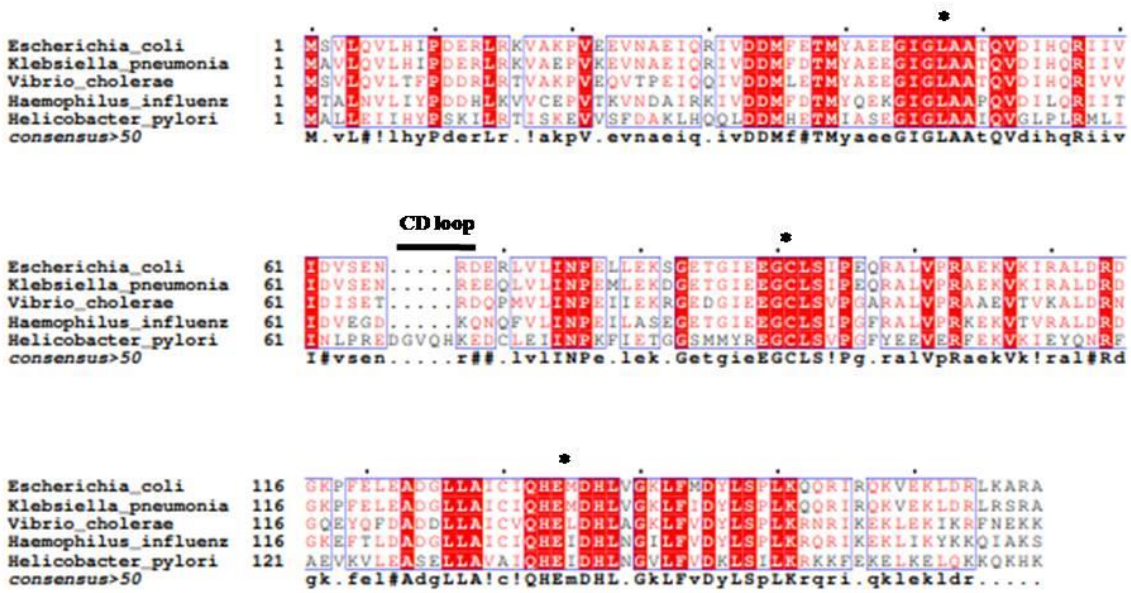
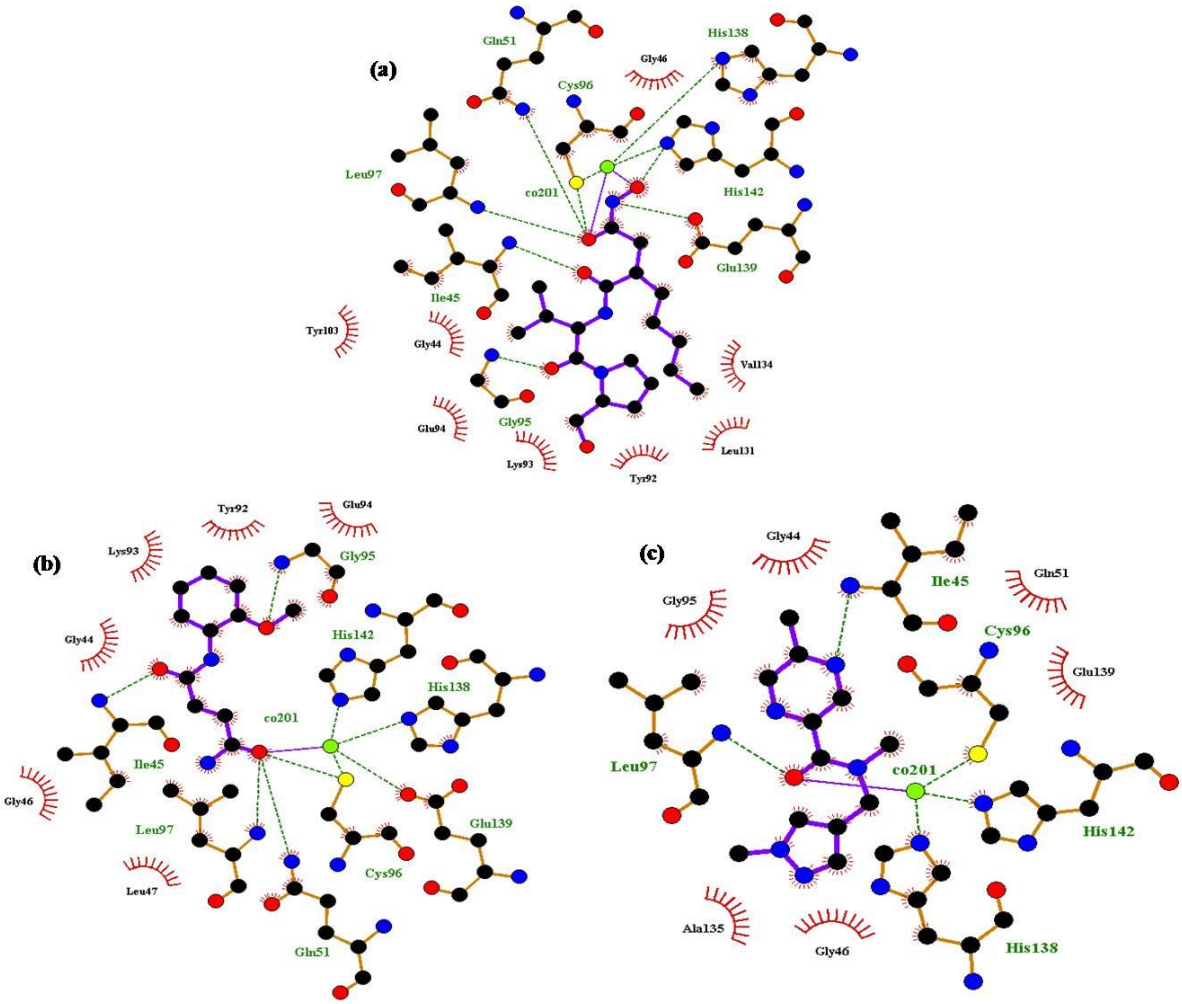
Supplementary Figures and Tables



