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# Quality in the Lifesciences: software and much more

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# Alma mater

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Санкт-Петербургский государственный университет

Институт химии

Universität Rostock

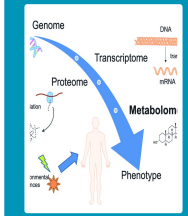
gegründet 1419

Traditio et Innovatio

ITMO UNIVERSITY

# Life science

## Life science




Domain


Requirements

# Life science: areas

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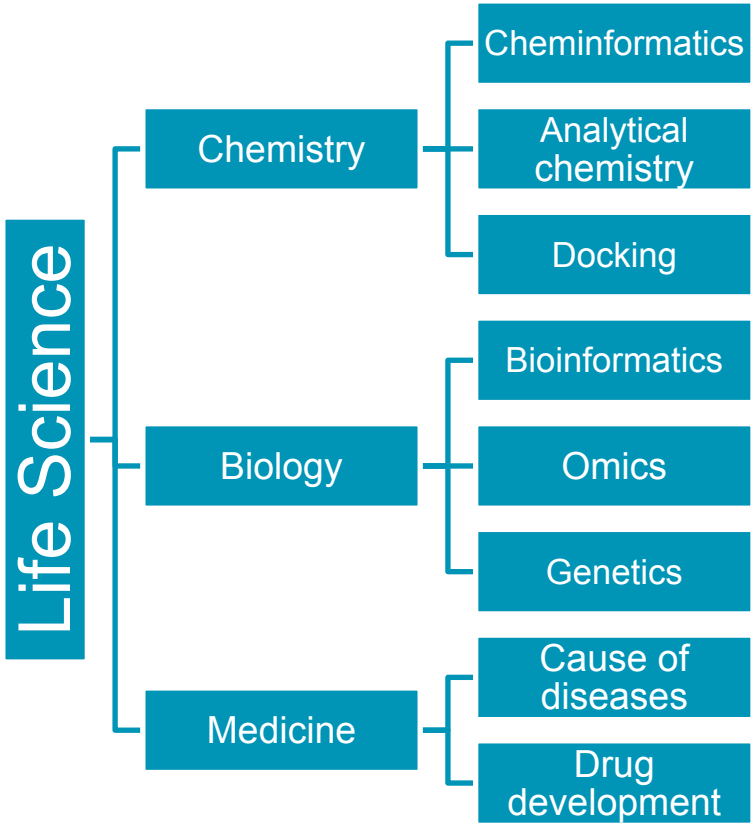


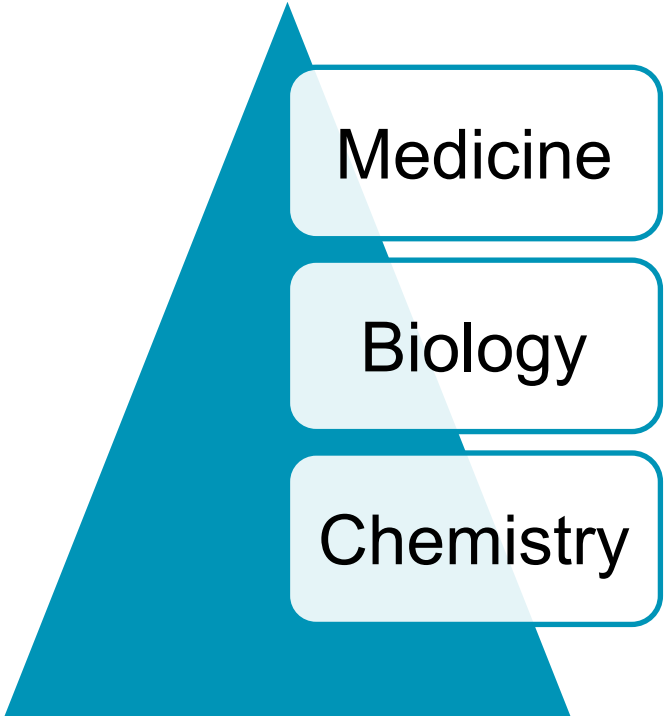

# Life science: what do we do

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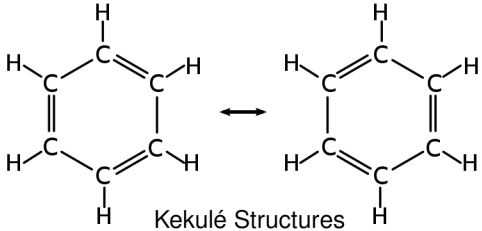
## Cheminformatics

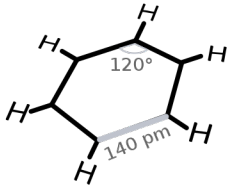
Simplified molecular -input line-entry system

$C_6H_6$

Benzene
Molecular formula

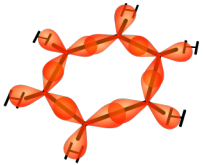


Kekulé Structures
(Resonance Forms)

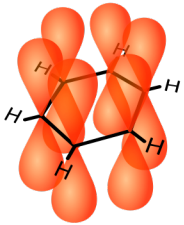



Planar Hexagon
Bond Length 140 pm

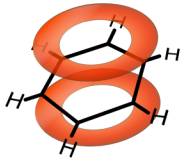
SMILES:
c1ccccc1



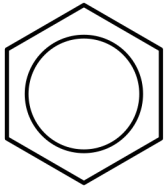
Sigma Bonds
$sp^2$ Hybridized orbitals



6 $p_z$ orbitals



delocalized pi system



Benzene ring
Simplified depiction

InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

# Life science: what do we do

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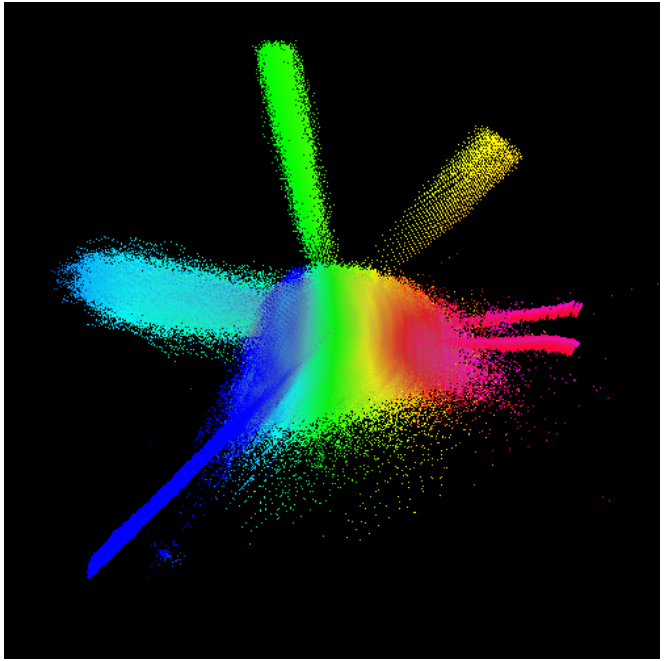
Cheminformatics

Chemical space ~ $10^{60}$ molecules

vs

Age of Universe ~ $10^{17}$ seconds



# Life science: what do we do – testing

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## Cheminformatics

How do we approach chemical features testing?

