Indicator Displacement Assays and Mixed-Host Sensor Arrays: A Simulation-Based Study of Classification Efficiency

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1 Introduction

In certain instances, a species requires classification into a specific class. To achieve this, we must gather information about our species, which is facilitated by a sensor. Chemosensors are sensors that operate based on the principles of chemical equilibrium. The signal produced by these sensors varies depending on the equilibrium conditions, specifically the initial concentrations and equilibrium constants. In this discussion, we will explore IDAs (Indicator Displacement Assays) and mixed-host sensor arrays, examining the conditions under which these yield optimal classification efficiency.

2 Sensor Architectures

IDAs and mixed-host sensors generate signals through variations in the concentrations of signal-producing species. These variations are then measured.

$$\mathrm{H} + \mathrm{D} \rightleftharpoons \mathrm{HD} \qquad K_{HD} \tag{1}$$

$$\mathrm{H} + \mathrm{G}_1 \rightleftharpoons \mathrm{HG}_1 \qquad K_{HG_1} \tag{2}$$

$$\mathrm{H} + \mathrm{G}_2 \rightleftharpoons \mathrm{HG}_2 \qquad K_{HG_2} \tag{3}$$

Mixed-host sensors are IDAs with an additional competitive reaction between the Guest and the Dye

$$\mathrm{D} + \mathrm{G}_1 \rightleftharpoons \mathrm{DG}_1 \qquad K_{GD_1} \tag{4}$$

$$\mathrm{D} + \mathrm{G}_2 \rightleftharpoons \mathrm{DG}_2 \qquad K_{GD_2} \tag{5}$$

Each sensor array consists of two sensor elements. The host (H) and the dye (D) are present at equal initial concentrations C_s, while the Guest (G) is introduced at concentration C_0.

3 Constants

Table 1: Formation constants defining the IDA sensor arrays.

Constant	Notation
$\log(K_{HD}^{(1)})$	K_1
$\log(K_{HG_1}^{(1)})$	K_2
$\log(K_{HG_2}^{(1)})$	K_3
$\log(K_{HD}^{(2)})$	K_4
$\log(K_{HG_1}^{(2)})$	K_5
$\log(K_{HG_2}^{(2)})$	K_6
$\frac{\log(K_{HD}^{(1)})+\log(K_{HD}^{(2)})}{2}$	$\overline{K}_{HD}$
$\log(K_{HD}^{(2)}) - \log(K_{HD}^{(1)})$	ΔK_{HD}
$\log(K_{HG_2}^{(i)}) - \log(K_{HG_1}^{(i)})$	$\Delta K^{(i)}$
$\min(\log(K_{HG_1}^{(i)}), \log(K_{HG_2}^{(i)})) - \log(K_{HD}^{(i)})$	$\Delta D^{(i)}$

4 Class Definitions

Two classes are defined:

- **Class 1**: Species with smaller K_{HG} in the first sensor element.
- **Class 2**: Species with larger K_{HG} in the first sensor element.

5 Methods

Formation constants are drawn from

$$P = \{1, 2.5, 4, 5.5, 7, 8.5, 10, 11.5, 13\}.$$

For each permutation, 90 concentrations per class are sampled for C_0, keeping C_s fixed. UV–vis signals for free Dye (D) and complexed Dye (HD) are simulated, yielding signal vectors. Data are split into training and test sets, and classification is performed using PLS-DA.

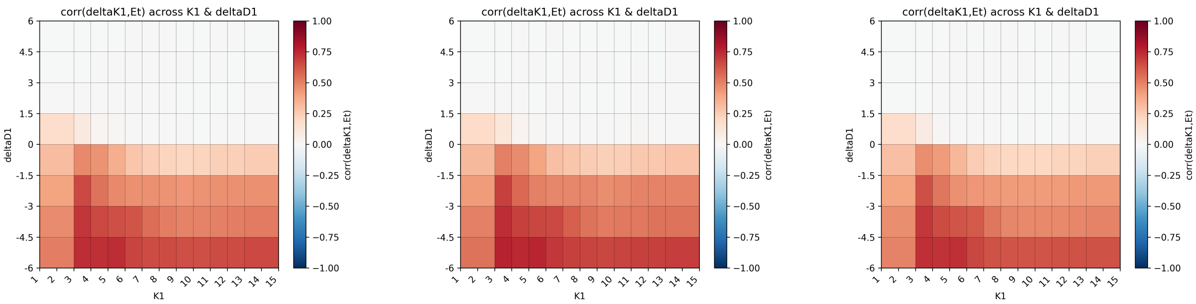
6 Efficiency Subsets

Sets are partitioned into:

- **P**: $\log K_{HG_2} - \log K_{HG_1} \geq 0$
- **N**: $\log K_{HG_2} - \log K_{HG_1} \leq 0$
- **U**: Union of **P** and **N**

7 Correlation Analysis

Mean test efficiency mean(E_t) is analyzed against various parameters.



(a) U (b) N (c) P

Figure 1: Figure N: description

8 Conclusions

The two sensor elements behave nearly independently. Optimal classification efficiency is achieved by:

- Maintaining $\log K_{HD} \approx 8$
- Maximizing ΔK
- Minimizing ΔD such that strong guest binding approaches K_{HD}

9 Confirmatory Simulation

A secondary simulation uses $\overline{K}_{HD}$ and ΔK_{HD} as design variables.

Table 2: Factor pools used in the confirmatory simulation.

Factor	Range
MeanHD	$5:1:11$
ΔHD	$-8:2:8$
ΔD	$-6:1.5:6$
ΔK	$0:2:14$

10 Results

Two deviations from the primary trends are observed:

1. At least one ΔD must be negative
2. Optimal performance favors $\Delta D_1 < 0$ and $\Delta D_2 > 0$