

## Langmuir-Freundlich Fit

Experimental Values							Fitting Parameters and Summary Statistics			
F	B	log F	log B	log B*	R <sub>E</sub>	T <sub>S</sub>	1	a	m	
0.0126	0.0485	-1.8999	-1.3146	-1.2758	0.00151	0.2887	1	130.8324		
0.0200	0.0685	-1.7000	-1.1645	-1.1797	0.00023	0.1499	a	0.0033		
0.0232	0.0755	-1.6340	-1.1223	-1.1480	0.00066	0.1190	m	0.4808		
0.0440	0.0960	-1.3561	-1.0179	-1.0145	0.00001	0.0579	RSS	0.0036		
0.0646	0.1157	-1.1898	-0.9368	-0.9346	0.00000	0.0254	TSS	1.2805		
0.1413	0.1745	-0.8498	-0.7583	-0.7713	0.00017	0.0004	R <sup>2</sup>	0.9972		
0.2740	0.2234	-0.5623	-0.6509	-0.6333	0.00031	0.0160				
0.4440	0.2997	-0.3527	-0.5233	-0.5327	0.00009	0.0645				
0.5949	0.3479	-0.2329	-0.4586	-0.4752	0.00028	0.1016				
1.0595	0.4458	0.0251	-0.3509	-0.3515	0.00000	0.1819				
1.8621	0.5589	0.2700	-0.2526	-0.2342	0.00034	0.2753				

Definitions		Binding Isotherm	
F	concentration of free guest (mM)		
B	concentration of bound guest (mM)		
B*	calculated concentration of bound guest (mM)		
B* = taF^m/(1+aF^m)			
RS	square of the residual		
SR = (log B - log B*) <sup>2</sup>			
TS	square of the total deviation from the mean		
TS = (log B - average log B*) <sup>2</sup>			
RSS	residual sum of squares		
RSS = SUM(RS)			
TSS	total sum of squares		
TSS = SUM(TS)			
R <sup>2</sup>	coefficient of determination		
R <sup>2</sup> = 1 - RSS/TSS			

To use this worksheet, input the experimental data (B and F) in the green area.  
Use the solver function (under the tools menu) to set R<sup>2</sup> (in blue) to a value of 1.00 by changing the fitting coefficients 1, a and m (in red).

