**The Identification of Emerging Psychoactive Substances**

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**Aims & Objectives:**
- Confirm the structures of six synthetic cannabinoids (Figure 3) by mass spectrometry, and determine their fragmentation patterns.
- Develop a repeatable method for simultaneous identification of a range of synthetic cannabinoids, after their extraction from biological matrices.
- Use this method to identify the presence of NPSs and/or their metabolites in clinical samples.

**Methods:**
- Extracted I3C samples from plasma and urine, and used the mass spectra to confirm the structures of each of the 6 compounds.
- Reverse phase C18 HPLC (high performance liquid chromatography) was used to separate compounds.
- Detected which NPS may be present in blood samples from hospital patients by use of HPLC-MS/MS.
- The process of mass spectrometry (MS) is illustrated in Figure 2.

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**Introduction:**
Indole- and indazole-3-carboxylates (I3Cs) are types of synthetic cannabinoids (SCs). SCs are a class of novel psychoactive substances (NPS) or 'legal highs'. Their incidence of use is increasing [1] as they are often difficult to detect. Currently, their structures and properties are not fully known, as well as their pharmacokinetics [2]. This means that their effects cannot be characterised, making them potentially dangerous. This is a cause for concern, especially while they remain largely undetectable.

This research is motivated towards confirmation and continuation of previous work (3) and aimed to identify any potential diagnostic analytes, as well as to develop a method for detection, which could prove useful in the fields of forensics and toxicology.

**Results:**
- Results were recorded and displayed using Analyst and PeakView respectively. An example PeakView trace is shown in Figure 4, showing that SF-SDB-005 has a parent ion of 377.2Da and major fragments of 233.0Da, 213.06Da, and 144.9Da.
- MRM result from a blood sample (Figure 5) showed a transition from 310.2Da to 265.1Da, indicating the presence of methadone.
- MRM of the clinical sample did not detect heroin or any I3Cs.
- A scan of another clinical sample suggested the presence of SF-AKB-48, which is a novel synthetic cannabinoid [4].

**Conclusions & Discussion:**
- Successfully developed a repeatable LC-MS method for analysis of a mixture of drugs, when extracted from biological matrices.
- Confirmed structures of synthetic cannabinoids identified in [3] and their fragmentation patterns, as well as an isomer of SF-SDB-005.
- The blood sample which was screened for the presence of NPSs tested positive for methadone, but negative for heroin and I3Cs.
- Another sample suggested that a non-I3C cannabinoid (SF-AKB-48) may have been present, but the ratio between peaks was too great to be confident about this result.
- Results were confirmed to prove that the LC-MS method was successful.
- Future research could be directed towards furthering knowledge by producing full descriptions of the pharmacokinetics of NPSs.

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**References:**

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**Sample extraction by isolute SLE+ solid phase extraction**

**Liquid chromatography with H2O/MeOH + 0.1% FA gradient**

**Mass spectrometry including MS/MS, MRM, EIC, ESI, product ion scan, precursor scan, and MRM-triggered MS/MS**

**Data collection by Analyst and review with PeakView software**

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