Supplementary Figure: 1 Peptide deformylase Sequence comparison. Peptide deformylase sequence analysed for conserved and least conserved regions with four Gram negative bacteria.Red colour box indicates conserved residues through the group. CD loop region between residue 68- 72, shows least conserved residues for *H.pylori*. Major three motif regions indicated with a star. Sequence alignment was done using ESpript3 software (https://espript.ibcp.fr/ESPript/ESPript/).



Supplementary Figure: 2 Schematic 2-dimensional representation of binding mode of ZINC ligands with HpPDF S1 active site residues: (a) Actionin, (b) ZINC00225109, (c) ZINC44896875. Cobalt metal is represented in green colour. Hydrogen bonds formed indicated in dotted lines. Major binding site residues in contact with ligand represented as ball and sticks, other residues within the active site are labeled. LIGPLOT software was employed to visualize the interactions.

Table: S1 XP docking score of Known antagonist of PDF enzyme docked on HpPDF S1 binding Site.

S:No	Compound	Glide G Score Xp
1.	Actinonin	-9.730
2.	VRC3375	-9.306
3.	N-[(3-amino-3-oxopropyl)carbamoyl]-1-[(2R)-3-cyclopentyl-2-[[formyl(hydroxy)amino]methyl]propanoyl]-L-prolinamide	-9.171
4.	1-[(2R)-3-cyclopentyl-2-[[formyl(hydroxy)amino]methyl]propanoyl]-N-(2,2-dimethylpropanoyl)-L-prolinamide	-9.033
5.	(2R)-N-[(2S)-1-(dimethylamino)-3,3-dimethyl-1-oxobutan-2-yl]-2-[[formyl(hydroxy)amino]methyl]hexanamide	-8.940
6.	N-Caffeoyltyramine	-8.933
7.	(RS)-3-(phenylsulfonyl)heptanoic acid hydroxyamide	-11.553
8.	BB-3497	-8.752
9.	(3R)-3-[3-[(1-benzofuran-3-yl)methyl]-1,2,4-oxadiazol-5-yl]-5-cyclopentyl-N-hydroxypentanamide	-8.074
10.	(3R)-3-[[(2S)-2-(1,3-benzoxazol-2-yl)pyrrolidin-1-yl]carbonyl]-N-hydroxyheptanamide	-7.965
11.	2-(2,2-dioxido-1,4-dihydro-3H-2,1,3-benzothiadiazin-3-yl)-N-hydroxyacetamide	-10.074
12.	5281787	-7.803
13.	(RS)- and (SR)-3-[(RS)-benzenesulfinyl]heptanoic acid hydroxyamide	-10.366
14.	2-[5-chloro-2,2-dioxido-1-(3-phenylpropyl)-1,4-dihydro-3H-2,1,3-benzothiadiazin-3-yl]-N-hydroxyacetamide	-9.610
15.	(3R)-3-[3-[(1,3-benzothiazol-2-yl)methyl]-1,2,4-oxadiazol-5-yl]-N-hydroxyheptanamide	-7.198
16.	n-formyln-hydroxy-3phenylpropailamine	-6.327
17.	2-(5-bromo-1-cyclopropyl-2,2-dioxido-1,4-dihydro-3H-2,1,3-benzothiadiazin-3-yl)-N-hydroxyacetamide	-6.250
18.	2-(5-fluoro-2-oxo-1,4-dihydroquinazolin-3(2H)-yl)-N-hydroxyacetamide	-8.673
19.	2-(5-chloro-2-oxo-1,4-dihydroquinazolin-3(2H)-yl)acetohydrazide	-5.995
20.	N-formyl-N-hydroxy-2-(3-benzoylphenoxy)ethylamine	-7.149

