

**Table S1. A $\beta$  -binding A and B chains of FDH by H-bond. Donor = H donor; Receptor = H receptor.**

Protein (P)	Ligand (L)	Donor	Receptor	Bond Length
<b>1TEH_AB</b>	<b>1Z0Q</b>	P_A: ASN225:HND21	L: GLU11:OE2	2.375
		P_A: LYS226: HNZ1	L: VAL12: O	1.770
		P_A: HIS363:HD1	L: GLU3:OE2	2.437
		P_B: LYS330:HZ1	L: ARG5: O	1.996
		P_B: LYS330:HZ2	L: ARG5: O	1.659
		L: ARG5: HE	P_B: GLU326:OE2	2.292
		L: HIS6:HD1	P_B: GLU326:OE1	2.292
		L: HIS13:HE2	P_B: ASP161:OD1	1.540
		L: HIS14:HD1	P_B: LYS82: O	2.466
		L:GLN15:HE21	P_A: ASP227:OD2	1.671
<b>1TEH_AB-Zn</b>	(Under vacuum conditions)	P_A: ASN225:ND2	L: GLU11:OE2	2.973
		P_A: LYS226:NZ	L: VAL12: O	2.572
		P_B: GLU326: N	L: TYR10: OH	3.054
		P_B: LYS330:NZ	L: ARG5: O	2.216
		P_B: LYS330:NZ	L: SER8: OG	3.198
		L: ARG5: HE	P_B: GLU326:OE2	2.289
		L: HIS6:HD1	P_B: GLU326:OE1	2.292
		L: HIS13:HE2	P_B: ASP161:OD1	1.537
		L: HIS14:HD1	P_B: LYS82: O	2.462
		L:GLN15:HE21	P_A: ASP227:OD2	1.670
<b>1TEH_AB-eq</b>		P_A: HIS47:HE2	L: GLU3: O	2.406
		P_A: SER54: HG	L: ASP7:OD1	2.127
		P_B: LYS82:HZ2	L: HIS13:NE22	2.335
		L: SER8: HG	P_A: HIS363: O	1.757
		L: HIS14:HD1	P_A:GLY18:O	2.357
<b>1TEH_AB-Zn-eq</b>	<b>1Z0Q-eq</b> (Under the condition of ion equilibrium)	P_A: LYS226:HZ1	L: VAL12: O	1.776
		P_A: LYS366:HZ1	L: GLU11:OE1	2.169
		P_A: LYS366:HZ1	L: GLU11:OE2	1.851
		P_A: LYS366:HZ2	L: GLU11:OE1	1.556
		P_A: LYS366:HZ2	L: GLU11:OE2	1.333
		P_A: LYS366:HZ3	L: GLU11:OE2	1.579
		P_B: LYS82:HZ1	L: ALA2: O	1.995
		P_B: LYS82:HZ2	L: ASP1:OD2	2.487
		P_B: GLY98:HN	L:ASP1: O	2.061
		P_B: LYS159:HZ3	L: HIS14:NE2	1.752
		P_B: GLU326:HN	<b>L: HIS63:NE2</b>	1.619
		<b>L: ASP1:HT1</b>	<b>P_B: GLN96: O</b>	0.819
		<b>L: ASP1:HT2</b>	<b>P_B: GLN96: O</b>	1.294
		<b>L: ASP1:HT3</b>	<b>P_B: GLN96: O</b>	1.730
L:GLN15:HE21	P_A: ASP227:OD2	2.393		

**Table S2: Changes in the cysteine residues of CYS45, CYS90, CYS100, and CYS111 residues of the samples of hFDH, A $\beta$ +FDH, and RL+A $\beta$ +FDH.**

<b>Cysteine status</b>	<b>Sample 1: FDH</b>	<b>Sample 2: A<math>\beta</math>+FDH</b>	<b>Sample 3: RL+A<math>\beta</math>+FDH</b>
<b>Cys 43</b>	%	%	%
<b>SH</b>	96.8	95.3	94.6
<b>MTHIO</b>	3.2	4.2	4.3
<b>SOxH</b>		0.4	1.1
<b>Cys 97,100</b>			
<b>SH</b>	100.0	100.0	100.0
<b>MTHIO</b>			
<b>SOxH</b>			0.3
<b>S-S</b>		1.4	
<b>Cys 111</b>	%	%	%
<b>SH</b>	76.7	93.2	92.1
<b>MTHIO</b>	53.2	6.8	5.3
<b>S-S</b>	5.9		2.6

