CHNOSZ via Rpad

Web interface to stability diagrams

Follow this link for help

setup environment

redoxin choose example

```
WWW: REnvSetup ( 1 )
WWW: this example provides 5 of 226 proteins in the database.
```

search thermodynamic data

```
WWW: SetupSearch ( 1 )
search by name, formula, or species number
```

GO

```
WWW: ProcessSearch ( 1 )
NULL
```

select thermodynamic data

```
WWW: SelectData ( 1 )
enter data source codes and/or species numbers
```

69,1,68,2,70,3,1,70,2,3,2210,70,22,26,1008

GO

```
WWW: ProcessData ( 1 )
WWW: 10 of 3001 data entries activated
```

select basis species

```
WWW: SelectBasis ( 1 )
basis species / logarithm of activity
```

CO2 aq	-5
water liq	0
NH3 aq	-4
e- aq	-7
H2S aq	-12
H+ aq	-7
	0

GO

```
WWW: ProcessBasis ( 1 )
    C H N O S  Z ispecies logact state
CO2 1 0 0 2 0  0       69     -5    aq
H2O 0 2 0 1 0  0        1      0   liq
NH3 0 3 1 0 0  0       68     -4    aq
e-  0 0 0 0 0 -1        2     -7    aq
H2S 0 2 0 0 1  0       70    -12    aq
H+  0 1 0 0 0  1        3     -7    aq
```

add protein sequences

WWW: SelectProteins (1)
protein sequence / name

	PROT1_NEW
	PROT2_NEW
	PROT3_NEW
	PROT4_NEW
	PROT5_NEW
	PROT6_NEW
	PROT7_NEW
	PROT8_NEW

GO

WWW: ProcessProteins (1)

select species of interest

WWW: SelectSpecies (1)
reaction coefficient / species / logarithm of activity

-1/110	GLRX1_YEAST aq	-6
1/143	GLRX2_YEAST aq	-6
0	GLRX3_YEAST aq	-6
0	GLRX4_YEAST aq	-6
0	GLRX5_YEAST aq	-6
0		0
0		0
0		0
0		0
0		0
0		0
0		0

GO

WWW: ProcessSpecies (1)

	CO2	H2O	NH3	e-	H2S	H+	ispecies	logact	state	name
1	549	-928	146	2296	4	2296	3002	-6	aq	GLRX1_YEAST
2	715	-1217	181	3042	5	3042	3003	-6	aq	GLRX2_YEAST
3	1444	-2425	371	5912	10	5912	3004	-6	aq	GLRX3_YEAST
4	1226	-2063	316	5076	6	5076	3005	-6	aq	GLRX4_YEAST
5	762	-1297	196	3194	6	3194	3006	-6	aq	GLRX5_YEAST

setup and plot diagram

WWW: SelectTP (1)

25	Temperature, degC
1	Pressure, bar

WWW: SelectVariables (1)

X,min,max	pH	0	14
Y,min,max	Eh	-0.6	0.6

WWW: SetupDiagram (1)

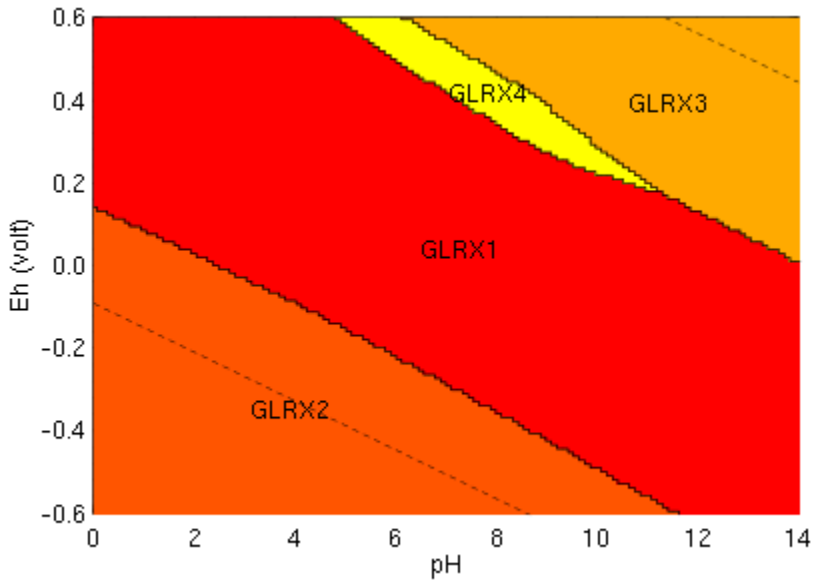
all plots: ☑ show graph ☑ use residues ☑ draw names