- Experience based exploratory testing
- Data driven testing
- Extensive DB querying
- Test automation

# Life science: what do we do – exploratory testing

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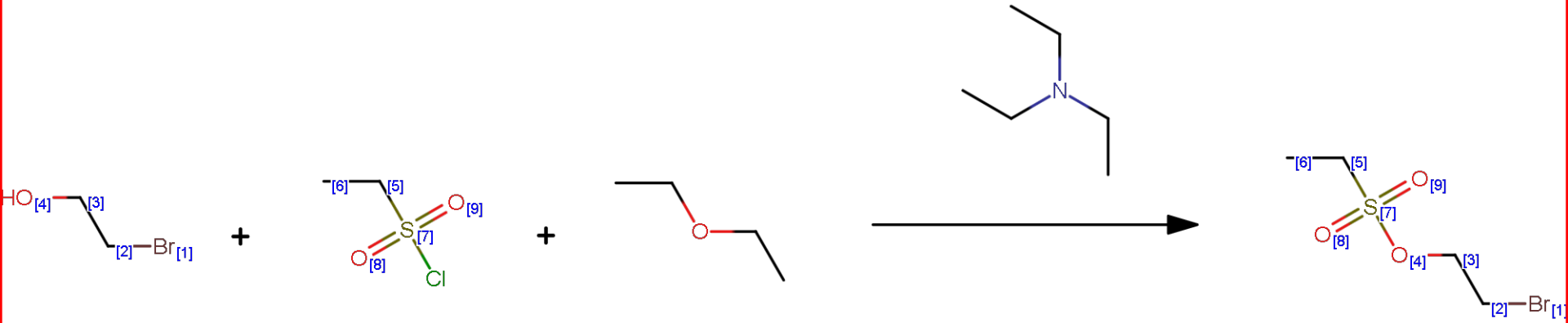
## Cheminformatics

[OH:4][CH2:3][CH2:2][Br:1].[CH3:6][CH2:5][S:7](Cl)(=[O:9])=[O:8].CCOCC>CCN(CC)CC>[CH3:6][CH2:5][S:7](=[O:9])(=[O:8])[O:4][CH2:3][CH2:2][Br:1]



# Life science: what do we do – data driven testing

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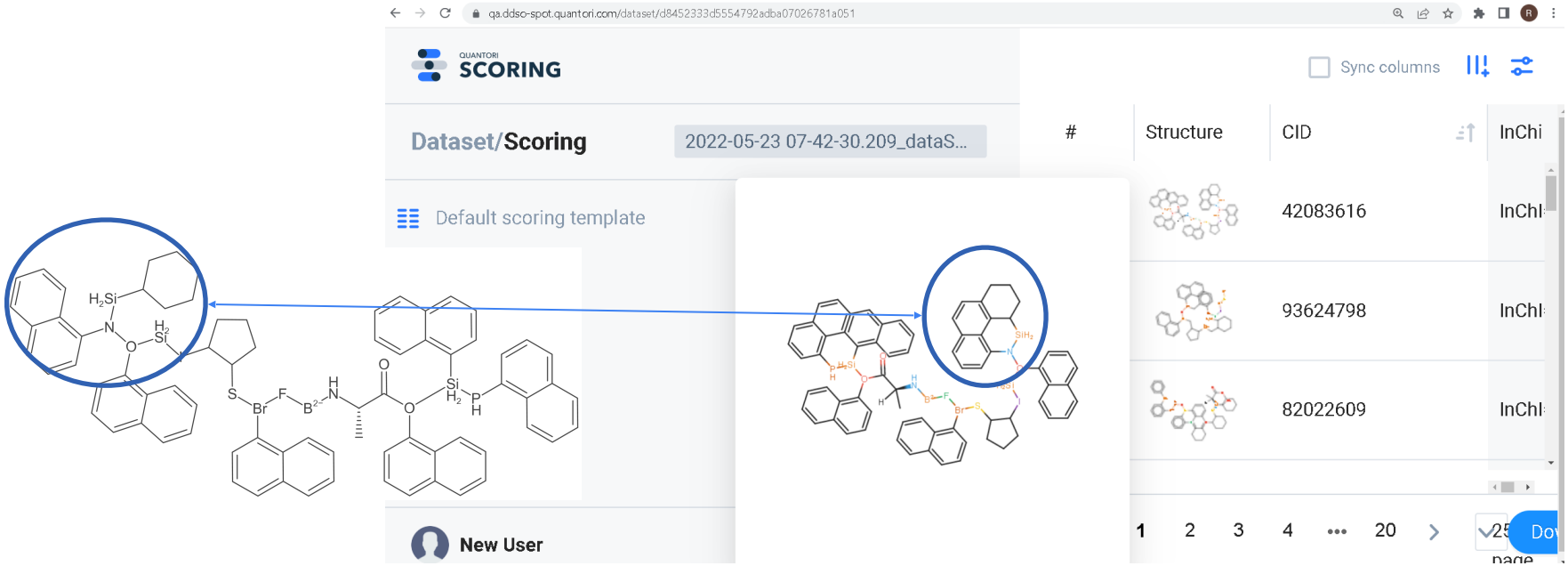
## Cheminformatics



# Life science: what do we do – DB queries

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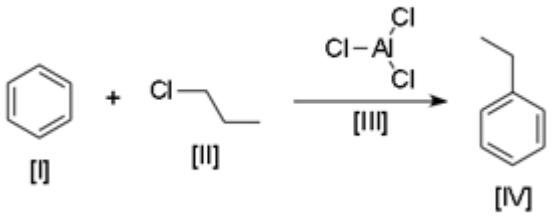
## Cheminformatics




```
select reactant.quantity from reaction where reactant.smiles like 'c1ccccc1'

select reactant.equiv
from description
inner join reaction
on reaction.reactant.smiles = description.reactant.smiles
where description.reactant.smiles like 'c1ccccc1'
and description.temperature between 30 and 50
```

# Life science: how do we do

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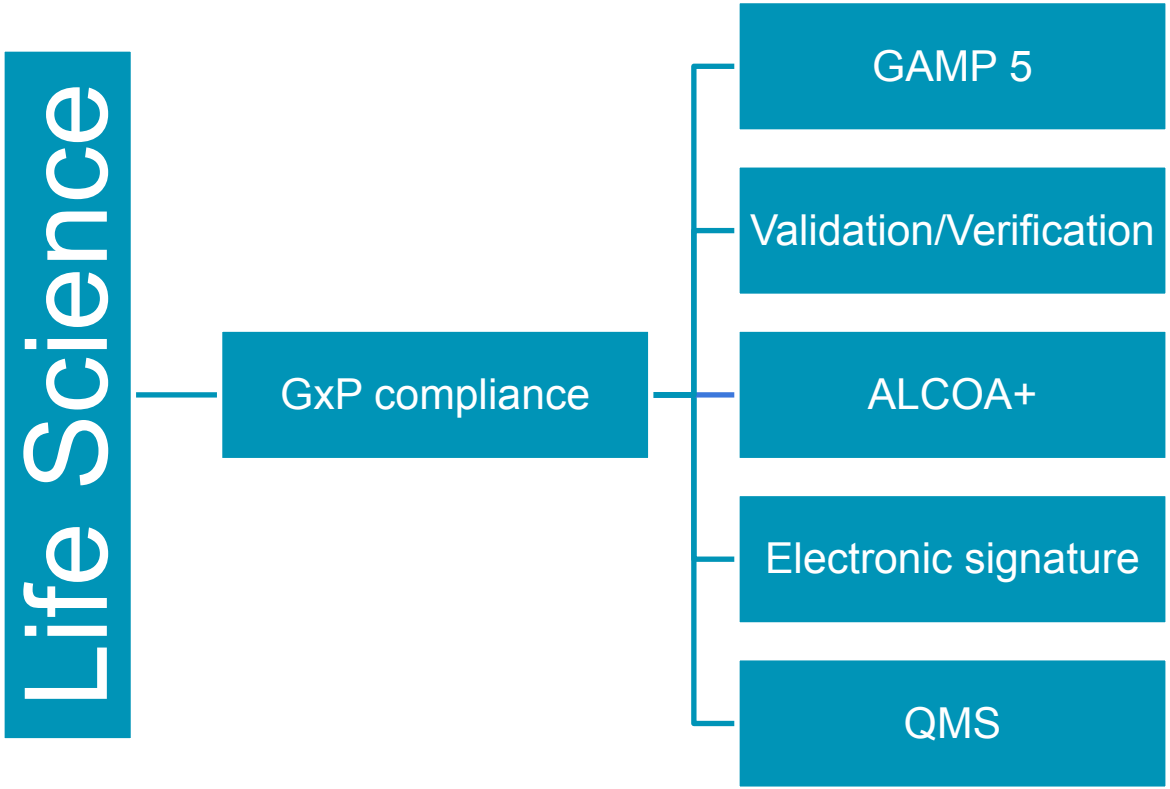

