

Supplemental Table S1: Data collection and refinement statistics			
	InhA+AN2918	InhA+AN3438	InhA+AN12855
Protein	InhA (R5645)	InhA	InhA
Compound	AN2918.01 / NAD ⁺	AN3438.02 / NADH	AN12855 (EBSI 41882)
Beamline	APS-21-ID-F	APS-21-ID-G	APS 21 ID-F
Space Group	SG=5; C2	SG=20; C2221	I ₄ 22
Unit Cell	a=125.35Å	a=81.66Å	a=94.08Å
	b=92.68Å	b=100.94Å	b=94.08Å
	c=101.93Å	c=377.82Å	c=184.43Å
	β=105.539		
Solvent content	50.41%	45.70%	
V_m	2.48 Å ³ /Da	2.26 Å ³ /Da	
Resolution	49.09-2.50Å (2.565-2.500)	48.76-2.55Å (2.62-2.55)	50-2.65Å (2.72-2.65)
I/σ	22.82 (4.63)	11.72 (3.14)	26.8 (3.85)
Completeness	99.9% (100.1%)	99.4% (99.7%)	99.6% (100%)
Rmerge	0.059 (0.515)	0.121 (0.506)	0.063 (0.502)
Multiplicity	6.8 (7.5)	5.3 (5.1)	9.6 (9.8)
Reflections	38978 (2872)	51162 (3740)	12,408 (896)
Mosaicity	0.21	0.30	0.20
R	0.191 (0.263)	0.235 (0.301)	0.172 (0.245)
R_{free}	0.221 (0.327)	0.273 (0.342)	0.198 (0.243)
Ramachandran			
Favored	94.69%	96.23%	248 (95.8%)
Allowed	100.0%	100.0%	9 (3.5%)
Outliers			2 (0.8%), none per molprobability
Molprobability Score	1.18 (100th percentile)	1.65 (99th percentile)	1.31 (100 th percentile)
PDB File	5VRM	5VRM	5VRL