**Table S3: Changes in the cysteine residues of CYS45, CYS90, CYS100, and CYS111 residues of sample 1-hFDH.**

Modifications	Area		Area	%
C4(Carbamidomethyl)	1525305SH	Cys 43		
C4(Carbamidomethyl)	4162714SH	SH	4717766 0	96.80317
C4(Methylthio)	1557996MTHIO	MTHIO	1557996	3.196829
C4(Carbamidomethyl)	41489641SH			
		Cys 97,100		
C5(Carbamidomethyl); M6(Oxidation); C8(Carbamidomethyl)	3868177SH	SH	4373136	100
C6(Methylthio)	218750.3MTHIO	Cys 111	Area	%
C1(Dehydro); C9(Dehydro)	286208.3S-S	SH	1224353 9	76.67404
C1(Dehydro)	244006S-S	MTHIO	8490884	53.17338
C1(Methylthio); C9(Methylthio)	2293431MTHIO	S-S	949382.4	5.94542
C1(Methylthio); C9(Methylthio)	364871.5MTHIO			
C1(Methylthio); C9(Carbamidomethyl)	4346956SH	MTHIO		
C1(Carbamidomethyl); C9(Methylthio)	803793.8SH	MTHIO		
C1(Carbamidomethyl); C9(Methylthio)	145588.7SH	MTHIO		
	1422834SH			
C6(Methylthio)	317492.7MTHIO			
C6(Carbamidomethyl)	5524366SH			

**Table S4: Changes in the cysteine residues of CYS45, CYS90, CYS100, and CYS111 residues of sample 2- A $\beta$ +FDH.**

Modifications	Area					
C4(Methylthio)	3593866	MTHIO	Cys 43	Area	%	
C4(Carbamidomethyl)	92585621	SH	SH	2.28E+08	95.31692	
C4(Methylthio)	4375416	MTHIO	MTHIO	1016290	4.24385	
C4(Methylthio)	2193622	MTHIO	SOxH	1051846	0.439232	
C4(Trioxidation)	1051846	SOxH	S-S	ND		
C4(Carbamidomethyl)	1.02E+08	SH				
C4(Carbamidomethyl)	33906144	SH				
C5(Carbamidomethyl); C8(Dehydro)	157720.2	SH	S-S	Cys 97,100		
C5(Carbamidomethyl); C8(Carbamidomethyl)	586814.6	SH	SH	SH	1107675	100
					4	
C5(Carbamidomethyl); M6(Oxidation); C8(Carbamidomethyl)	9845248	SH	SH	S-S	157720.2	1.423884
C4(Carbamidomethyl); M5(Oxidation); C7(Carbamidomethyl)	486971.5	SH	SH			
C6(Methylthio)	507735.2	MTHIO	Cys 111	Area	%	
C6(Carbamidomethyl)	3917935	SH	SH	1699928	93.20222	
	1097808	SH	MTHIO	1239857	6.797781	
C6(Methylthio)	732121.5	MTHIO	SOxH	ND		
C6(Carbamidomethyl)	11983539	SH	S-S	ND		

**Table S5: Changes in the cysteine residues of CYS45, CYS90, CYS100, and CYS111 residues of sample 3-RL+A $\beta$ +FDH.**

Modifications	Area				
C4(Dioxidation)	6033516SOxH	Cys 43	Area	%	
C4(Methylthio)	21570859MTHIO	SH	7.33E+08	94.61604	
C4(Methylthio)	8948802MTHIO	MTHIO	33327636	4.30004	
C4(Trioxidation)	2367469SOxH	SOxH	8400985	1.083922	
C4(Carbamidomethyl)	4.63E+08SH	S-S	ND		
C4(Carbamidomethyl)	1.67E+08SH				
C4(Methylthio)	2807975MTHIO				
C4(Carbamidomethyl)	1.03E+08SH				
C5(Dioxidation); M6(Oxidation); C8(Carbamidomethyl)	69652.33SH	SOxH	Cys 97,100		
C5(Carbamidomethyl); C8(Carbamidomethyl)	9525196SH	SH	SH	2061331 8	100
C5(Carbamidomethyl); M6(Oxidation); C8(Carbamidomethyl)	9729114SH	SH	SOxH	69652.33	0.3379
C4(Carbamidomethyl); C7(Carbamidomethyl)	797207.1SH	SH			
C4(Carbamidomethyl); M5(Oxidation); C7(Carbamidomethyl)	492148.6SH	SH			
C6(Methylthio)	323035.8MTHIO	Cys 111	Area	%	
C6(Carbamidomethyl)	3874670SH	SH	1504216 5	92.05637	
C1(Dehydro); C9(Dehydro)	432942.9S-S	MTHIO	8650605.294071		
C6(Methylthio)	542024.2MTHIO	SOxH	ND		
C6(Carbamidomethyl)	11167495SH	S-S	432942.9	2.649562	