# Life science: how do we do

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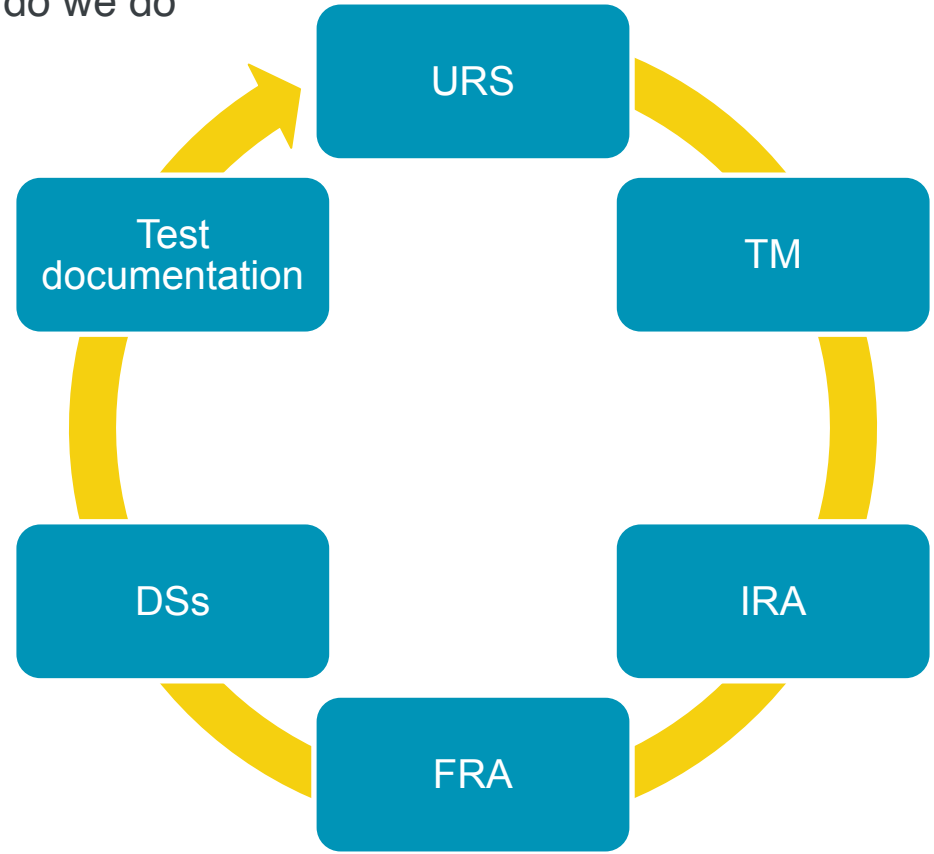

# Life science: how do we do

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FRA

| S/P | High | Medium | Low |
|---|---|---|---|
| High | High | High | Medium |
| Medium | High | Medium | Low |
| Low | Medium | Low | Low |

# LS and life quality

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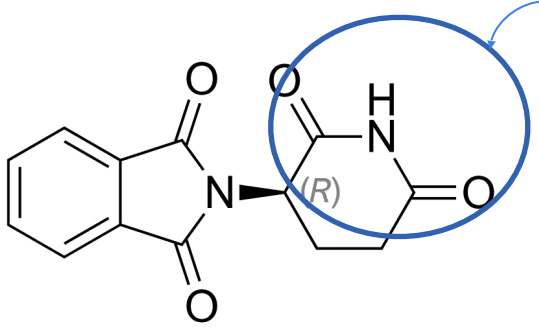
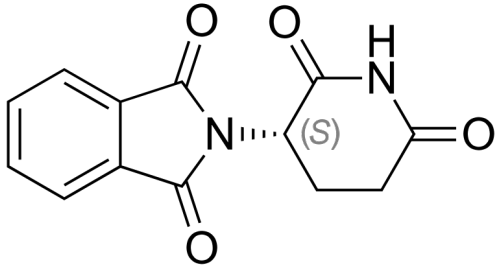
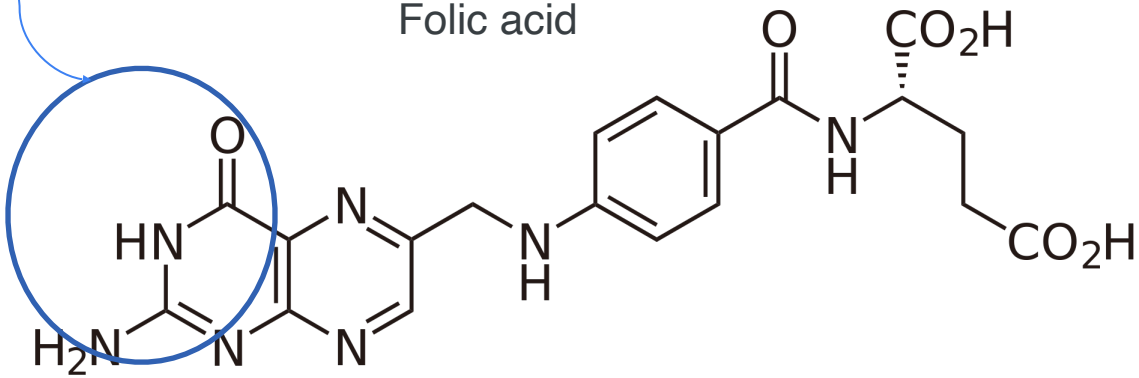
## Thalidomide scandal



