A Computational Approach to pH Selective Reactions in the Extracellular Fluid of Cancer Cells Based in the Gibbs Free Energy Minimization Approach

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Significance

The dissociation of calcium sulfide into its ions and other apoptotic agents, as well as the distribution of the sulfides, as a function of pH is important for the mimicking of the extracellular environment of cancer and benign cells.

Innovation

Previous findings in the lab suggest that CaS dissociates selectively in the acidic extracellular environment of malign cells and not in the basic environment of benign cells.

Approach

Input

pH, volume, temperature, and initial moles of the following species: H_2O *(l)*, H_2S *(g)*, S^{2-} *(aq)*, Ca^{2+} *(aq)*, CaS *(aq)*, H_3O^+ *(aq)*, H_2S *(aq)*, HS^- *(aq)*, OH^- *(aq)*

Standard Gibbs free energy of formation of possible products

python

Output

Moles in equilibrium of the following species: H_2O *(l)*, H_2S *(g)*, S^{2-} *(aq)*, Ca^{2+} *(aq)*, CaS *(aq)*, H_3O^+ *(aq)*, H_2S *(aq)*, HS^- *(aq)*, OH^- *(aq)*.

Gibbs energy minimization:

- Guess value from computer algorithm
- Constraint in mass balance
- Constraint in value of each equilibrium

Results

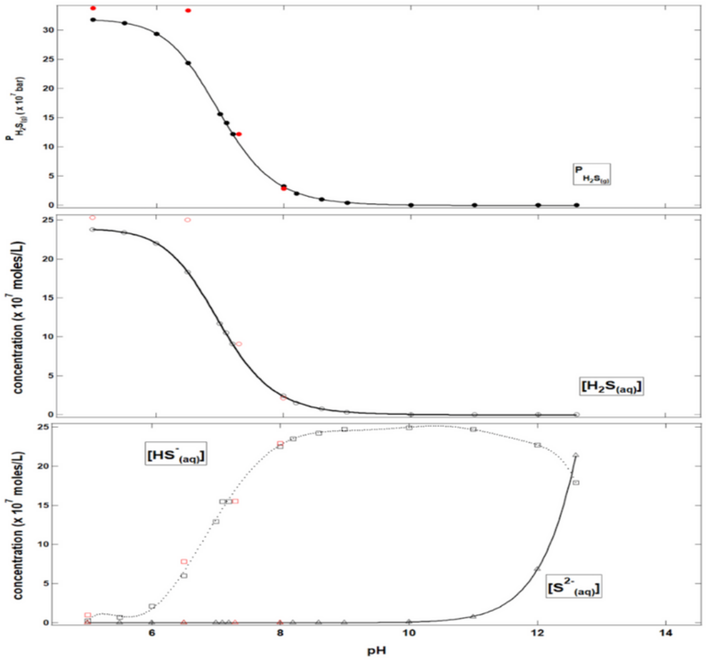

Figure 1. H2S (aq), H2S (g), HS- (aq) and S2-(aq) concentrations in equilibrium as a function of pH for an initial [S2-] of 2.5 x 10-8 M. Data in red represents the calculated equilibrium concentrations when an initial concentration of 2.5 x 10-8 M of CaS is employed.

pH	[CaS]
5.0	1.0191E-23
6.5	2.24703E-21
7.3	1.24703E-19
8.0	2.82468E-19

Table 1. Calculated equilibrium concentrations of CaS as a function of pH. The initial [CaS] is 2.5 x 10-8 M.

Conclusion

- The total Gibbs minimization approach was used for a wide range of pH values to mimic different biological environments.
- The results are not consistent with the hypothesis since CaS dissociates in basic environments.

Future work

- We also wish to extend the total Gibbs minimization approach to other cellular processes as well as to study these findings in living cells.

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