Supplementary Materials

Distinct Conformational Behaviors of Four Mammalian Dual-Flavin Reductases (Cytochrome P450 Reductase, Methionine Synthase Reductase, Neuronal Nitric Oxide Synthase, Endothelial Nitric Oxide Synthase) Determine their Unique Catalytic Profiles

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Table S1: Residue contacts in different dual-flavin enzymes.

	Cytochrome P450 reductase (1AMO) residue contacts			
	FMN domain		**FNR domain**	
1.	LYS	72	ASN	356
2.	LYS	75	GLU	354
3.	ARG	78	ASP	352
4.	GLN	87	TYR	455
5.	GLN	87	ARG	514
6.	THR	88	GLN	452
7.	THR	90	ARG	382
8.	PHE	94	ARG	382
9.	ASN	96	GLN	244
10.	ARG	97	ARG	382
11.	ARG	97	THR	383
12.	ARG	97	ASN	384
13.	LYS	100	ARG	243
14.	LYS	100	GLN	244
15.	ARG	108	ASP	352
16.	SER	111	LYS	357
17.	GLU	116	ASN	356
18.	ASP	147	ARG	514
19.	THR	177	ALA	633
20.	TYR	178	TRP	677
21.	GLU	179	GLN	641
22.	GLU	179	LYS	664
23.	GLU	179	MET	667
24.	GLU	213	ARG	382
25.	GLU	213	THR	383
26.	GLU	213	TYR	416
27.	GLU	214	SER	407
28.	GLU	214	LYS	413
29.	GLU	214	TYR	416
30.	ILE	217	THR	383
31.	ILE	217	ALA	406
32.	GLU	221	SER	408

Neuronal Nitric Oxide Synthase (1TLL) Residue contacts				
	FMN domain		**FNR domain**	
1.	GLU	762	GLN	1171
2.	GLU	762	ARG	1229
3.	THR	763	GLN	1171
4.	GLU	775	ASP	961
5.	GLU	775	ARG	962
6.	ASN	811	GLU	1392
7.	GLU	816	ARG	1229
8.	SER	840	ASP	1386
9.	LYS	842	ARG	1385
10.	VAL	843	ASP	1386
11.	ASN	846	ARG	1385
12.	VAL	848	GLN	1363
13.	VAL	848	GLY	1378
14.	ALA	888	VAL	1352
15.	ALA	888	VAL	1397
16.	ALA	888	LEU	1408
17.	TYR	889	VAL	1352
18.	TYR	889	GLY	1396
19.	TYR	889	VAL	1397
20.	PRO	890	VAL	1352
21.	GLU	919	TRP	1140
22.	LEU	920	TRP	1140
23.	LEU	920	LEU	1408
24.	LEU	920	ARG	1409
25.	CYS	921	GLU	1136
26.	CYS	921	ILE	1413
27.	GLY	922	GLU	1136
28.	GLU	924	PRO	1106
29.	GLU	925	LYS	1130
30.	GLU	925	GLY	1131
31.	ARG	928	SER	1129
32.	ARG	928	LYS	1130

Endothelial Nitric Oxide Synthase (Model, 1TLL template) Residue contacts				
	FMN domain		FNR domain	
1.	GLU	529	GLN	938
2.	GLU	529	TYR	941
3.	GLU	529	ARG	996
4.	THR	530	GLN	938
5.	ARG	542	LYS	729
6.	ARG	545	LYS	836
7.	ASN	578	ARG	1152
8.	ASN	578	GLU	1159
9.	ASN	578	ILE	1161
10.	GLU	583	ARG	996
11.	VAL	618	GLY	1145
12.	VAL	618	ARG	1152
13.	ARG	657	ILE	1175
14.	ARG	657	SER	1179
15.	ALA	658	VAL	1119
16.	TYR	659	VAL	1119
17.	TYR	659	GLY	1163
18.	PRO	660	THR	1123
19.	HIS	661	ARG	1152
20.	GLU	689	TRP	907
21.	LEU	690	GLU	903
22.	LEU	690	TRP	907
23.	LEU	690	ILE	1175
24.	LEU	690	ARG	1176
25.	CYS	691	GLU	903
26.	CYS	691	PHE	1180
27.	GLY	692	ASP	898
28.	GLY	692	GLU	903
29.	GLU	694	PRO	873
30.	GLU	694	ASP	898
31.	GLU	695	GLN	897
32.	GLU	695	ASP	898
33.	ARG	698	PRO	873
34.	ARG	698	ARG	877
35.	ARG	698	SER	896
36.	ARG	698	GLN	897

Methionine synthase reductase (Model, 1AMO template) Residue contacts				
	FMN domain		**FNR domain**	
1.	ARG	2	THR	349
2.	ARG	2	LYS	350
3.	GLN	11	ARG	525
4.	GLN	12	GLN	449
5.	GLU	20	LYS	352
6.	GLU	21	LYS	381
7.	ASP	34	LYS	350
8.	ASP	34	LYS	351
9.	ASP	34	LYS	352
10.	LEU	35	LYS	352
11.	LEU	35	GLY	353
12.	HIS	36	GLY	353
13.	CYS	37	GLY	353
14.	GLU	40	GLY	353
15.	GLU	40	ALA	354
16.	ASP	67	ARG	525
17.	GLU	100	ALA	653
18.	GLU	100	LYS	654
19.	GLU	100	SER	698
20.	TYR	101	ILE	696
21.	TYR	101	TRP	697
22.	VAL	133	ARG	418
23.	GLU	136	LYS	381
24.	GLU	136	LYS	382
25.	GLU	136	TYR	413
26.	LEU	137	LYS	382
27.	GLU	140	CYS	405

Methionine synthase reductase (Model, 1TLL template) Residue contacts				
	FMN domain		**FNR domain**	
1.	TYR	8	LEU	245
2.	GLN	11	PRO	346
3.	GLN	12	PRO	246
4.	GLN	12	GLN	449
5.	LYS	16	LEU	245
6.	ASP	34	ASN	210
7.	GLY	61	ILE	696
8.	THR	62	GLN	694
9.	ASP	67	ARG	525
10.	GLN	79	GLU	688
11.	THR	80	GLU	688
12.	VAL	83	GLU	688
13.	GLU	100	LYS	654
14.	TYR	101	ALA	653
15.	THR	102	LYS	658
16.	GLU	136	LYS	382
17.	LEU	137	GLN	408