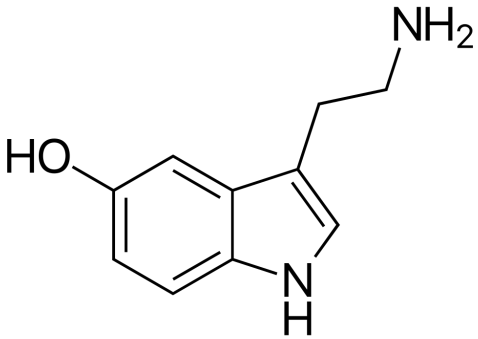



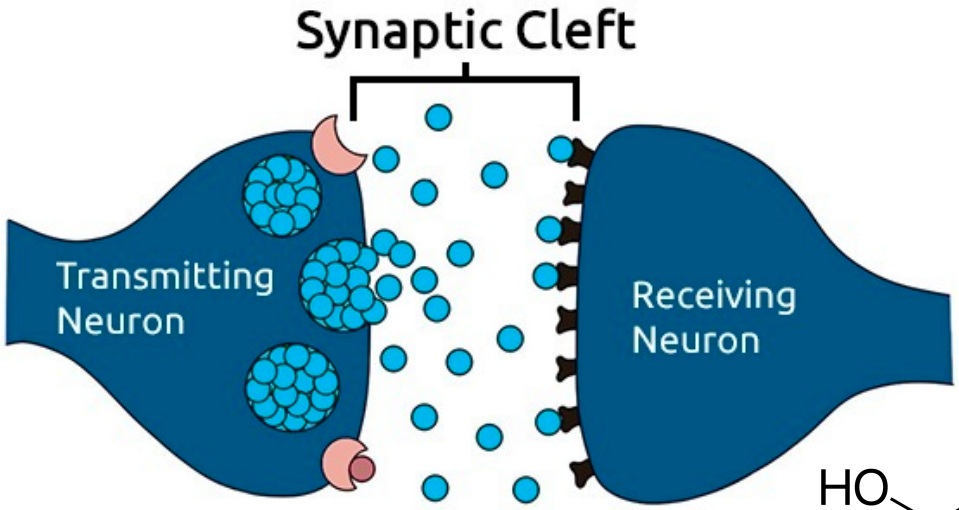

Folic acid

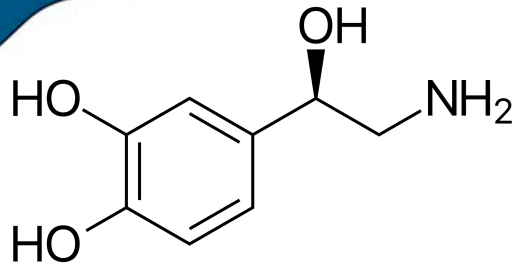


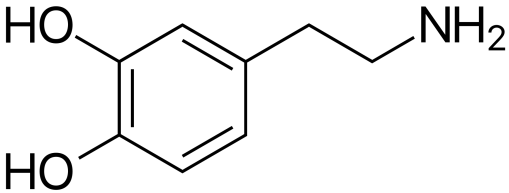
# LS and life quality

## Depression and anxiety



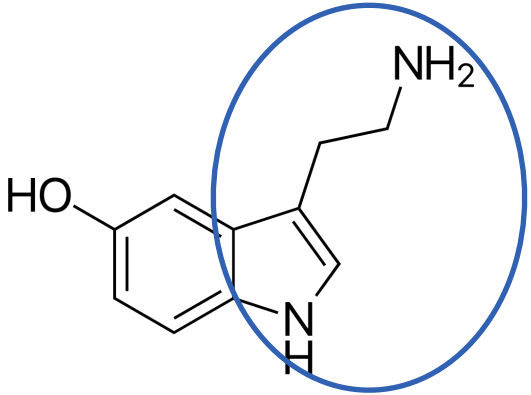



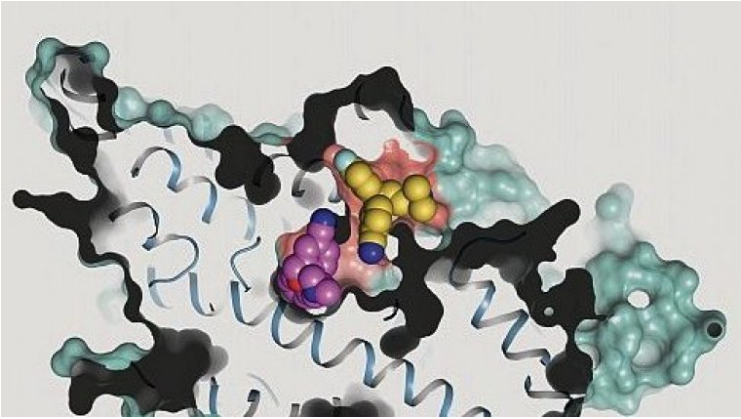



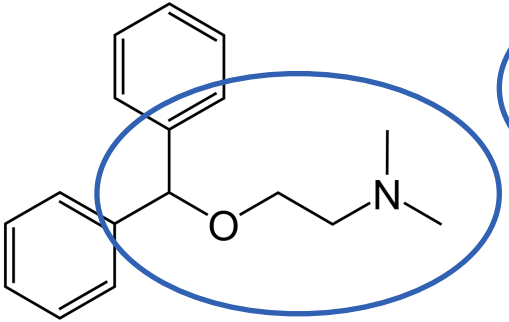



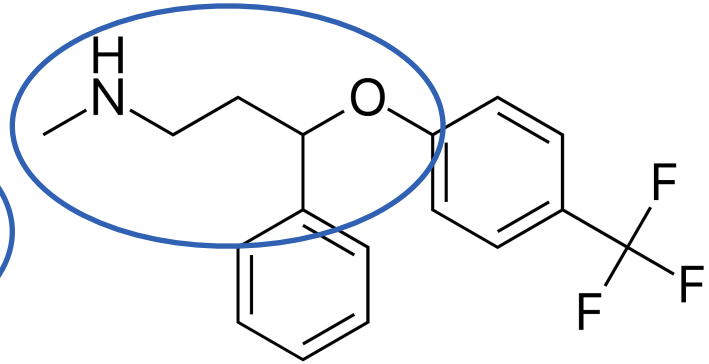
# LS and life quality

## Depression and anxiety





# Chemistry and SD

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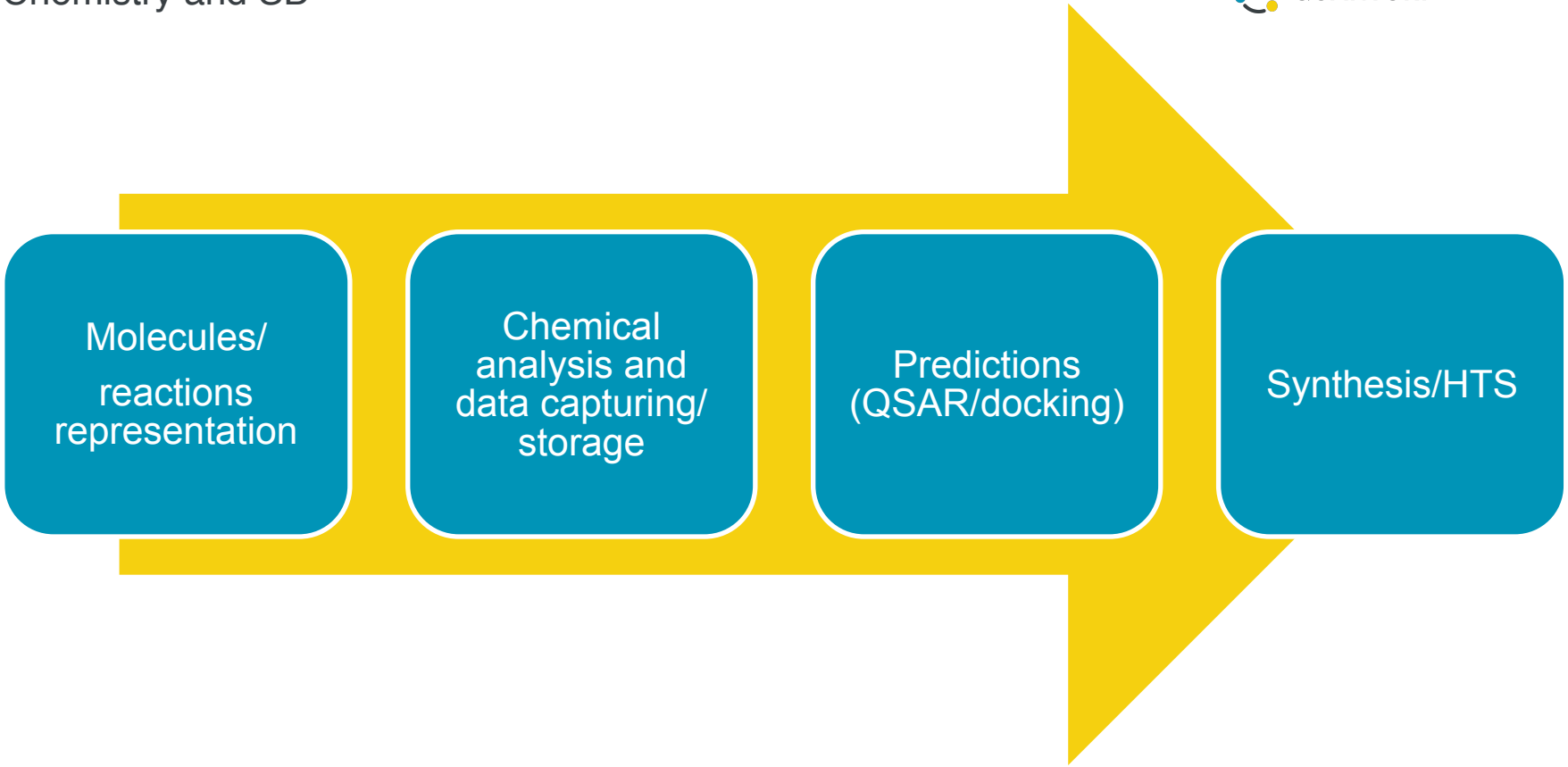

