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FACULTY OF PHARMACEUTICAL SCIENCES

THE USE OF UHPLC COUPLED TO SINGLE QUAD MS DETECTION IN FRANZ DIFFUSION CELL METHODOLOGIES

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INTRODUCTION and OBJECTIVES

Ultraviolet/visible (UV/VIS) detector
- High detection limits
- Lack of selectivity: co-eluting compounds having similar structures and UV spectra

Single quad MS detector
- Easy to use
- Increased efficiency
- Additional detection possibilities compared to UV/VIS
- Scan selected mass range
- Single ion monitoring (SIM)
- Identification and quantification of compounds

✓ Quantification biologically active compounds in **plant extracts**
✓ In cosmetics for topical use

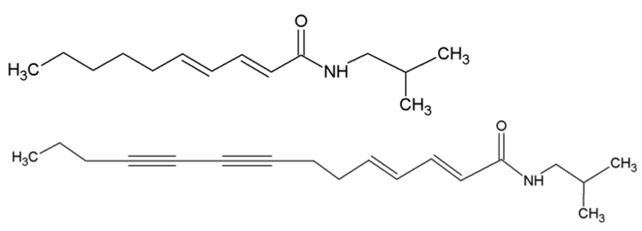
✓ ***Anacyclus pyrethrum*** plant extract containing the ***N*-alkylamides** (NAAs) pellitorine and anacycline

✓ ***Spilanthes acmella*** plant extract containing the NAA spilanthol

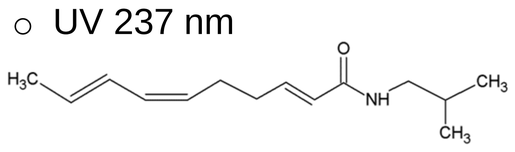
✓ Investigation transdermal behavior of *N*-alkylamides using *in vitro* Franz diffusion cell (FDC) experiment
✓ Quantification with UHPLC coupled to single quad MS detector

EXPERIMENTAL

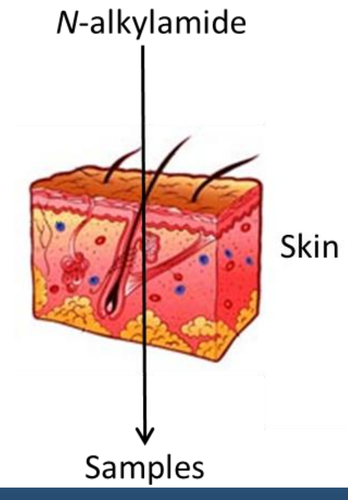
✓ Investigation transdermal behaviour of *N*-alkylamides using *in vitro* **FDC** experiment [1]
✓ Human skin
✓ Samples analysed with UHPLC-single quad MS/UV
✓ ***Anacyclus pyrethrum* extract**
- Split 1/10 MS/UV
- SIM pellitorine (*m/z* 224.36)
- SIM anacycline (*m/z* 272.40)
- UV 258 nm



✓ ***Spilanthes acmella* extract**
- SIM spilanthol (*m/z* 222.15)
- UV 237 nm

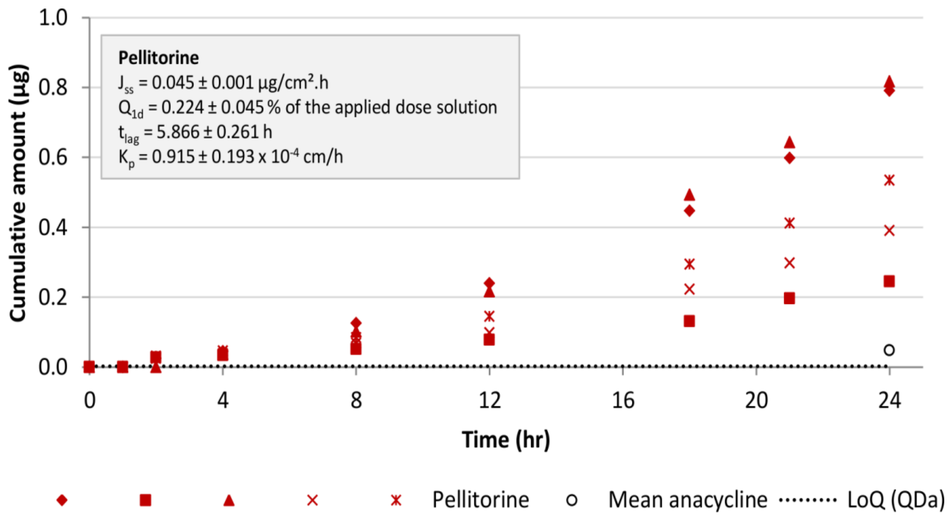


✓ Calculation skin parameters:
- Permeability coefficient (K_p), lag time (t_{lag}), flux (J_{ss}), percentage penetrated after 1 day (Q_{1d})

