

SADIG GOJAYEV

Report

Detection of polycyclic aromatic  
hydrocarbons by fluorescence lifetime  
measurements

Department of  
Computer Science  
CS-017



2021

# Methodology

The mixture data files are given in binary file, which contains 10,000 values. In formula it seems easily that when time is zero, there will be only sum of A (the maximal fluorescence signal) values. First of all, for trying to guess composition of mixture, the fluorescence signal (only exponential part, because in mixtures the maximal signal values is unknown and not constant) of each molecule should be calculate with times that measured (0 to 1 microsecond with 100 pico second steps. In next stage in two nested loops, for each combination of A value and molecule lifetime the errors (differences greater than  $10^{-10}$  between original and guessed data) calculated and combination with the least error is selected as the composition of mixtures. There are two types of conditions. In mixture1 and 4 number of molecules is known, but in the second and third it is not like this. For this state one loop is added for iterate for finding number of molecules

## Functions that were implemented

1. `florescent(time, lifetime)` - return value that calculated from exponential part of formula
2. `test_error(value1, value2)` - if absolute of value1-value2 is greater than  $10^{-10}$ , it returns True
3. `errors(test, data_test)` - returns list of error indexes
4. `show_errors(error_list, test, data_test, numbers)` - show errors whcih found in previous function
5. `get_sum(a_vals, index_list)` - get A combination and molecule indexes, returns guessed data
6. `A_list (size, n)` - get sum of A values and number of molecelus, returns all possible A combinations
7. `mixture_composition( data_test, num_mixture )` - takes original mixture data and number of molecules in it, prints components of mixture and A values, return number of errors
8. `mixture_composition2 (data_test)` - same procedure with previous one, but the number of molecules is find by function itself (specially for mixture 2 and 3)

```
Mixture 1
  Naphtalene ( 2.009e-07 )  A=1.0
  Benzofluoranthene ( 8.9e-09 )  A=3.0
with 0 errors
-----
Mixture 2
  Anthracene ( 5.8e-09 )  A=2.0
  Pyrene ( 5.162e-07 )  A=1.0
  Chrysene ( 5.78e-08 )  A=5.0
with 0 errors
-----
Mixture 3
  Naphtalene ( 2.009e-07 )  A=1.0
  Pyrene ( 5.162e-07 )  A=1.0
with 0 errors
-----
Mixture 4
  Naphtalene ( 2.009e-07 )  A=1.0
  Benzopyrene ( 3.86e-08 )  A=2.0
  Benzofluoranthene ( 8.9e-09 )  A=3.0
with 0 errors
```

Figure 1: Result