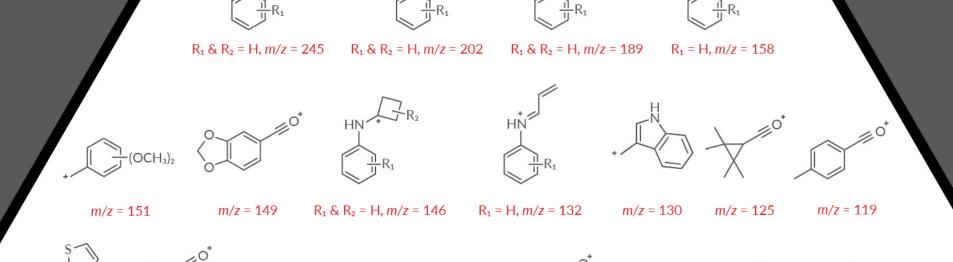
## Common Fentanyl MS Fragments

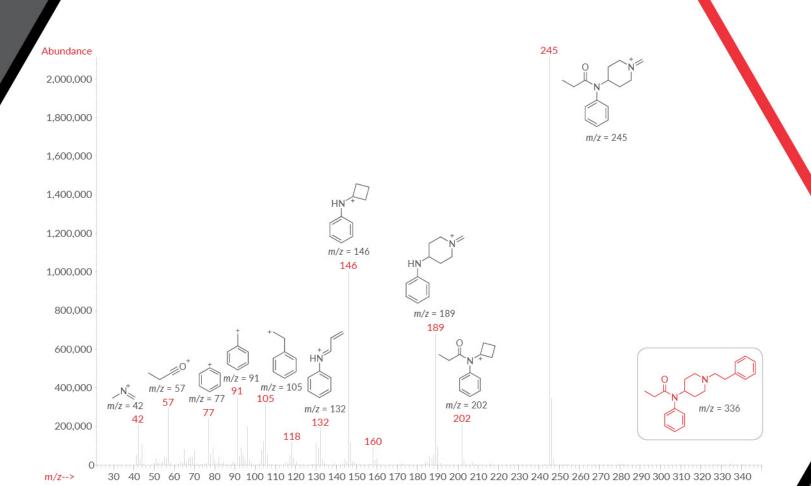


m/z = 85 m/z = 83 m/z = 83 m/z = 81 m/z = 77 m/z = 73 m/z = 71 m/z = 71

m/z = 69 m/z = 69 m/z = 69 m/z = 69 m/z = 67 m/z = 59 m/z = 59

m/z = 57 m/z = 55 m/z = 55 m/z = 45 m/z = 43 m/z = 43 m/z = 42

# Mass Spectrum of Fentanyl and Tips for Interpretation



#### Tips for GC-MS Interpretation:

Here are some common substituents to replace an H (such as where  $R_1$  and  $R_2$  are noted in the Common MS Fragments section above):

- R<sub>1</sub> (aniline ring):
- R<sub>2</sub> (piperidine ring):  $\cdot$  If R<sub>2</sub> = CH<sub>3</sub>, the m/z is +14 · If  $R_1 = CH_3$ , the m/z is +14
- $\cdot$  If R<sub>2</sub> = F, the m/z is +18
- · If  $R_1 = F$ , the m/z is +18
- · If  $R_1 = OCH_3$ , the m/z is +30
- $\cdot$  If R<sub>1</sub> = Cl, the m/z is +34
- · If  $R_1 = CH(CH_3)_2$ , the m/z is +42
- · If  $R_1$  = Br, the m/z is +78

# Laboratory Guide for

Identification, Naming, and Metabolism

# Standardized Naming of Substituted Fentanyls

N-Alkyl Chain

### Simple substituents on the fentanyl skeleton (by region):

Amide Group

- Amide group substituents occur at either the  $\alpha'$  or  $\beta'$  position.
- Aniline ring substituents occur at the ortho, meta, and/or para positions.
- · Piperidine ring substituents occur at the 2, 3, and/or 4 positions.
- $\cdot$  N-alkyl chain substituents occur at either the  $\alpha$  or  $\beta$  points on the carbon chain linker and/or the 2', 3', or 4' position of the associated phenyl ring.

Read more about our standardized naming convention and explore examples and exceptions at www.caymanchem.com/fentanylnaming



# Major Fentanyl Predictive Patterns

Benzodioxole fentanyl, MW 428

**Pattern 1:** Fentanyl-like compounds cleave between the  $\alpha$  and  $\beta$  carbons of the ethyl heterocyclic linker, which results in the base peak (BP) ion.

- · Fentanyls with a hydroxyl group in the β position observe a MW minus 18 (M-18) fragment for
- Pattern 2: Additional cleavage of the BP ion occurs along the piperidine ring and at the amide C-N bond.
- Pattern 3: Subsequent cleavage at either the piperidine ring or the amide C-N bond of the secondary fragments results in a third characteristic fragment.
- Pattern 4: Cleavage at the amide C-N bond will generate the BP if a highly stabilized or highly substituted group is in the acyl region.
  - Learn more about our predictive patterns for identifying unknown fentanyls at www.caymanchem.com/fentanylpatterns

## Fentanyl Metabolism: Typical Phase I Metabolites

Biotransformation Pathway:

A) N-Dealkylation B) Hydrolysis C) Hydroxylation D) O-Monomethylation

- · The known routes of fentanyl metabolism include N-dealkylation to form norfentanyl (1), hydrolysis to form 4-ANPP (2), and numerous sites for hydroxylation.
  - · Many of these phase I metabolites undergo phase II metabolism to form the corresponding glucuronides or sulfates.
    - · Coincidentally, norfentanyl and 4-ANPP can also be considered synthetic precursors.
    - Learn more about what is known about the metabolism of fentanyls at www.caymanchem.com/fentanylmetabolism