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QSAR/QSPR approach of aroma compounds behaviour in food products

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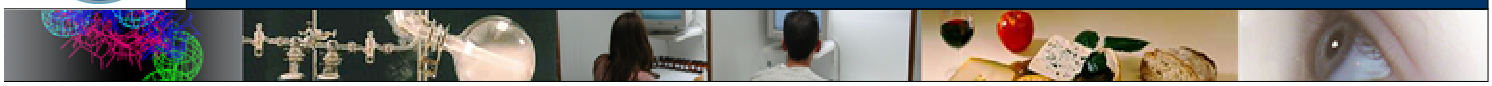


Introduction

- Improved standard of living and lifestyle ☛ demand for food products with less or no fat, sugars
- Equilibrium flavour retention/flavour release depends:
  - on the components of the food matrix
  - on the physicochemical properties of the flavour compound
- Reducing the fat content of a food system ☛ modifications in flavour release and perception
- To retain the properties of a product when the fat is removed, fat-substitutes are used (starch, pectin…)

Influence of texturing agents is unclear

Use QSPR approach to evaluate the influence of texturing agent and the chemical structure of aroma compounds on the partition coefficient of aroma compounds between food product and vapour phase

Quantitative Structure-Activities Relationships (QSAR)
Quantitative Structure-Properties Relationships (QSPR)
} assumption: changes in molecular properties elicit different responses

QSAR

QSPR

links

dependant variable:
"activity" or "property":
Experimental Response

independent variable:
molecular features $p_1, p_2, \ldots p_n$
Molecular Descriptors

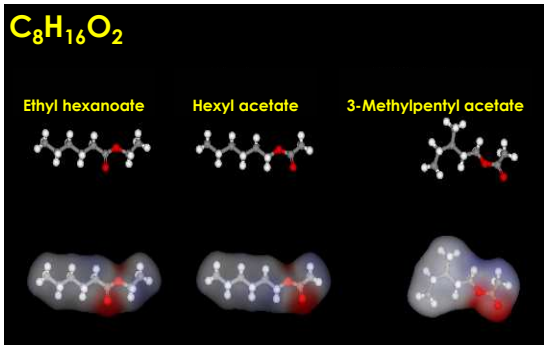
Generates a relationship

ER = « activity » = $f(p_1, p_2, \ldots, p_n)$ *f* linear or non-linear function

Molecular descriptors are intrinsic molecular features

Ex: Molar Weight (MW) Hydrophobicity (AlogP98)
Polarisability (Apol) Dipolar Moment (Dipole –X, Y, Z)

Surface Descriptors:
« Jurs » descriptors surface and charged surface descriptors



Determination of the partition coefficients for yogurt
➢ headspace analysis at equilibrium using solid-phase micro extraction.

$$K_{ret} = \frac{\text{chromatographic area reference}}{\text{chromatographic area thicheners}}$$

QSPR study:
- molecular descriptors calculations
- equations constructions

carried out using Cerius² (Accelrys Inc.)

$$JursWNSA-1 = \sum_s \text{surfaces areas of all negatively charged atoms} \times \frac{\text{total molecular solvent} - \text{accesible area}}{1000}$$

20 descriptors selected ☛ present at least a dependable correlation with the partition coefficient values K_{ret}(Starch0.1%)
For higher amounts of starch (0.4 and 0.6%) and pectin (0.04, 0.1, and 0.15%)

all of the previous correlations are severely disturbed

☛ **no reliable correlation between the descriptors and log K_{ret} values**

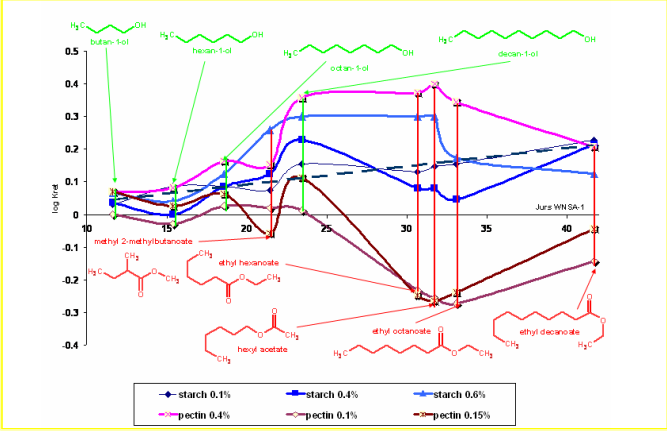
surface descriptor Jurs WNSA-1 is a particular interest

Jurs WNSA-1 encodes the surface negatively charged area weighted by the total surface area
For the same chemical class negatively charged areas similar
- lower values ☛ smallest molecules ☛ low hydrophobicity
- higher values ☛ biggest molecule ☛ high hydrophobicity

only true for Starch 0.1%

Increase in the amount of starch disrupts "hydrophobic effect" in favour of other natures of interactions

Jurs WNSA-1 values highlights the existence of two groups:
- **ethyl hexanoate, hexyl acetate, ethyl octoanoate**, and **ethyl decanoate**
- **butanol, hexanol, octanol, decanol** and **methyl 2-methylbutanoate**



Conclusion : QSPR study shows an intricate role due to adding both starch at concentrations higher than 0.1% and pectin
puts forward the power of negatively charged surface areas
suggests the existence of competitive interactions, hydrophobic and polar binding

QSPR approach constitutes a promising tool for characterizing the interactions involved in complex food matrices
Experiments are now in progress to obtain true partition coefficient values involving a larger range of chemical structures

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