

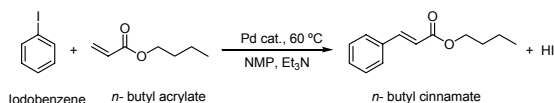


# Less Calibration in HTE!

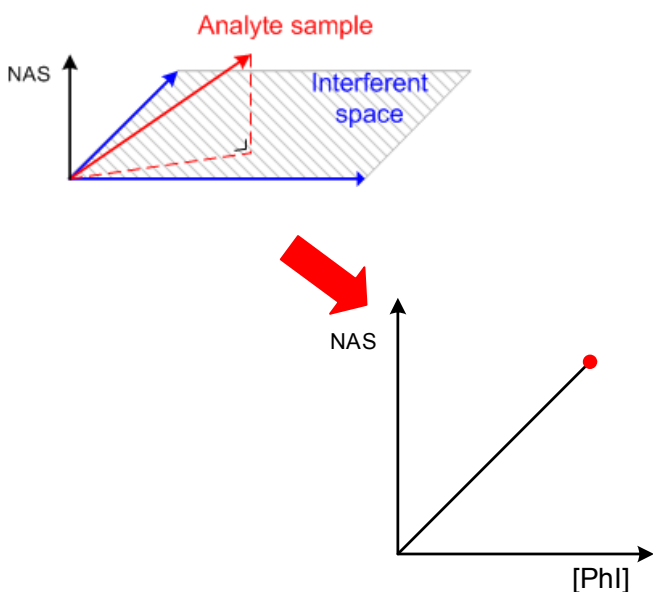
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Combinatorial catalysis is a new field that brings together rational design and High Throughput Experimentation (HTE). Much effort is focused on new methods for the synthesis and screening of catalyst libraries using novel techniques.

The Heck reaction was monitored at 60 °C using FT-NIR spectroscopy. A PLS calibration model for Iodobenzene (PhI) quantification based on GC results was built using **32** samples.



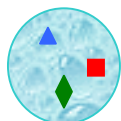
We use the Net Analyte Signal (**NAS**) approach<sup>1</sup> to build a calibration model for FT-NIR measurements using a minimum number of calibration samples.



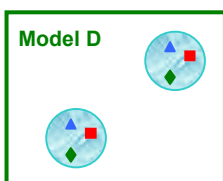
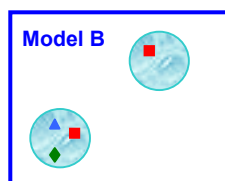
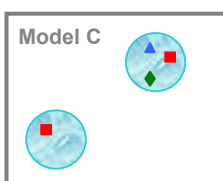
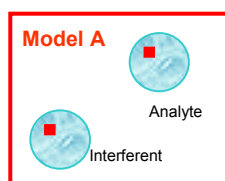
Which **type** of samples?



Single-component samples

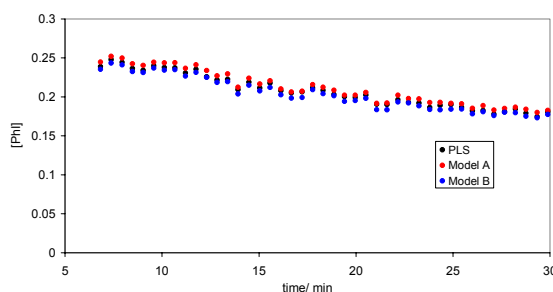
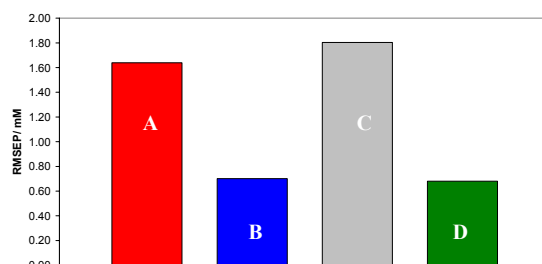


Multi-component samples



## Results

5 chemical compounds  $\rightarrow$  5 calibration samples



## Conclusions

- Multi-component samples are preferred in the interferent space. The analyte sample composition has a limited effect.
- Calibration reduced from 32 to 5 samples.

1. Cruz, S.C.; Aarnoutse, P. J.; Rothenberg, G.; Westerhuis, J.A.; Smilde, A.K., Blik, A. *Phys. Chem. Chem. Phys.*, **2003**, 5, 4455-3360.