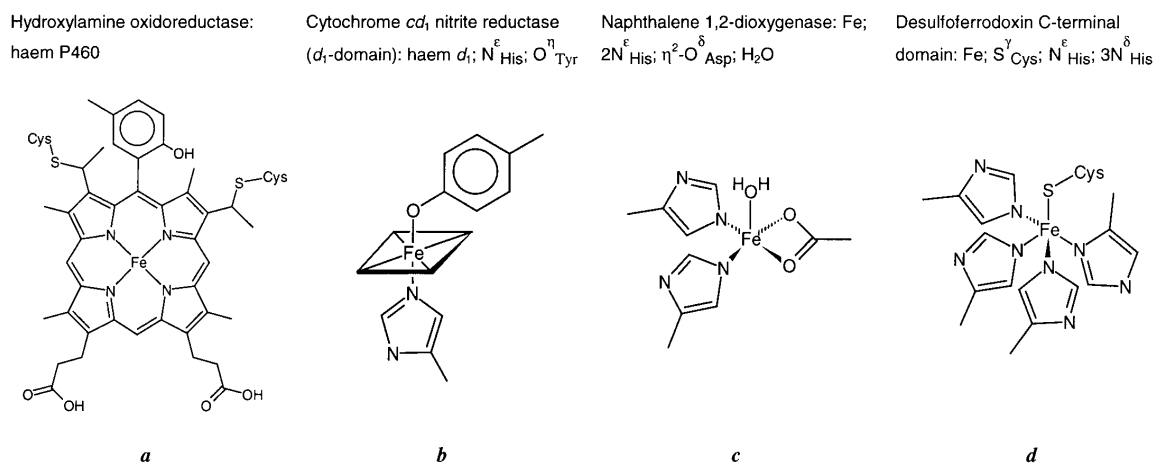


Figure 1. Examples of novel prosthetic groups and bioinorganic motifs: (a) haem P460 of hydroxylamine oxidoreductase (8); (b) cytochrome *cd*₁ nitrite reductase (9); (c) naphthalene 1,2-dioxygenase (10); (d) desulfoferrodoxin (11).

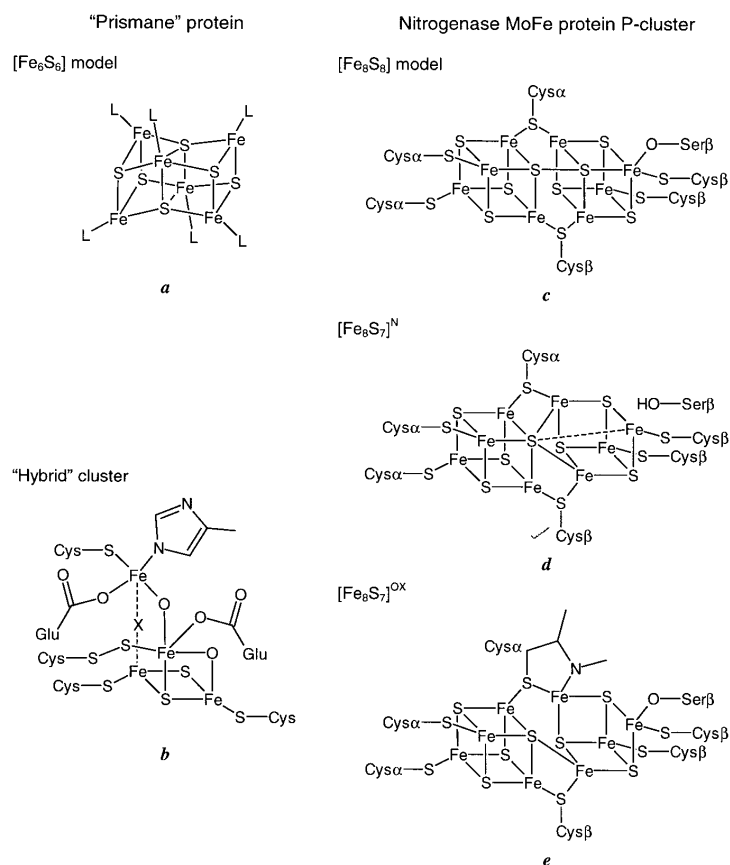


Figure 2. (a) [Fe₆S₆] model for iron cluster in prismane protein (4); (b) ‘hybrid’ cluster in prismane protein as revealed by X-ray crystallography and spectroscopy (5); (c) [Fe₈S₈] model for P-cluster of nitrogenase molybdenum–iron protein (6); (d) [Fe₈S₇]^N, model for reduced P-cluster (7); (e) [Fe₈S₇]^{OX}, model for oxidised P-cluster (7).