													Notes
experiment title	VP-ITC CBS-CAII												
date	10/25/2012												
user	John D. Chodera												
titrant:titrand filename	102512a.itc												
titrant:buffer filename	102512b.itc												
EXPERIMENTAL DETAILS													
temperature		25	**C**										
estimated Ka		1.00E+06	**1/M**										
sample cell volume (approximate)		1.4	mL										
number of injections		10											
injection volume		10	**uL**										
dilution factor for single injection (d)		0.9928571429											
dilution factor after final injection (d^n)		0.9308241571											
		desired						**actual**		**error**		**percent error**	
cell concentration		10.00	**uM**					10.01	**uM**	0.09	**uM**	0.87%	
c-value		10.00						12.01		0.03		0.26%	
optimal Rm		5.34						4.98					
syringe concentration		718.29	**uM**					718.23	**uM**	8.69	**uM**	1.21%	
LIGAND													
compound name	4-Carboxybenzenesulfonamide (CBS)												
description	4-sulfonylbenzoic acid at 97% purity												**Color key**
vendor	Sigma-Aldrich												fill in before experiment
product no.	000944798												fill in during experiment
lot no.	#MKBF3323V												automatically computed
purity		97.00%											
molecular weight		201.2	**g/mol**										
solubility		453	**mg/L**	2,251.49	**uM**								
Stock solution preparation													
		desired		**typical error**		**typical percent error**		**actual**		**error**		**percent error**	
target compound mass	**(most balances need min 10 mg)**	10	**mg**	0.1	**mg**	1.00%		10.01	**mg**	0.1	**mg**	1.00%	balance tared to 50 mL Falcon tube + holder near 0.1 mg uncertainty
buffer volume needed for target mass	**(for planning buffer usage)**	32.14	**mL**										
buffer volume needed for actual mass	**(use this for actual preparation)**	32.17	**mL**	0.64	**mL**	2.00%		32.17	**mL**	0.21	**mL**	0.65%	via P5000: 4x5 mL + 4.130 mL + 2x4.020 mL
purity-corrected stock solution concentration	**(be careful not to exceed solubility)**	1,500.00	**uM**	33.54	**uM**	2.24%		1,500.12	**uM**	17.90	**uM**	1.19%	
Syringe solution preparation													
		desired		**typical error**		**typical percent error**		**actual**		**error**		**percent error**	
dilution factor from stock to titrant solution		0.479		0.004		0.74%		0.47878		0.00094		0.20%	
stock solution volume		4.309	**mL**	0.04	**mL**	1.00%		4.309	**mL**	0.012	**mL**	0.28%	via P5000: 4.309 mL
buffer volume		4.691	**mL**	0.05	**mL**	1.00%		4.691	**mL**	0.012	**mL**	0.26%	via P5000: 4.691 mL
total volume for titrant	**(need min 350 uL for VP-ITC)**	9	**mL**	0.06	**mL**	0.71%		9	**mL**	0.017	**mL**	0.19%	
titrant concentration		718.29	**uM**	17	**uM**	2.35%		718	**uM**	9	**uM**	1.21%	(this error is included in the 'actual error' in thermodynamic parameters below)
PROTEIN													
protein name	carbonic anhydrase II (CAII)												
source	Sigma-Aldrich C2522-25mg												
lot no.													
molar extinction coefficient		50070	**M-1 cm-1**										
protein purity (or 100% if unknown)		100.00%											
Dialyzed stock solution concentration													
								actual		**error**			
absorbance measurement for 1 cm path length	**(e.g. NanoDrop)**							11.768	**A**	0.03	**A**	0.25%	used error from spec manual (for 200-350nm)
concentration of stock solution								235.03	**uM**	0.60	**uM**	0.25%	
purity-corrected concentration of stock solution								235.03	**uM**	0.60	**uM**	0.25%	
Cell solution preparation													**Add a section for UV-VIS measurement of protein final dilution**
		desired		**typical error**				**actual**		**error**		**percent error**	
dilution factor		0.04255		0.00058				0.04258		0.00036		0.83%	
stock solution volume		0.511	**mL**	0.005	**mL**			0.511	**mL**	0.004	**mL**	0.78%	via P1000
buffer volume		11.489	**mL**	0.11	**mL**			11.489	**mL**	0.044	**mL**	0.38%	via P5000: 2x5 + 1.489
total volume for titrate	**(need min 2.1 mL for VP-ITC)**	12.00	**mL**	0.12	**mL**			12.00	**mL**	0.044	**mL**	0.37%	
titrate concentration		10.00	**uM**	0.14	**uM**			10.01	**uM**	0.087	**uM**	0.87%	(this error is absorbed into the n parameter in the ITC fit)
THERMODYNAMIC PARAMETERS													
		reported from fit		**error from fit**		**percent error from fit**		**actual**		**error**		**percent error**	
n (stoichiometry, purity, and V0 correction)		0.915		0.003		0.37%		0.915		0.004		0.42%	Origin fit used purity-corrected protein concentration in cell
K (association constant)		1.20E+06	**M-1**	2.78E+04	**M-1**	2.32%		1.20E+06	**M-1**	3.14E+04	**M-1**	2.61%	
Kd (dissociation constant)		8.33E-07	**M**	1.93E-08	**M**	2.32%		8.33E-07	**M**	2.18E-08	**M**	2.61%	
DeltaH		-11.27	**kcal/mol**	0.05721	**kcal/mol**	0.51%		-11.27	**kcal/mol**	0.15	**kcal/mol**	1.31%	
TDeltaS		-2.97	**kcal/mol**	0.06	**kcal/mol**	1.98%		-2.97	**kcal/mol**	0.15	**kcal/mol**	5.00%	
DeltaG		-8.30	**kcal/mol**	0.01	**kcal/mol**	0.17%		-8.30	**kcal/mol**	0.02	**kcal/mol**	0.19%	