2-D plots: ☑ fill areas black line color

1-D plots: 1 number of line types

Calculate

```
WWW: ShowDiagram ( 1 )
affinity: temperature is 25 C.
affinity: pressure is 1 bar.
affinity: y-axis is Eh at 128 increments from -0.6 to 0.6.
affinity: x-axis is H+ at 128 increments from 0 to 14.
affinity: loading ionizable protein groups.
subcrt: 28 species at 298.15 K and 1 bar (wet).
diagram: balance method - per mole of protein backbone.
diagram: balance coefficients are 110 143 285 244 150.
diagram: using residues (balance vector reset to ones).
subcrt: 3 species at 298.15 K and 1 bar (wet).
subcrt: 4 species at 2 values of T and P (wet).
subcrt: 4 species at 2 values of T and P (wet).
opens in new window output from affinity()
opens in new window output from diagram()
```



calculate properties

WWW: SetupProperty (1)

Tmin,Tmax 24 99

Pmin,Pmax 1

Calculate

```
WWW: CalculateProperty ( 1 )
subcrt: 2 species at 11 values of T and P (wet).
subcrt: reaction is not balanced; it is missing this composition:
            C          H           N           O           S
 -0.009090909 -0.06433566 0.06153846 0.05594406 0.001398601
subcrt: adding missing composition from basis definition and restarting...
subcrt: 8 species at 11 values of T and P (wet).
$reaction
            coeff        name              formula state ispecies logact
3002 -0.009090909 GLRX1_YEAST  C549H886N146O170S4    aq     3002     -6
3003  0.006993007 GLRX2_YEAST C715H1161N181O213S5    aq     3003     -6
69   -0.009090909         CO2                 CO2    aq       69     -5
1     0.074125874       water                 H2O   liq        1      0
68    0.061538462         NH3                 NH3    aq       68     -4
2    -0.400000000          e-                 Z-1    aq        2     -7
70    0.001398601         H2S                 H2S    aq       70    -12
3    -0.400000000          H+                  H+    aq        3     -7

$out
      T P      logK          G         H         S        V       Cp     logQ         A
1  24.0 1 0.8806139 -1197.3428 -2563.274 -4.612072 1.953315 2.675641 5.395105 -6138.211
2  31.5 1 0.8343022 -1163.0057 -2542.940 -4.544495 1.951973 2.743288 5.395105 -6357.696
3  39.0 1 0.7905705 -1129.1748 -2522.167 -4.477137 1.952133 2.793850 5.395105 -6576.674
4  46.5 1 0.7492350 -1095.8473 -2501.061 -4.410324 1.953535 2.832828 5.395105 -6795.150
5  54.0 1 0.7101277 -1063.0181 -2479.694 -4.344253 1.956000 2.863871 5.395105 -7013.126
```

```
6  61.5 1 0.6730949 -1030.6813 -2458.117 -4.279042 1.959402 2.889424 5.395105 -7230.611
7  69.0 1 0.6379958  -998.8302 -2436.363 -4.214755 1.963650 2.911125 5.395105 -7447.610
8  76.5 1 0.6047016  -967.4576 -2414.457 -4.151423 1.968680 2.930084 5.395105 -7664.130
9  84.0 1 0.5730942  -936.5564 -2392.416 -4.089055 1.974444 2.947060 5.395105 -7880.179
10 91.5 1 0.5430652  -906.1194 -2370.254 -4.027646 1.980913 2.962587 5.395105 -8095.764
11 99.0 1 0.5145148  -876.1394 -2347.980 -3.967182 1.988065 2.977055 5.395105 -8310.892
```

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