Application of Quantitative Structure-Property Relationships (QSPR) approach to aroma release study

Anne Tromelin, A. Chana-Lopez, Samuel Lubbers, Isabelle Andriot, Elisabeth Guichard

Application of Quantitative Structure-Property Relationships (QSPR) approach to aroma release study

A. Tromelin[a], A. Chana-Lopez[b], S. Lubbers[a], I. Andriot[a] and E. Guichard[a]

[a]UMR-FLAVIC - Institut National de la Recherche Agronomique, 17, rue Sully, BP 86510, 21065 Dijon Cedex, France
[b]Istituto di Ricerce Farmacologiche, Via Eritrea 62, 20157 Milano, Italy
tromelin@dijon.inra.fr

Introduction

Improved standard of living and lifestyle ☛ demand for food products with less or no fat, sugars

Equilibrium flavor retention/flavor release depends:
- on the components of the food matrix
- on the physicochemical properties of the flavor compound

Reducing the fat content of a food system ☛ modifications in flavor 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 vapor phase**

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

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

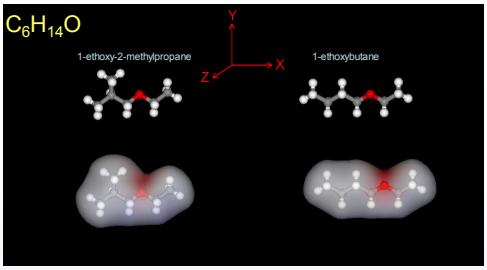
QSAR
QSPR
⟷
links

independent variables:
molecular features p1, p2, …, pn
Molecular Descriptors

Generate a relationship
ER = « activity » = $f(p_1, p_2, ..., p_n)$ *f* linear or non-linear function

Molecular descriptor are intrinsic molecular features

Ex: Molar Weight (MW) — logP (hydrophobicity) AlogP98
Polarisability (Apol) — Dipolar Moment (Dipole –X, Y, Z)
Shape and Surface Descriptors:
Radius of Gyration (Rad of Gyration)
« Shadow-XY »: calculated by projecting the molecular surface on the perpendicular plane XY
« Jurs » descriptors surface and charged surface descriptors



Determination of the partition coefficients ➥ headspace analysis at equilibrium:
- directly by vapor phase samples assay by gas chromatography for both ι-carrageenan gel and saline solution
- using solid-phase micro extraction for yogurt.

QSPR study:
- molecular descriptors calculations
- equation constructions

carried out using Cerius² (Accelrys Inc.)

For dairy gel (fat-free stirred yogurt): linear correlations observed between the ratio of partition coefficient related to increasing amount of thickener and selected descriptors show that:

➢ **with increasing amount of starch**
- ✓ increasing molecular volume and polarizability improve retention of aroma molecules
- ☛ is indicative of van der Waals hydrophobic interactions

➢ **with increasing amount of pectin**
- ✓ **positive molecular partial charges**
  - ☛ **negative effect** of the inductive donor effect of carbon chain to the retention of aroma
- ✓ **carbonyl dipole**
  - ☛ **favorable effect** to the retention of aroma

☛ point forward the power of dipole-dipole interaction and hydrogen bonding in the retention of aroma by pectin

For saline solution as for ι-carrageenan gel: equation generation performed by Genetic Function Approximation

Involved descriptors both in gel and water encode:
- ➢ electronic properties of charges repartition on the molecule
- ➢ molecules shapes

☛ **key factors for the aroma release in both gel and water are:**
- ✓ chain branching and spherical chain shape ☛ decreases the retention
- ✓ molecular charge ☛ increases the retention

✕ Best fitting for carrageenan gel is obtained with a quadratic relation:
- ✓ seems to indicate a different mechanism of aroma release in gel than in water
- ✓ suggests that the effect of carrageenan polymers only modules but does not change interaction of aroma compounds with water molecules

Conclusion

QSPR approach allows highlighting the nature of the interactions due to various components of the food matrix and constitutes a promising way to better understand the nature of intermolecular interactions involved between macromolecules and aroma compounds in food matrices

References

A. Chana, A. Tromelin, I. Andriot, E. Guichard (2006) *J. Agr. Food Chem.* **54,** 3679 -3685.
A. Tromelin, E. Guichard (2004) *QSAR Comb. Sci.* **23,** 214-233.
M. E. Carey, T. Asquith, R. S. T. Linforth, A. J. Taylor (2002) *J. Agr. Food Chem.* **50,** 1985-1990.
E. Guichard (2002) *Food Rev. Int.* **18,** 49-70.

IUFOST XIII[th] Congress of Food Science & Technology, 17-21 September 2006, Nantes, France