# Chemistry and SD

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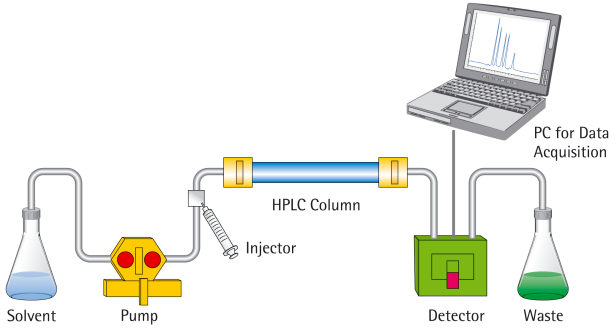
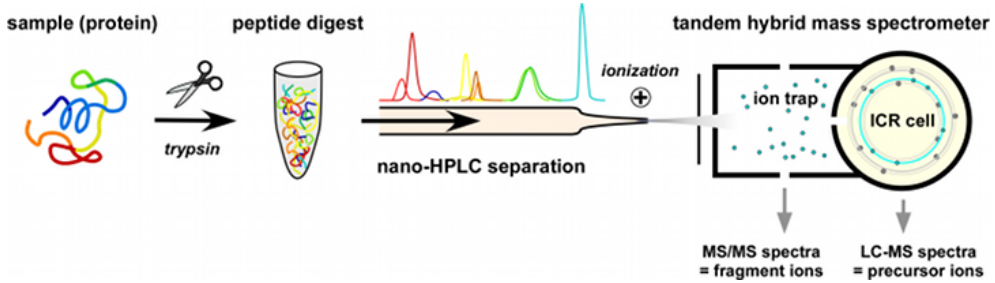
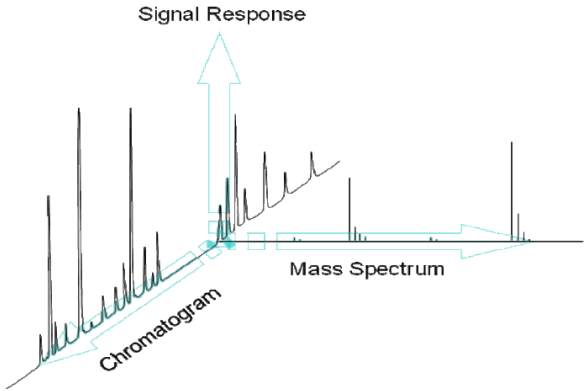
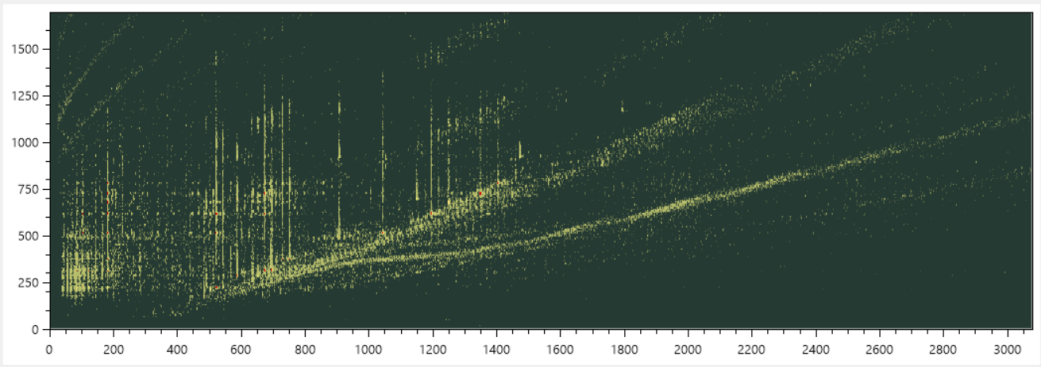
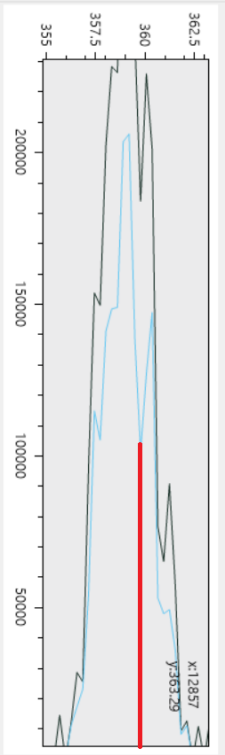


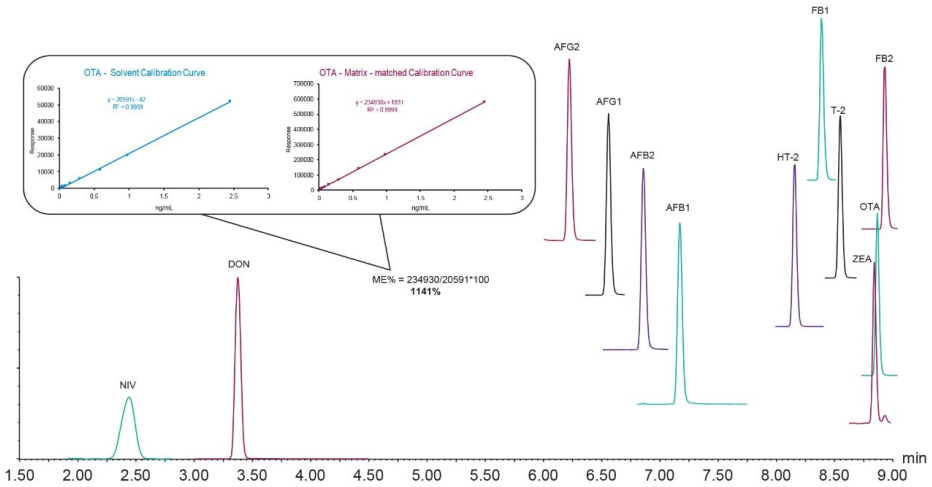
# Chemistry and SD




Chromatography:
- Quantitative analysis
- Qualitative analysis

The issue we faced: peak properties miscalculation
Is this one substance? Two substances? How to assess the quantity?

Actual peak properties:
- Are they calculated correctly?
- Algorithm to deconvolute?



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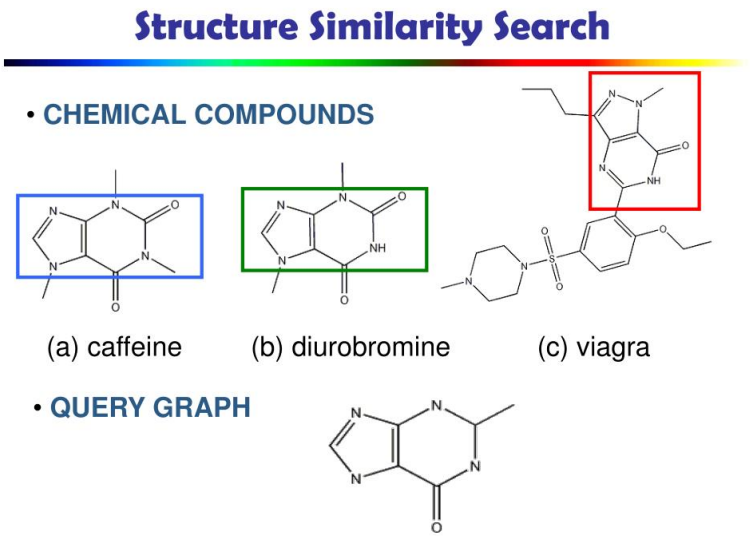
## Similarity problem




