

Adaptive Spectroscopy and Molecular Feature Extraction for Real-Time High- Throughput Chemical Analysis

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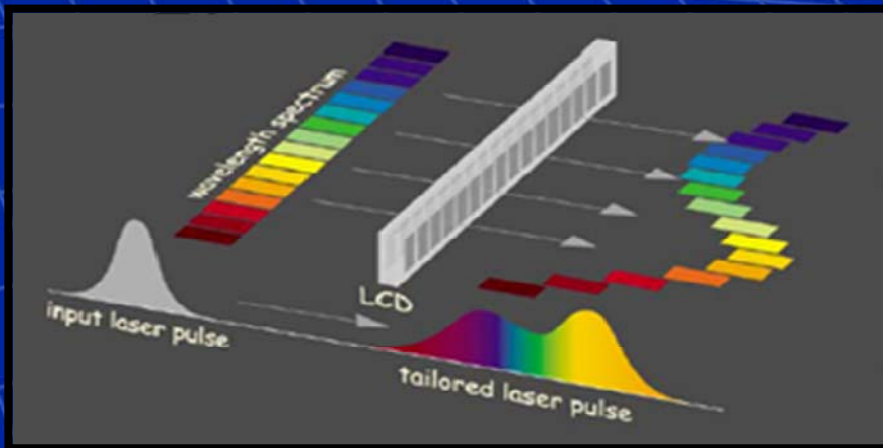
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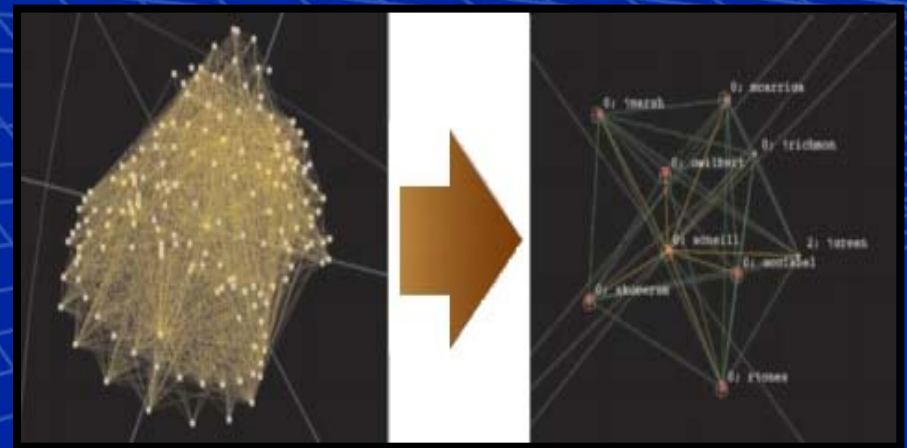


- **Advanced Sensing**
- **Signature Detection**
Chemical and Biological
Defense and Response

- **Dynamic Systems**
- **Adaptive Systems**
- **Reconfigurable Systems**
Information Exploitation



Cutting Edge
Chemical Security



Next-generation Real-time
Decision-driven Systems

Adaptive Intelligent Feature Extraction

Challenges

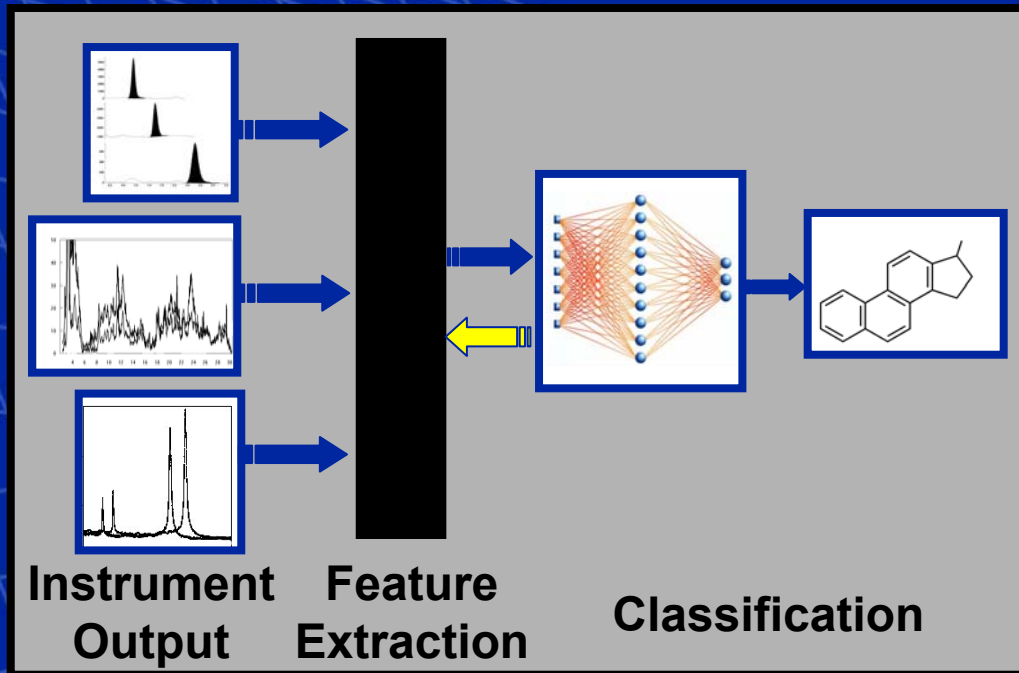
Raw data **too complex** for direct classification

Traditional feature extraction **too time consuming**

Changes in instrument array traditionally require re-tooling feature extraction approach

Features should be optimal for classification algorithm, not human inspection

**Adaptive • Intelligent • Fast
Robust • Dynamic**



Our Feature Extraction Method:

Ignores unimportant details

Adapts to vast changes in input

Agnostic about choice of instruments

Listens to feedback from the classifier

Quantum Control

- Flexibility of detection type(s)
 - Shaped laser pulse to drive optimal signature
 - One excitation pulse → simultaneous & multiple spectral signatures
 - Feature extraction in parallel – machine learning “in loop” with experimental for dual optimization
- Discrimination capability
 - Separate extremely similar & complex molecules
 - Probing functional group landscape for identification of classes & unknowns
- High duty cycle (1 kHz laser)
 - RIEDAR goal – reduced or no signal averaging
 - Laser hardware improvements in last 5 years
 - Energy / pulse, repetition rate, stability, bandwidth, shaping
- Dual optimization of experimental signature with computational feature extraction

