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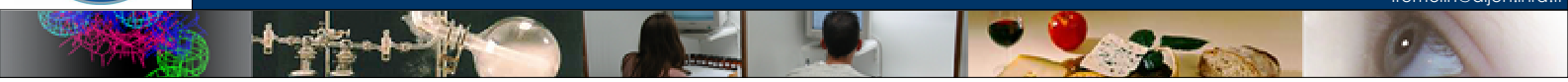


Introduction

- 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

Influence of texturing agents is unclear

Aim of this work:

study and compare respective effects on the aroma release of two common used thickeners pectin and ι-carrageenan

↳ Use QSPR approach to evaluate the influence of the chemical structure of aroma compounds on retention/release equilibrium between vapour phase and gels

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

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

QSAR / QSPR links

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

Generates a relationship

ER = « activity » = *f* (p_1, p_2, …., p_n) *f* linear or non-linear function

Molecular descriptors are intrinsic molecular features

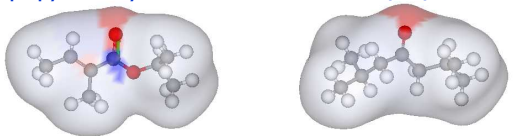
Ex: Molar Weight (MW) Hydrophobicity (AlogP98)
Polarisability (Apol) Dipolar Moment (Dipole –X, Y, Z)

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

MW=142.1 g mol^{-1}

$C_8H_{14}O_2$ isopropyl 2-methyl-2-butenoate

$C_9H_{18}O$ 2,6-dimethylheptan-4-one



Determination of the partition coefficients:

- 13 aroma compounds (7 esters, 4 ketones, 2 aldehydes) for ι-carrageenan gel, pectin gel, and water (reference medium)
  - ➢ headspace analysis at equilibrium using Phase Ratio Variation method calculation (Ettre, *Chromatographia*, 1993)

QSPR study:

- molecular descriptor calculations
- equation constructions
  - ➢ carried out using Cerius²(Accelrys Inc.)

involved descriptors loading retention informations in QSPR equations:

water and ι-carrageenan gel

Jurs-PNSA-1 and Jurs-WNSA-2

Jurs-PNSA-1 ☛ sum of the solvent-accessible surface area of all negatively charged atoms

$$Jurs-PNSA-1 = \sum_s SA_s^-$$

Jurs-WNSA-2 ☛ partial negative solvent-accessible surface area multiplied by the total negative charge multiplied by the total molecular solvent-accessible surface area and divided by 1000

$$Jurs-WNSA-2 = Q^- \cdot \sum_s SA_s^- \times \frac{Solvent\ Accessible\ Surface\ Area}{1000}$$

➢ ι-carrageenan polymer **not change the interaction** of aroma compounds with water molecules

➢ attractive interactions due to **negative charges and negatively charged surfaces** on the aroma molecules

pectin gel

Jurs-RPSA

Jurs-RPSA ☛ sum of solvent-accessible polar surfaces areas with absolute value of partial charges greater of equal to 0.2 divided by the solvent accessible surface area

$$Jurs-RPSA = \frac{\sum_a SA_a}{Solvent\ Accessible\ Surface\ Area} \qquad \forall a : |q| \geq 0.2$$

➢ pectin polymer **lightly modify the interaction** of aroma compounds with water molecules

➢ attractive interactions due to **both negative and positive polar surfaces** on the aroma molecules

Conclusion: QSPR study
- draws attention to the different molecular properties involved in attractive interactions of aroma compounds with ι-carrageenan and pectin gels
- highlights the role of positive polar effects on the retention of odorant molecules in pectin gel

QSPR approach constitutes a promising tool for characterizing the interactions involved in complex food matrices

Experiments are now in progress to obtain partition coefficient values involving a larger range of chemical structures in more complex mediums

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