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QSTAR Session - NCS2012 Potsdam

Quantitative Structure Transcriptional Activity Relationship

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Understanding New Molecules
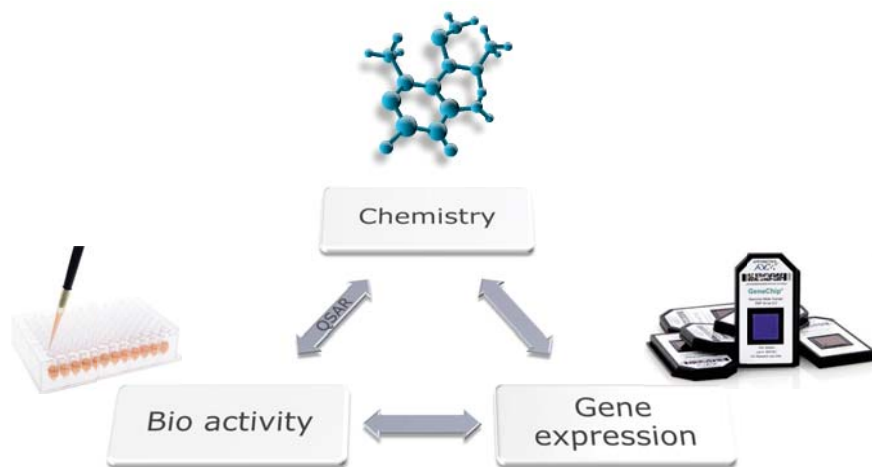
Chemistry

QSAR

Bio activity

Gene expression

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QSTAR Session - NCS2012 Potsdam

Quantitative Structure Transcriptional Activity Relationship

= QSAR + T

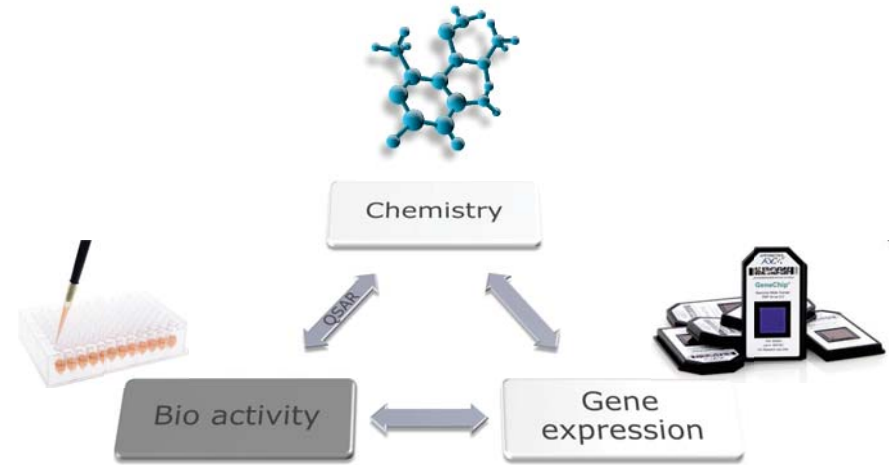janssen PHARMACEUTICAL COMPANIES of Johnson-Johnson