$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}.$$

# SD and domain knowledge

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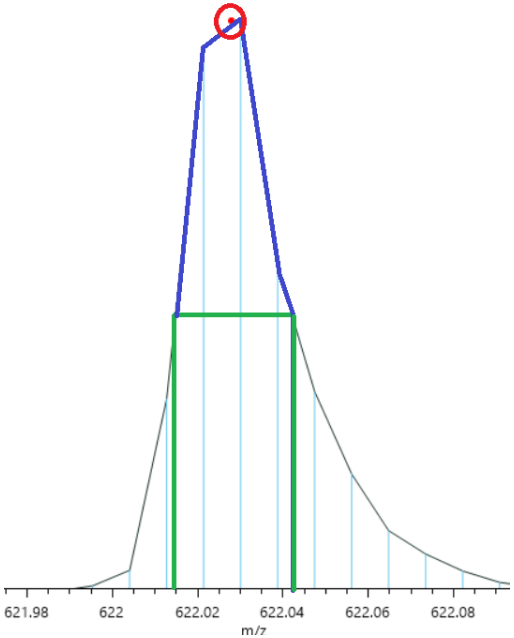
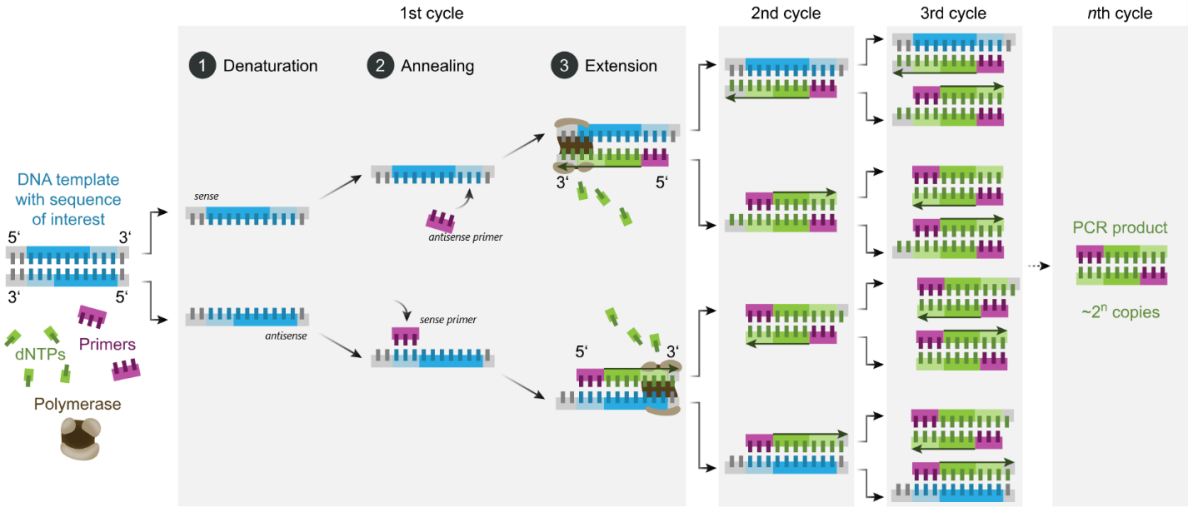
## Mass centroid problem




```python
@staticmethod
def calculate_centroid(x, y):
    thr = max(y) / 2
    y_cut = []
    x_cut = []
    area = []
    x_centr = []
    x_w = []
    incl = Centroid.filter_y(y)
    for i in range(1, len(incl) - 1):
        x_cut.append(Centroid.x_border(x, y, i, incl, thr))
        y_cut.append(Centroid.y_border(y, i, incl, thr))
    for i in range(len(x_cut) - 1):
        x_centr.append(Centroid.calc_trapezoid_centroid([x_cut[i], x_cut[i + 1]], [y_cut[i], y_cut[i + 1]]))
        area.append(Centroid.calc_area([x_cut[i], x_cut[i + 1]], [y_cut[i], y_cut[i + 1]]))
    area_tot = sum(area)
    for i in range(len(x_centr)):
        x_w.append(x_centr[i] * area[i] / area_tot)
    return sum(x_w)
```

# Scientists and science

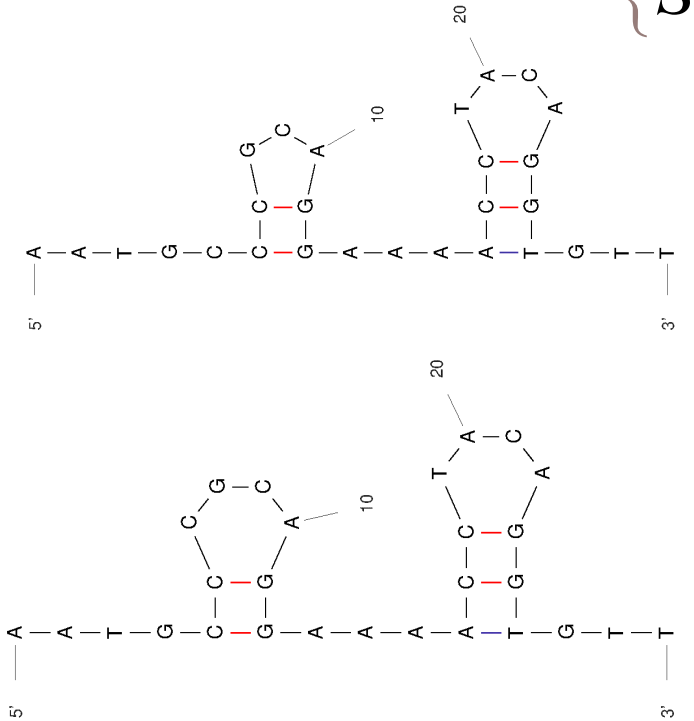


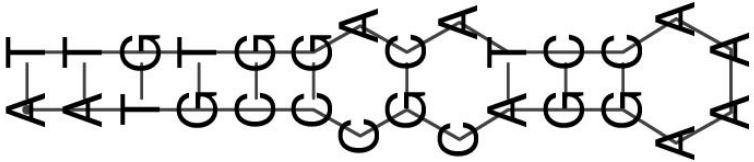

$$G(T, \boldsymbol{p}, S, \boldsymbol{c}) = \sum_{p, c_{p,min} \le c_p \le c_{p,max}} G_p(T, S, c_p) \to min$$

# Scientists and science

AATGCCCGCAGGAAAACCTACAGGTGTT

$$\{S_s\} = dG_f(p) < 0$$



/alignment(AATGCC-TTGTGG)/internalLoop(CGC-ACA)/alignment(AGG-TCC)/hairpin(AAAA)/

# QA and LS: compliance

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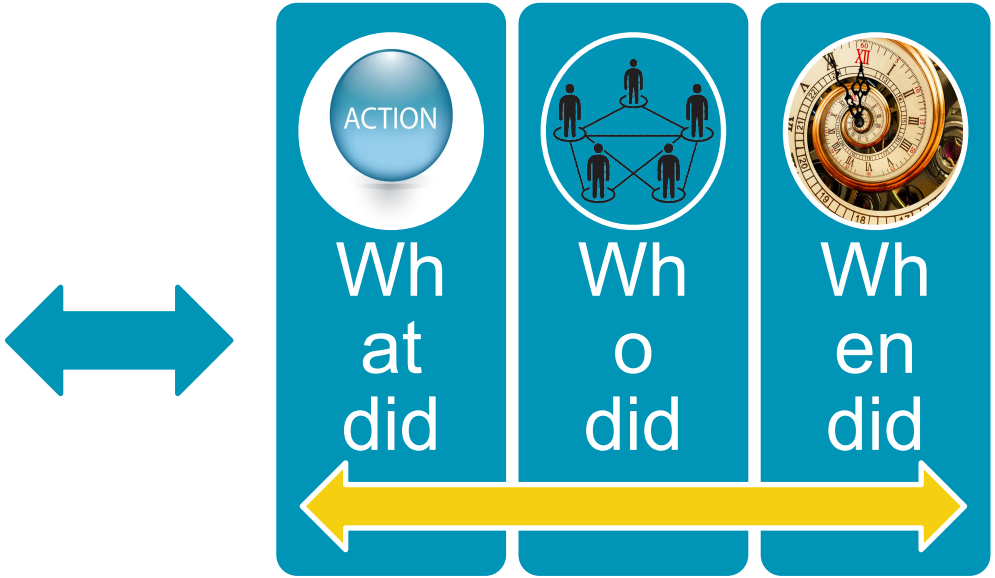
LS domain is in gross part related to health, therefore GAMP

# QA and LS: compliance

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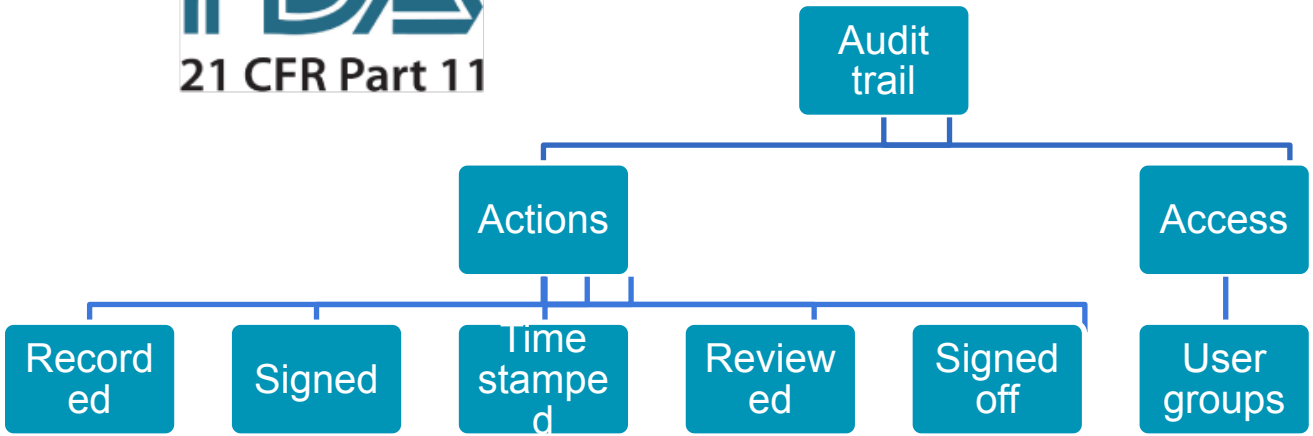