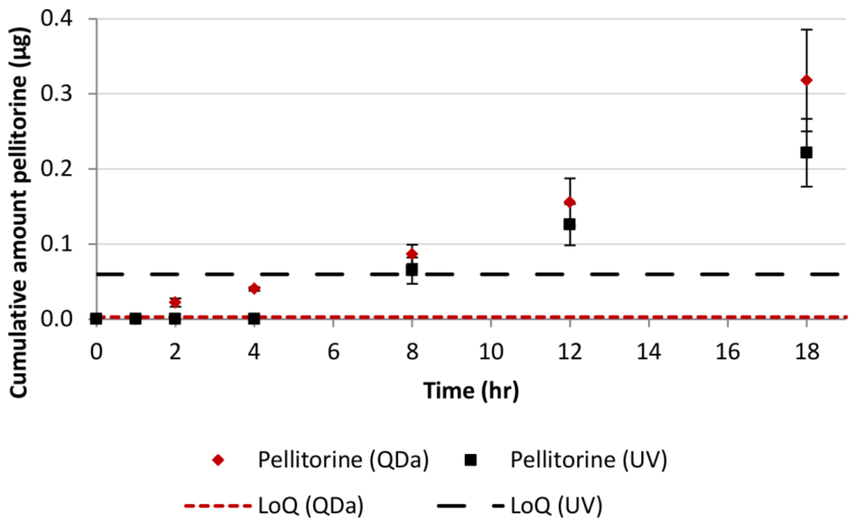


RESULTS and DISCUSSION

1. Transdermal results

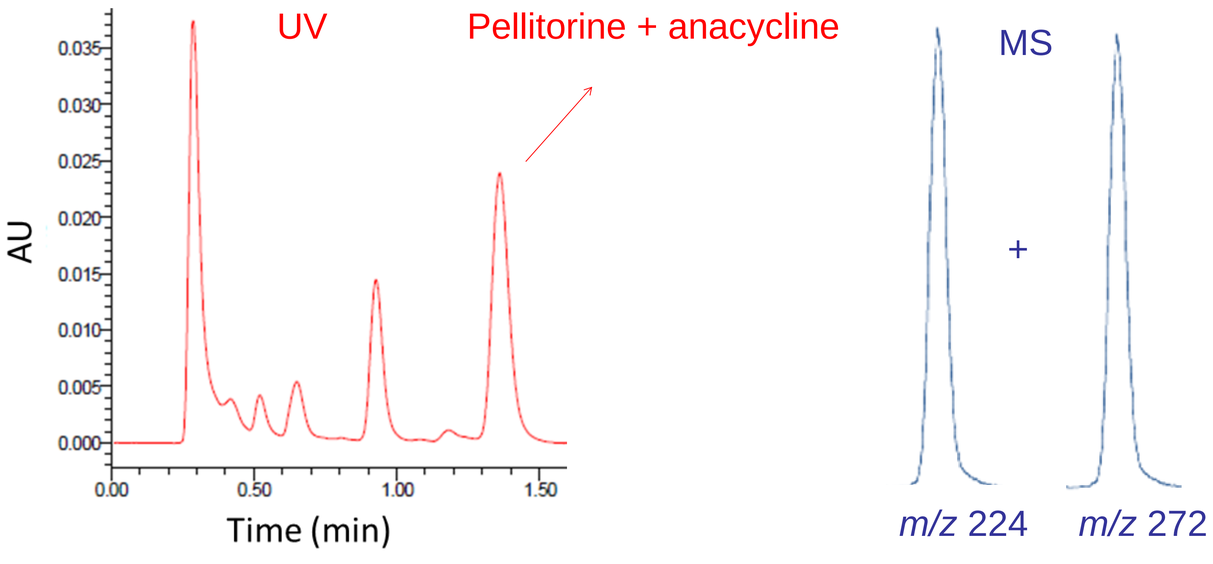


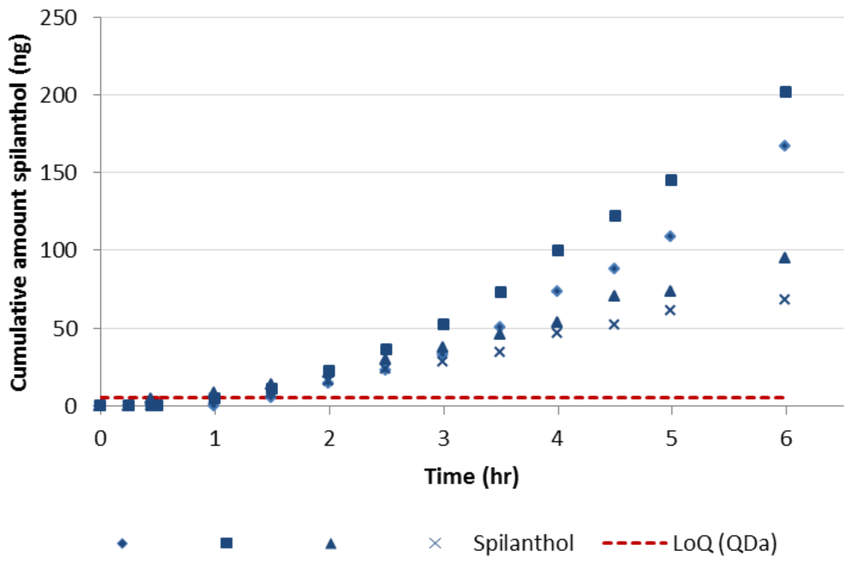
B) Lower LoQ values → better estimation of experimental t_{lag}



2. Advantages single quad MS compared to UV

A) Quantification possible without baseline separation in UV





CONCLUSIONS

✓ Quantification of different NAAs in plant extracts possible with UHPLC-single quad, even without baseline separation → better selectivity (versus UV)
✓ Low LoQ values are obtained with single quad MS → better estimation of lag time (versus UV)

REFERENCES

[1] Veryser L, Taevernier L, Roche N, Blondeel P, De Spiegeleer. 2015. Implementation of a single quad MS detector in high-throughput transdermal research of plant extracts. *Manuscript submitted for publication.*