Characterization of protein-aroma interactions at a molecular scale
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**Introduction:** β-lactoglobuline (β-LG) A variant
Flavour compounds of different chemical classes were tested.

The presence of 5% EtOH was proved by NMR analyses to induce no perturbation of amino acids involved in binding.

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**NMR spectroscopy**
- Bruker 500 MHz, 5 mm probe
- T=37°C
- 2D (1H, 1H) TOCSY-Watergate sequence with a mixing time of 40 ms
- β-LG in 12mM NaCl buffer, pH=2.3
  - addition of an aroma compound
  - >60% complexed protein

**FT-IR spectroscopy**
- FT6000 FT-IR spectrometer, ATR accessory
- T=25°C
- 512 scans, resolution of 2 cm⁻¹
- Analyses in 12mM NaCl buffer, 5% EtOH, pH=2
  - β-LG/aroma, >70% complexed protein
  - Aroma compound alone

**3D Molecular Modeling**
- Catalyst/Hypogen software
- Point of view of the receptor: Information only from the ligand
- 59 aroma characterized by their affinity data $K_b$ (2)

**Characteristics:** Hydrogen bond acceptor and Hydrobic

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**β-LG → amino acids assignment**
- NH/CHα = fingerprint region of protein

**Shift variation method:**
\[ \Delta \delta = \delta_{\text{complex}} - \delta_{\text{protein}} \]

**FTIR spectra:**
- Amide I band (1590-1700 cm⁻¹)
  - Screening of aroma compound in function of IR profile
- Differential spectra:
  - Complex spectrum – aroma spectrum
  - Amide I / Amide II = 1.46
  - Normalisation of Amide I band

**Identification of common structure of aroma having a probable common binding site**
- Generation of hypotheses
  - Set of features in 3D space
  - Estimation of affinity data
- Correlation $K_{B\text{Estimated}} / K_{B\text{Experimental}}$
- Alignment of aroma on the features
- Analyse cost

**Valid model**
- Division into pools

**2 binding sites**
- External site
- Central cavity

**2 binding behaviours**
- Significant perturbation of Amide I band
- No significant perturbation of Amide I band

**2 predictive models**
- Compact alignment
- Extended alignment
- Compact molecules
- Long acyl chain

**Conclusion:** Whatever the technique used, results confirmed the existence of at least two different binding sites for aroma compounds on β-LG: one binding site in the hydrophobic pocket for flavour molecules with a long acyl chain, and one external site for compact compounds.

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**References:**