

Supplementary Table 1

Data Collection and Refinement Statistics

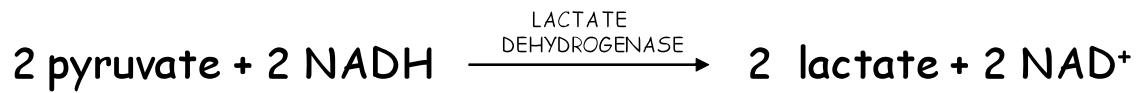
	<i>Pa</i> TMK 1	<i>Pa</i> TMK dFTM	<i>Pa</i> TMK 17
<i>Crystal Form</i>			
Space Group	<i>P2</i> ₁ <i>2</i> ₁ <i>2</i>	<i>P2</i>	<i>P2</i> ₁
Unit cell parameters			
a (Å)	74.3	73.9	46.2
b (Å)	118.1	41.5	56.0
c (Å)	42.0	117.9	82.1
α, β, γ (°)	90,90,90	90,90.02,90	90,95.3,90
No. Molecules per asymm. unit	2	4	2
<i>Data Collection</i>			
Resolution (Å)	41.9-1.9	24.6-1.9	32.1-1.7
No. of Unique Reflections	29,391	51,360	43,285
No. of Observations	110,874	177,972	155,047
R _{sym} * (%)	6.9(44.3)	6.4(32.2)	5.1(24.7)
I/σ_I	18.7(2.6)	15.5(3.3)	41.3(3.6)

Data Completeness (%)	99.7(100)	97.5(90.9)	94.1(61.5)
Mean Multiplicity	3.7(3.7)	3.5(3.0)	3.6(2.6)
<i>Refinement</i>			
No. of Reflections used in refinement	27,872	48,710	43,283
R _{cryst} [‡] (%)	19.5	17.5	19.2
R _{free} [‡] (%)	24.2	23.6	21.2
% Reflections used in R _{free} (F >0)	5.1	5.1	5.0
R.m.s. deviations, bond lengths (Å)	0.02	0.016	0.011
R.m.s. deviations, bond angles (°)	1.74	1.62	1.27
Ramachandran plot (% most favored, % additional allowed residues, % disallowed residues)	95.8 3.6 0.6	95.3 4.1 0.6	96.3 3.1 0.6
Average B-factors (Å ²)	28.2	24.2	34.1

* $R_{sym} = \frac{\sum_{hkl} \sum_i |I_i(hkl) - I(hkl)|}{\sum_{hkl} \sum_i I_i(hkl)}$ where $I_i(hkl)$ is the intensity of an individual measurement, and $I(hkl)$ is the mean intensity of this reflection. [‡]R factor = $\frac{\sum_{hkl} |F_{obs}| - |F_{calc}|}{\sum_{hkl} |F_{obs}|}$, where $|F_{obs}|$ and $|F_{calc}|$ are observed and calculated structure factor amplitudes, respectively. The values in parentheses for completeness, R_{sym} and $1/\sigma$ correspond to the highest resolution shell.

The four reactions which comprise this assay system are illustrated below.

COUPLED ASSAY:



measure $\text{OD}_{340 \text{ nm}}$