	VP-II C CBS-CAII							
date user EXDEDIMENTAL DETAILS	John D. Chodera <jchodera@berkeley. edu&gt;</jchodera@berkeley. 	12						
PERIMENTAL DETAILS								
temperature estimated Ka sample call volume (approximate)		25 C 1.00E+06 1/M 1.4 mL						
injection volume		10 uL						
dilution factor after final injection (d^n)		0.93082415714980						
cell concentration		desired uM			actual 10:01 uM	error 0.09 uM	percent error	
c-value		10.00			12.01	0.03	0.26%	
optimal Rm syringe concentration		5.34 718.29 uM			4.98 718.23 uM	8.69 uM	1.21%	
IGAND								
compound name	4-Carboxybenzenesulfonamide (CB							
description vendor	4-sulfonylbenzoic acid at 97% purity Sigma-Aldrich						Color key	viment
product no. lot no.	000944798 #MKBF3323V						fill in during experiment automatically computed	yiment mputed
purity		97.00%						
solubility		453 mg/L	2,251.49 uM					
Stock solution preparation								
et compound mass	(most balances need min 10 mg)	desired 10 mg	typical error	typical percent error	actual 10.01 mg	error 01 mg	percent error	balance tared to 50 ml. Falcon tube + holder near 0.1 mg uncertainty
buffer volume needed for target mass buffer volume needed for actual mass	(for planning buffer usage) (use this for actual preparation)	32.14 mL 32.17 mL	0.64 mL	2.00%	1	0.21 mL	0.65% via P5000: 4x5 m	
purity-corrected stock solution concentration	(be careful not to exceed solubility)	Mu 00.002,1	33.54 uM	2.24%	1,500.12 uM	17.90 uM	1.19%	
Syringe solution preparation								
dilution factor from stock to titrant solution		desired	typical error	typical percent error	actual 0.47878	error 0.00094	percent error	
stock solution volume buffer volume		4.309 mL 4.691 mL	0.04 mL 0.05 mL	1.00%	4.309 mL 4.691 mL	0.012 mL 0.012 mL	0.28% via P5000: 4.309 mL 0.26% via P5000: 4.691 mL	am.
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% (this error is inclu	ided in the 'actual error' in thermodynamic parameters
titrant concentration		718.29 uM	Mu 71	2.35%	718 uM	Wn 6	1.21% below)	below)
protein name	carbonic antrydrase II (CAII)							
source lof no	Sigma-Aldrich C2522-25mg							
molar extinction coefficient protein purity (or 100% if unknown)		50070 M-1 cm-1 100.00%						
Dialyzed stock solution concentration		l		İ				
absorbance measurement for 1 cm path length	(e.g. NanoDrop)				actual 11.768 A	error 0.03 A		used error from spec manual (for 200-350nm)
concentration of stock solution purity-corrected concentration of stock solution					235.03 uM 235.03 uM	09:0 MM	0.25%	
Cell solution preparation		desired	typical error		actual	епог	Add a section for percent error	Add a section for UV-VIS measurement of protein final dilution
dilution factor stock solution volume		0.04255 0.511 mL	0.0058 0.005 mL		0.04258 0.511 mL	0.00036 0.004 mL	0.83% 0.78% via P1000	
buffer volume total volume for titrate titrate concentration	(need min 2.1 mL for VP-ITC)	11.489 mL 12.00 mL 10.00 uM	0.11 mL 0.12 mL 0.14 uM		11.489 mL 12.00 mL 10.01 uM	0.044 mL 0.044 mL 0.087 uM	0.38% via P5000: 2x5 + 0.37% (this error is abso	via P5000; 2x5 + 1,489 (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	өттог	percent error	
n (stoichiometry, purity, and V0 correction) K (association constant)		0.915 1.20E+06 M-1	0.003 2.78E+04 M-1	0.37%	0.915 1.20E+06 M-1	0.004 3.14E+04 M-1	1%	Origin fit used purity-corrected protein concentration in cell
(dissociation constant)		8.33E-07 M -11.27 kcal/mol	1.93E-08 0.05721		8.33E-07 M -11.27 kcal/mol	2.18E-08 M 0.15 kcal/mol	2.61%	
eltaS		-2 97 kral/mol			lom/lood 70 c	landland 20 0	F 00%	