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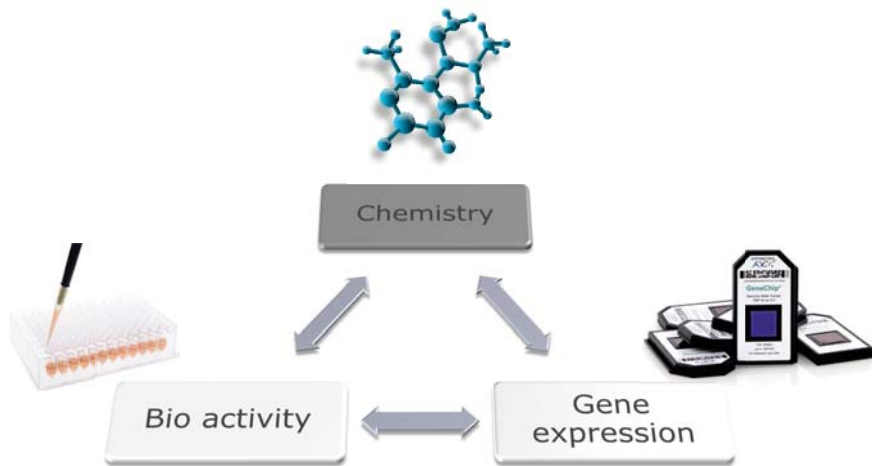Center of Excellence
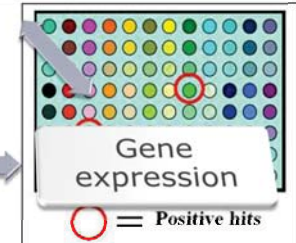
Bioassays – High Troughput Screening
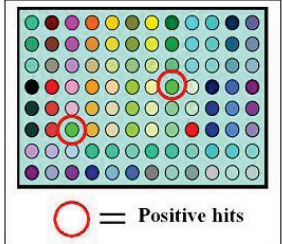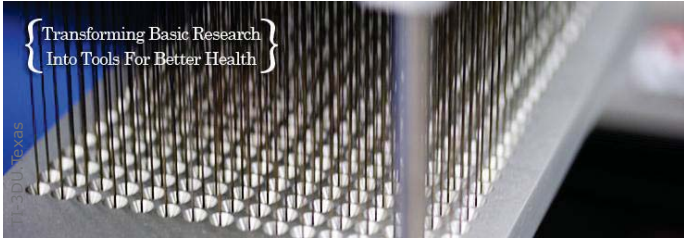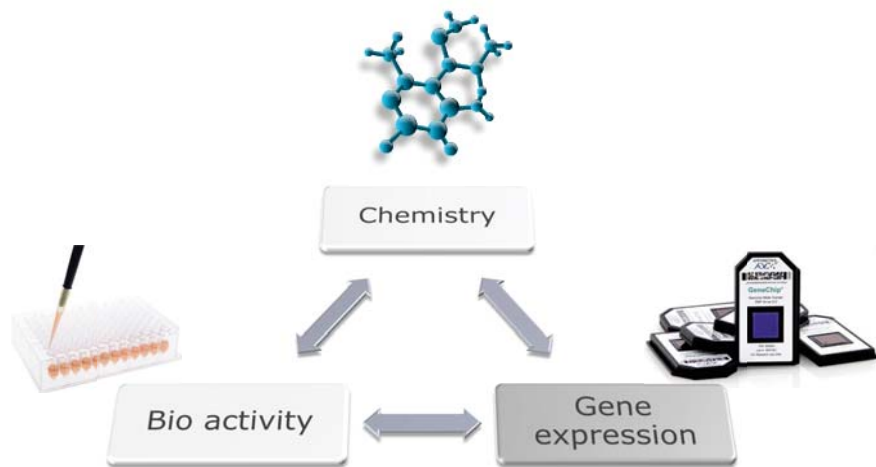