# QA and LS: compliance

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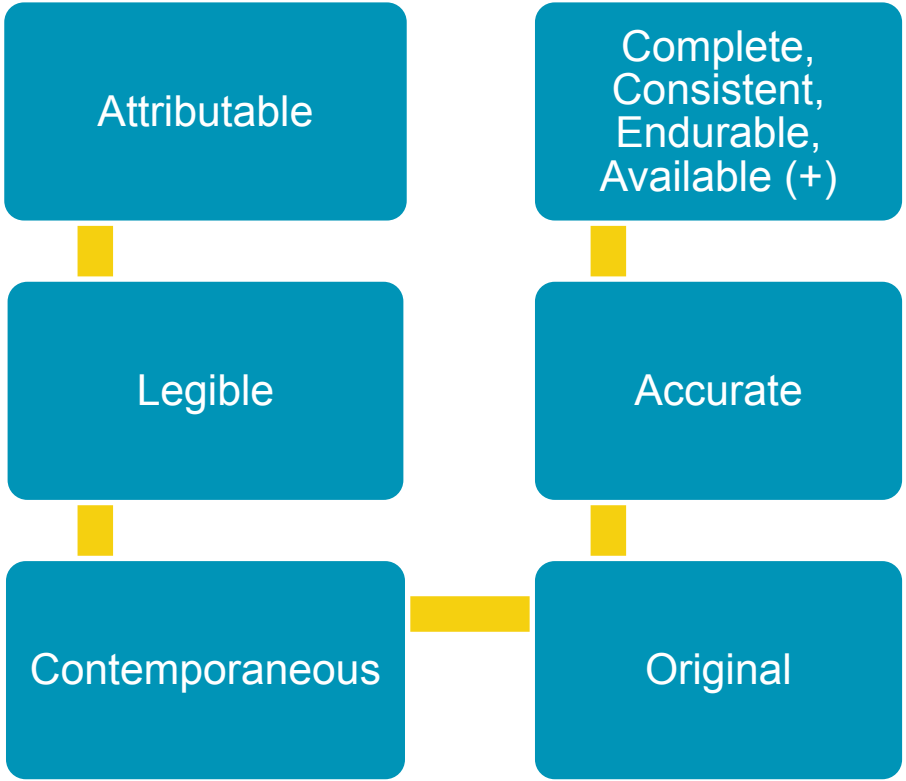


- System testing: check audit trail manually
- API testing: CUD operations
- DB querying (CUD operations, Access violation)
- Automated test scenarios: BDD + DDT

# QA and LS: compliance

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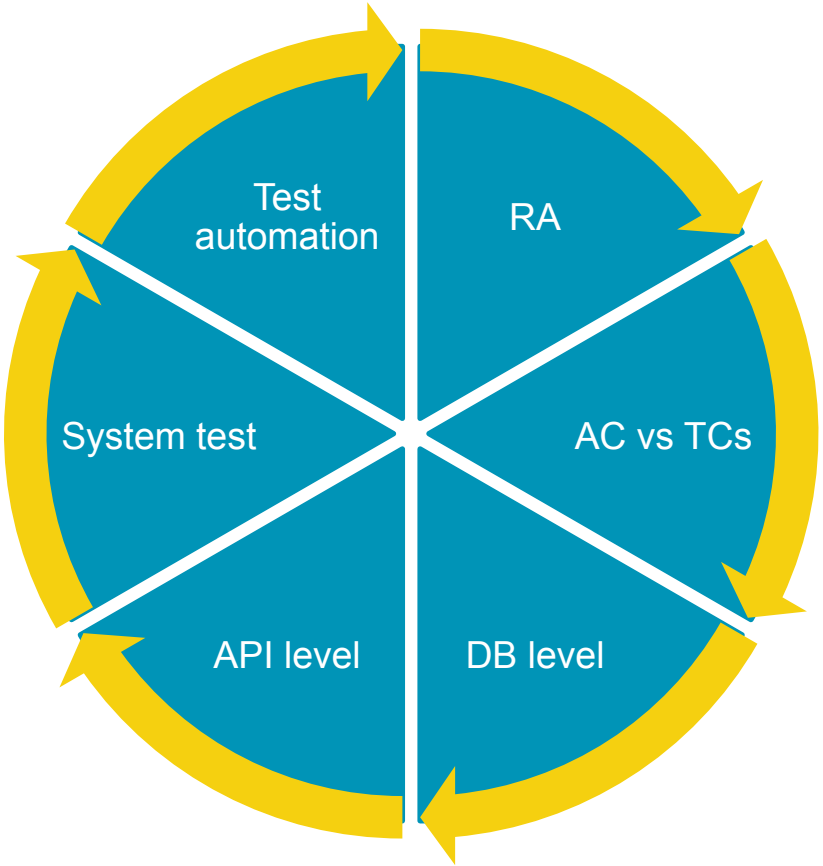


- System testing: check audit trail manually
- API testing: CUD operations
- DB querying (CUD operations, Access violation)
- Automated test scenarios: BDD + DDT

# QA and LS: complex problems

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- Design: planning and data preparation
- Validation: early decomposition into scenarios
- Verification: clear report
- Traceability: business requirements vs tests
- ALCOA+: collected test evidence

# QA and LS: complex problems

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- Requirements analysis
- Prototyping
- Data preparation
- Test scenarios collection
- Data driven testing

# QA and LS: complex problems

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## Requirements analysis

### URS

- Display file metadata

### AC

- As a user I want to be able to see the following properties…

### TC

- Import data file in the native format and display the following properties…

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## Prototyping

$$\frac{m}{z} = k \cdot (t - t_0)^2 + a_0 + a_1 \cdot t + a_2 \cdot t^2 + a_3 \cdot t^3 + a_4 \cdot t^4 + a_5 \cdot t^5$$

```
@staticmethod
def calibrate(data, calibration_json, peaks):
    centroids = Calibrate.find_centroids(data, peaks)
    tofs = Calibrate.centroids_to_tof(centroids, calibration_json)
    return Calibrate.find_parameters(tofs, peaks)
```

# QA and LS: complex problems

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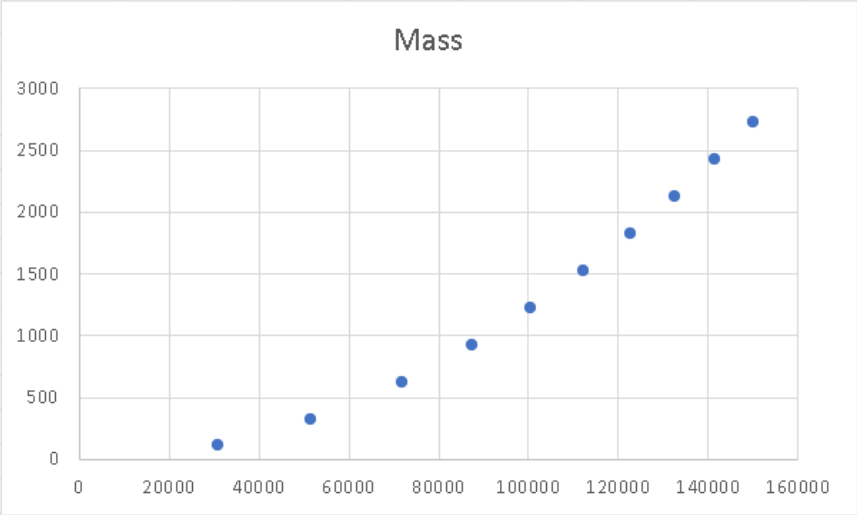
## Data preparation

| ToF | Mass |
|---|---|
| 30801.21 | 118.0863 |
| 51687.2 | 322.0481 |
| 71798.38 | 622.029 |
| 87393.47 | 922.0098 |
| 100597.2 | 1221.991 |
| 112257.2 | 1521.972 |
| 122814.4 | 1821.952 |
| 132532.7 | 2121.933 |
| 141585.1 | 2421.914 |
| 150091.9 | 2721.895 |



