

## K16 Determination of Chiral Cathinone in Fresh Samples of *Catha Edulis*

Abdulrhman M. Dhabbah, PhD\*, King Fahad Security College, Riyadh, SAUDI ARABIA

**Learning Overview:** The goals of this presentation are to show: (1) how using Menthyl Chloroformate (MCF) to derivatize cathinone enantiomers and yield two diastereomers; (2) the quantitative determination of *S* and *R* cathinone confirmed the presence of both enantiomers in all parts of the studied plant; (3) the screening of active constituents in different parts of the plant; and (4) the comparison of characteristic distribution between *S* and *R* cathinone in leaves and stems in Khat.

**Impact on the Forensic Science Community:** This presentation will impact the forensic science community by demonstrating: (1) the quantitative determination of *S* and *R* cathinone confirmed the presence of both enantiomers in all parts of the studied plant; (2) the concentration of *S*-cathinone was higher in stems while its values were lower in leaves; (3) the highest content of *S*-cathinone, which is the most psychoactive stereoisomer, was measured in the upper stems of the plant; and (4) the present study is the first quantitative investigation of the two cathinone enantiomers in different parts of fresh *Catha edulis*.

*Catha edulis* Forsk, commonly named Khat, is an evergreen wild shrub cultivated in East Africa and the Arabian Peninsula. It is traditionally consumed in these regions for its psychoactive properties. The main stimulating compound in Khat is cathinone, which consists of two enantiomers; several studies have established that *S*-(-)-cathinone is more stimulant than its *R* isomer. However, the quantitative determination of *R* and *S* cathinone in *Catha edulis* was not mentioned in previous papers. Moreover, there is still controversy about the presence of the *R* enantiomer in this plant. Thus, the present work aimed to determine the two cathinone enantiomers in different parts of fresh Khat samples.

Extraction of cathinone was carried out from different parts of fresh *Catha edulis*. The derivatization of cathinone enantiomers was done using MCF and yielded two diastereomers, which were separated by gas chromatography on a HP-5 capillary column with an excellent resolution factor (*R*s higher than 5). Figure 1 shows the chromatogram of a leaf extract after cathinone was derivatized with MCF. The three main peaks observed at 20.938, 31.857, and 33.887min. correspond to MCF, *S*-cathinone and *R*-cathinone derivatives, respectively. The structure of the two cathinone diastereomers was confirmed by mass spectrometry. Their mass spectra are shown in Figure 2; the same main fragments are observed in both spectra at *m/z* 83, 226, 105, 182, and 139, but with different abundances.

The quantitative measurements were based on a calibration curve obtained by injection of a series of standard solutions of *S*-(-)-cathinone in the concentration range from 1 to 100µg/mL. The quantitative results of *S* and *R* cathinone confirmed the presence of both enantiomers in all parts of the studied plant, while some previous studies mentioned that only *S*-cathinone was detected in this species. Also, the obtained results showed a characteristic distribution in the different parts of the plant. The concentration of *S*-cathinone was higher in stems while its values were lower in leaves. The concentrations were in the ranges 0.081-0.290mg/g and 0.087-0.211 mg/g for *S* and *R* isomers, respectively. On the other hand, the highest content of *S*-cathinone, which is the most psychoactive stereoisomer, was measured in the upper stems of the plant. The characteristic distribution of *S* and *R* cathinone was illustrated by their enantiomeric excess (ee%) in the different portions of the branch. The ee% values were positive in all stem samples of Khat, while in contrast they were negative in leaf samples. These results confirm the predominance of the most psychoactive *S*-cathinone in stems. The present study is the first quantitative investigation of the two cathinone enantiomers in different parts of fresh *Catha edulis*.

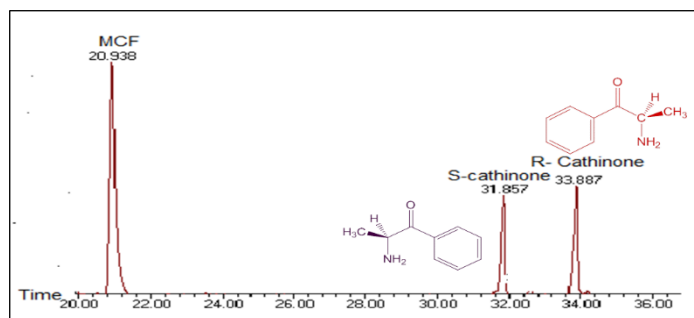


Figure 1: Chromatogram of leaf extract after derivatization with MCF

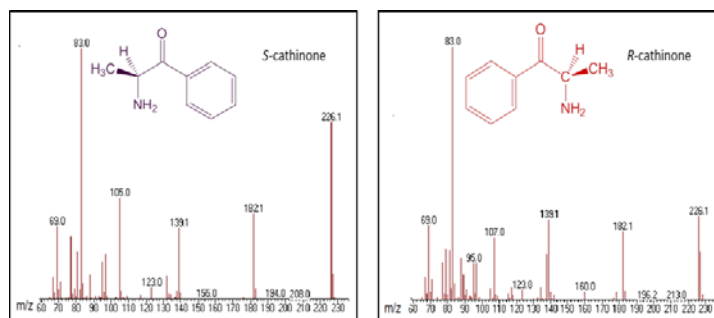


Figure 2: Mass spectra of cathinone diastereomers

The present study is the first quantitative investigation of the two cathinone enantiomers in different parts of fresh *Catha edulis*. The quantitative results of *S* and *R* cathinone confirmed the presence of both enantiomers in all parts of the studied plant, while some previous studies mentioned that only the most psychoactive stereoisomer *S*-cathinone was detected in this species. The concentration of *S*-cathinone was higher in stems while its values were lower in leaves. On the other hand, the highest content of *S*-cathinone was measured in the upper stems of the plant.

### S/R-Cathinone, Derivatization, GC/MS