Understanding New Molecules

Understanding New Molecules

Bioassays – High Troughput Screening

Understanding New Molecules
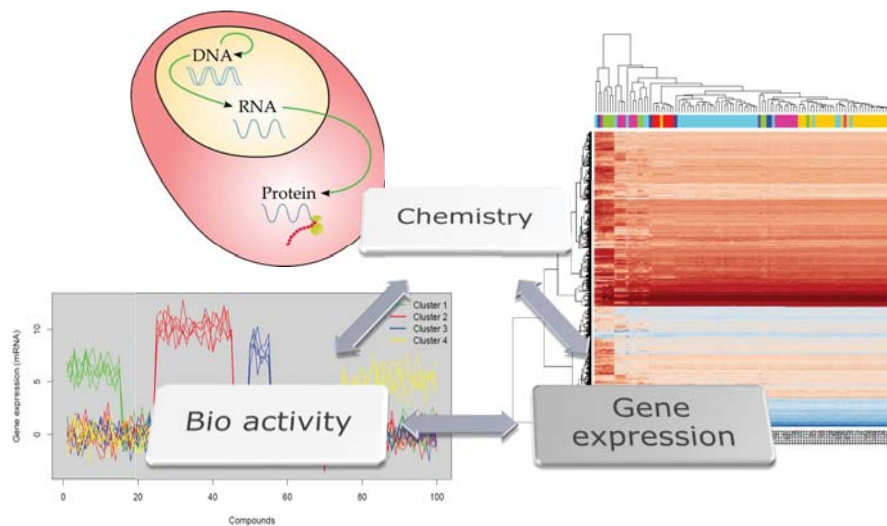
Chemistry

Bio activity ↔ Gene expression

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Chemical Structures

Paracetamol

Acid

Chemistry

Amide

Phenyl core

Hydroxyl

Phenyl core

Aspirin

Bio activity ↔ Gene expression

From Wikipedia

Legend
H, O, N, C

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Gene Expression Profiling

DNA
RNA
Protein

Chemistry

Bio activity

Gene expression

Cluster 1
Cluster 2
Cluster 3
Cluster 4

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Chemical Structures

Paracetamol

Acid

Amide

Phenyl core

Hydroxyl

Phenyl core

Aspirin

Ester

From Wikipedia

Legend
H, O, N, C

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QSTAR Session
Terminology

Gene Expression (GE)
  gene 001, gene 002, ...

Bio-Activity (BA)

Chemistry (CH)
  Compounds : cpd 001, cpd 002, ...
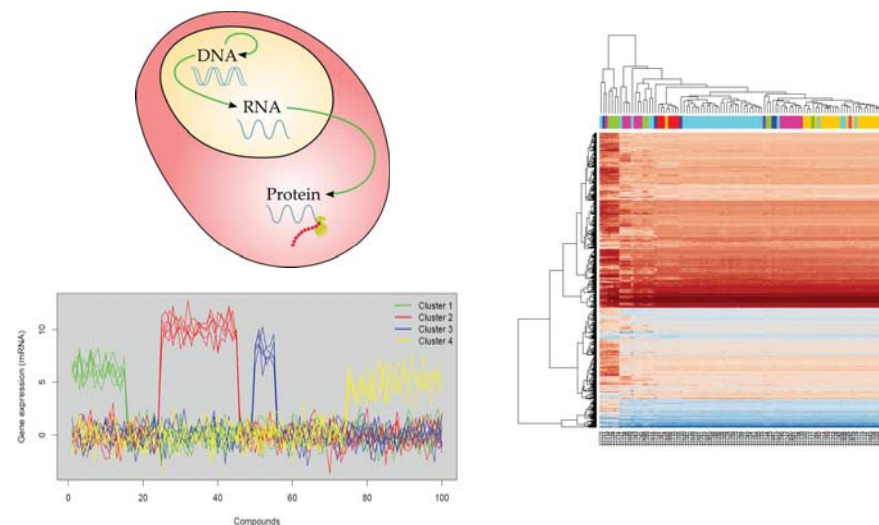 Finger print features : fpf 001, fpf 002, ...

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Gene Expression Profiling

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QSTAR Session Contents

Development of Predictive Models and Feature Selection Using LASSO and Elastic Net
Pushpike Thilakarathne

Analoging in large databases with structural fingerprint features
Martin Heusel

Integrated analysis of microarray data, biological data and chemical data in drug development
Nolen Joy Perualila

Biclustering in drug design
Djork-Arné Clevert

Integrated statistical analysis of three data sources for the detection of chemical fingerprint features that are simultaneously associated with bio-assay and transcriptomics data

Olivier Thas, Federico Mattiello

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Understanding New Molecules

+5,000 fingerprint features

Chemistry

QSAR ~20,000 compounds

Bio activity ←→ Gene expression

~1,000 screens +20,000 genes

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