# QA and LS: complex problems

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## Test scenarios collection

As a user I want to be able to apply mass calibration to data files

```
apply mass calibration to a file with the same polarity
apply negative polarity mass calibration to several files with the same polarity
apply positive polarity mass calibration to several files with the same polarity
try to apply mass calibration to a file with the opposite polarity
apply positive polarity mass calibration to several files with the different polarities
apply negative polarity mass calibration to several files with the different polarities
```

# QA and LS: complex problems

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## Data driven testing

As a user I want to be able to export mass calibration json

```
@Regression
  @Smoke
  @MassCalibration
  @Agilent

Scenario Outline: import Agilent calibration file "<calibrationFile>" and export the calibration json file

  Given the [redacted] application is opened
  And the calibration form is opened
  And the calibration is performed using "<polarityType>" Agilent "<calibrationFile>" file with "<peaks>" peaks toggled off
  When user exports the calibration file "<calResultFile>"
  Then the exported file "<calResultFile>" is identical to the reference file "<calReferenceFile>"

  Examples:
    | calibrationFile                                  | calResultFile                    | calReferenceFile          | peaks | polarityType |
    | [redacted]                                       | agilent_tunemix_mass_cal.json    | tunemix_mass_cal.json     | 2     | positive     |
    | [redacted]                                       | agilent_tunemix_pos_mass_cal.json | tunemix_pos_mass_cal.json | 2     | positive     |
    | [redacted]                                       | agilent_tunemix_neg_mass_cal.json | tunemix_neg_mass_cal.json | 0     | negative     |
```

# QA and LS: complex problems

QUANTORI

## BDD scenario to an Excel spreadsheet

| D | E | F | G | H | I | J | K | L | |
|---|---|---|---|---|---|---|---|---|---|
| Step # | Step description | Expected result | Actual result | Statu | Comment | Attachmen | Screenshot | Start time | End tir |
| 5 | Verify that the Processing details field contains the specified values. | | | fail | | | | 2022-05-22 20-46-49.757 +0400 | 2022- +0400 |
| 6 | user updates the feature table | | | not run | | | | | |
| 7 | the features table contains the provided values | | | not run | | | | | |
| 8 | the Processing Details field contains the following values | | | not run | | | | | |

# BDD

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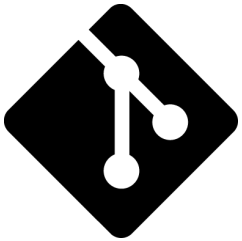
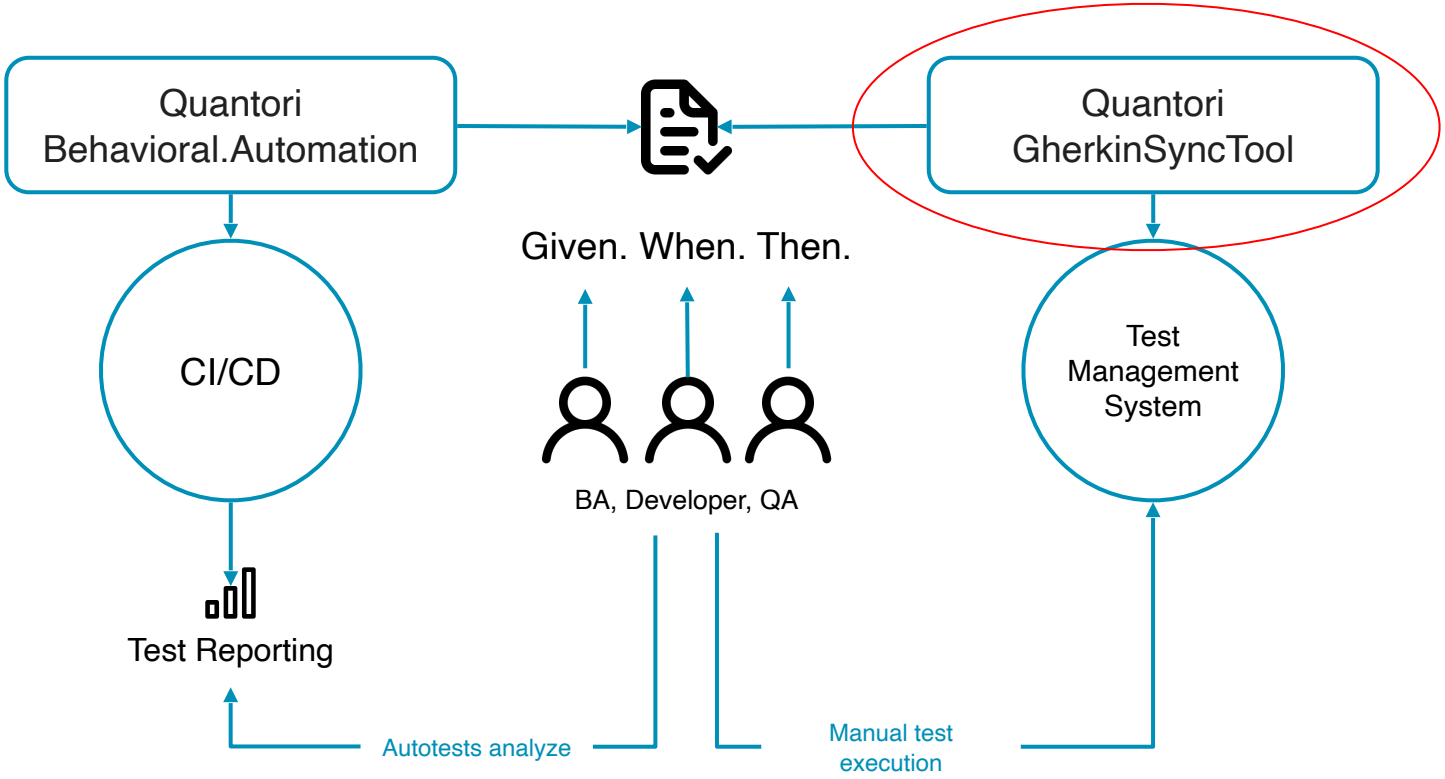
Up to date



Version control

Review

# BDD


Quantori
Behavioral.Automation
Quantori
GherkinSyncTool
Given. When. Then.
CI/CD
Test
Management
System
BA, Developer, QA
Test Reporting
Autotests analyze
Manual test
execution

# GherkinSyncTool

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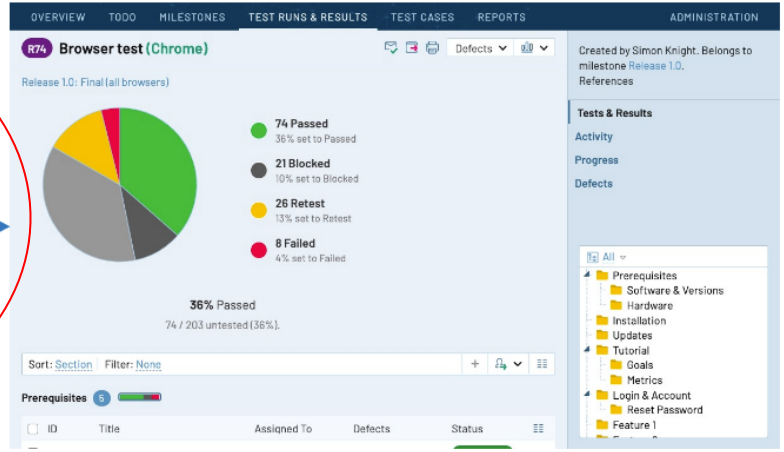
```
# Comment
@tag
Feature: Eating too many cucumbers may not be good for you

  Eating too much of anything may not be good for you.

  Scenario: Eating a few is no problem
    Given Alice is hungry
    When she eats 3 cucumbers
    Then she will be full
```

GherkinSyncTool




https://github.com/quantori/GherkinSyncTool

# Summary

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QA for a better life

Domain experience is a plus

Risk based approach is our all

BDD helps to collaborate