21.	1-[(2R)-3-cyclopentyl-2-[[formyl(hydroxy)amino]methyl]propanoyl]-N-(cyclopropylcarbonyl)-L-prolinamide	-7.062
22.	Thiophenol	-3.889

Table: S2 SIFT analysis of HpPDF binding site amino acids interaction with ZINC44896875

Amino acid	Backbone	Sidechain	Hydrophobic	Polar	Charged	Donor	Acceptor	Aromatic
Gly44	1	0	0	0	0	0	0	0
Ile45	1	1	1	0	0	0	0	0
Gly46	1	0	0	0	0	0	0	0
Tyr92	0	1	1	0	0	0	0	1
Lys93	1	0	0	0	0	0	0	0
Glu94	1	0	0	0	0	0	0	0
Gly95	1	0	0	0	0	1	0	0
Leu97	0	1	1	0	0	0	0	0
Leu131	0	1	1	0	0	0	0	0
Ala135	1	1	1	0	0	0	0	0
His138	0	1	0	1	0	0	0	0
Glu139	0	1	0	1	1	0	0	0

Table: S3 SIFT analysis of HpPDF binding site amino acids interaction with ZINC00225109

Amino acid	Backbone	Sidechain	Hydrophobic	Polar	Charged	Donor	Acceptor	Aromatic
ILE45	1	1	1	0	0	0	0	0
Gly46	1	0	0	0	0	0	0	0
Leu47	1	0	0	0	0	0	0	0
Gly51	0	1	0	1	0	1	1	0
Tyr92	0	1	1	0	0	0	0	1
Lys93	1	0	0	0	0	0	0	0
Glu94	1	0	0	0	0	0	0	0
Gly95	1	0	0	0	0	0	1	0
Cys96	1	1	1	0	0	0	0	0
Leu97	1	0	0	0	0	1	0	0
Leu131	0	1	1	0	0	0	0	0
Val134	0	1	1	0	0	0	0	0
His138	0	1	0	1	0	0	0	0
Glu139	0	1	0	1	1	0	1	0
Co201	0	1	0	0	0	0	0	0

Table: S4 SIFT analysis of HpPDF binding site amino acids interaction with Actinonin

Amino acid	Backbone	Side Chain	Hyrophobic	Polar	Charged	Donor	Acceptor	Aromatic
Gly44	1	1	1	0	0	0	0	0
Ile 45	1	1	1	0	0	0	0	0
Gly46	1	0	0	0	0	0	0	0
Gln51	0	1	0	1	0	1	0	0
Tyr92	0	1	1	0	0	1	0	1
Glu94	0	1	0	1	1	0	0	0
Gly95	1	0	0	0	0	0	0	0
Cys96	1	1	1	0	0	0	0	0
Leu97	1	1	1	0	0	1	0	0
Tyr103	0	1	1	0	0	0	0	1
Leu131	0	1	1	0	0	0	0	0
Val134	1	1	1	0	0	0	0	0
His138	0	1	0	1	0	0	0	0
Glu139	0	1	0	1	1	0	1	0
His142	0	1	0	1	0	0	0	0
Co201	0	1	0	0	0	0	0	0