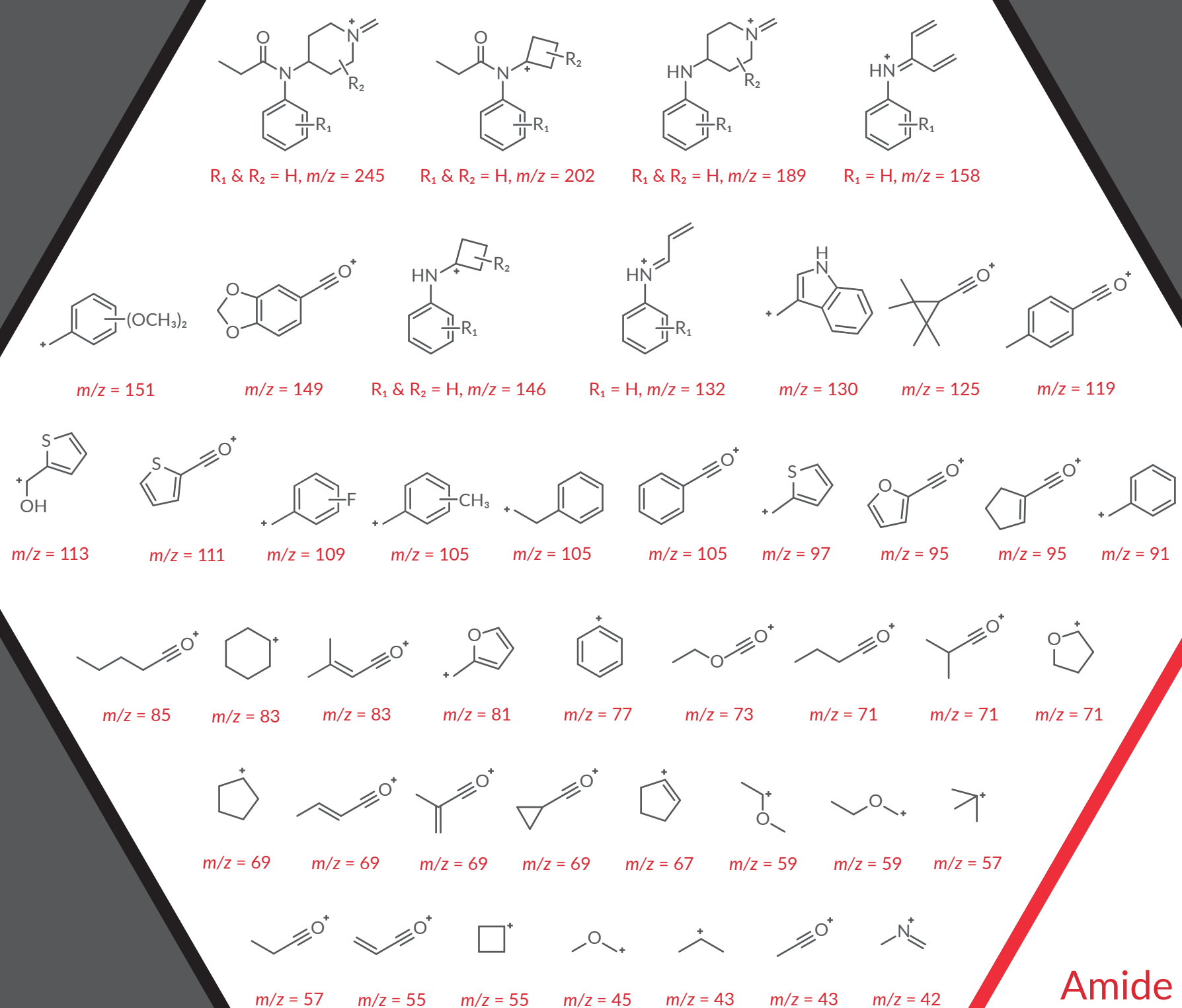
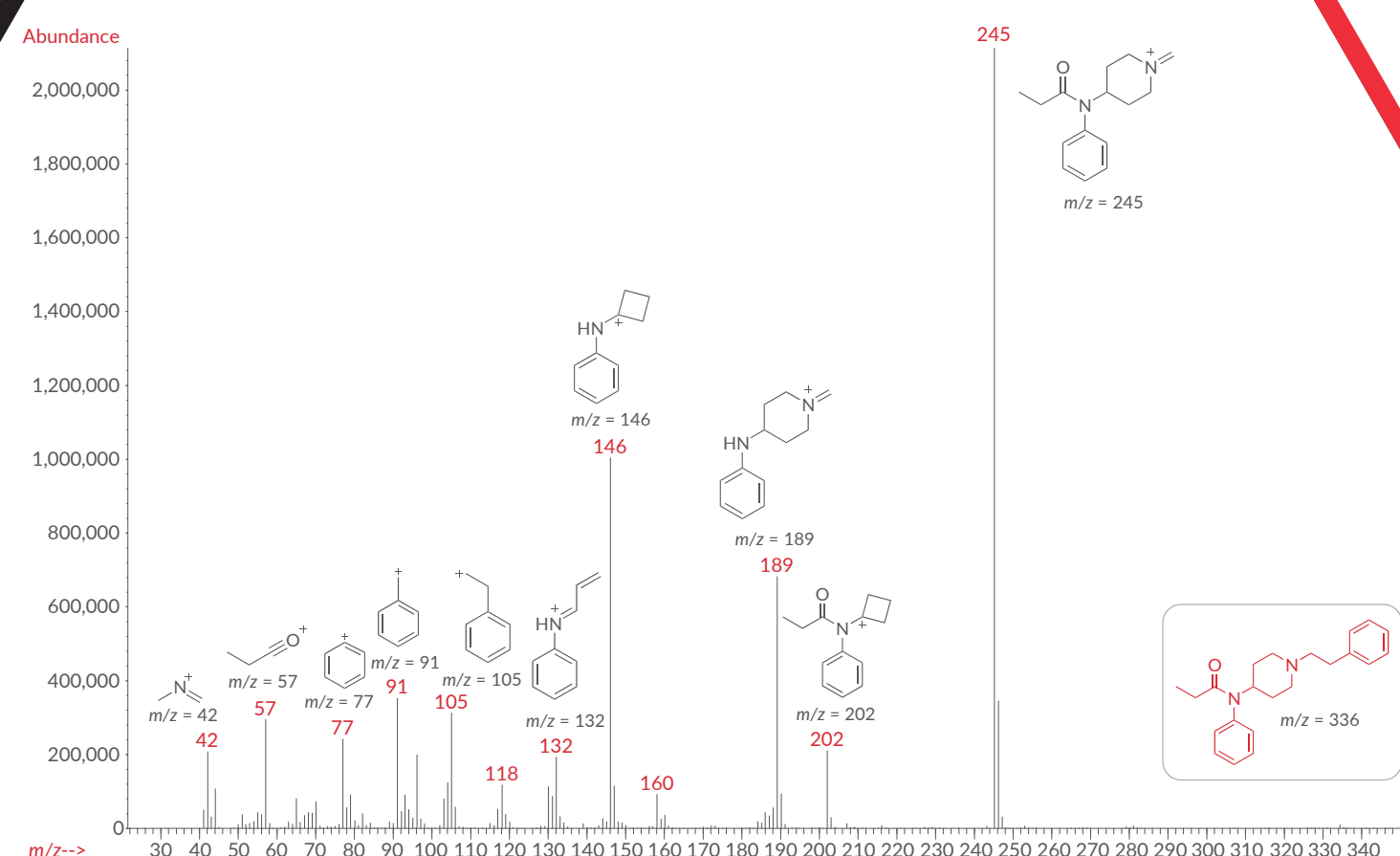


Common Fentanyl MS Fragments



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_1 (aniline ring):

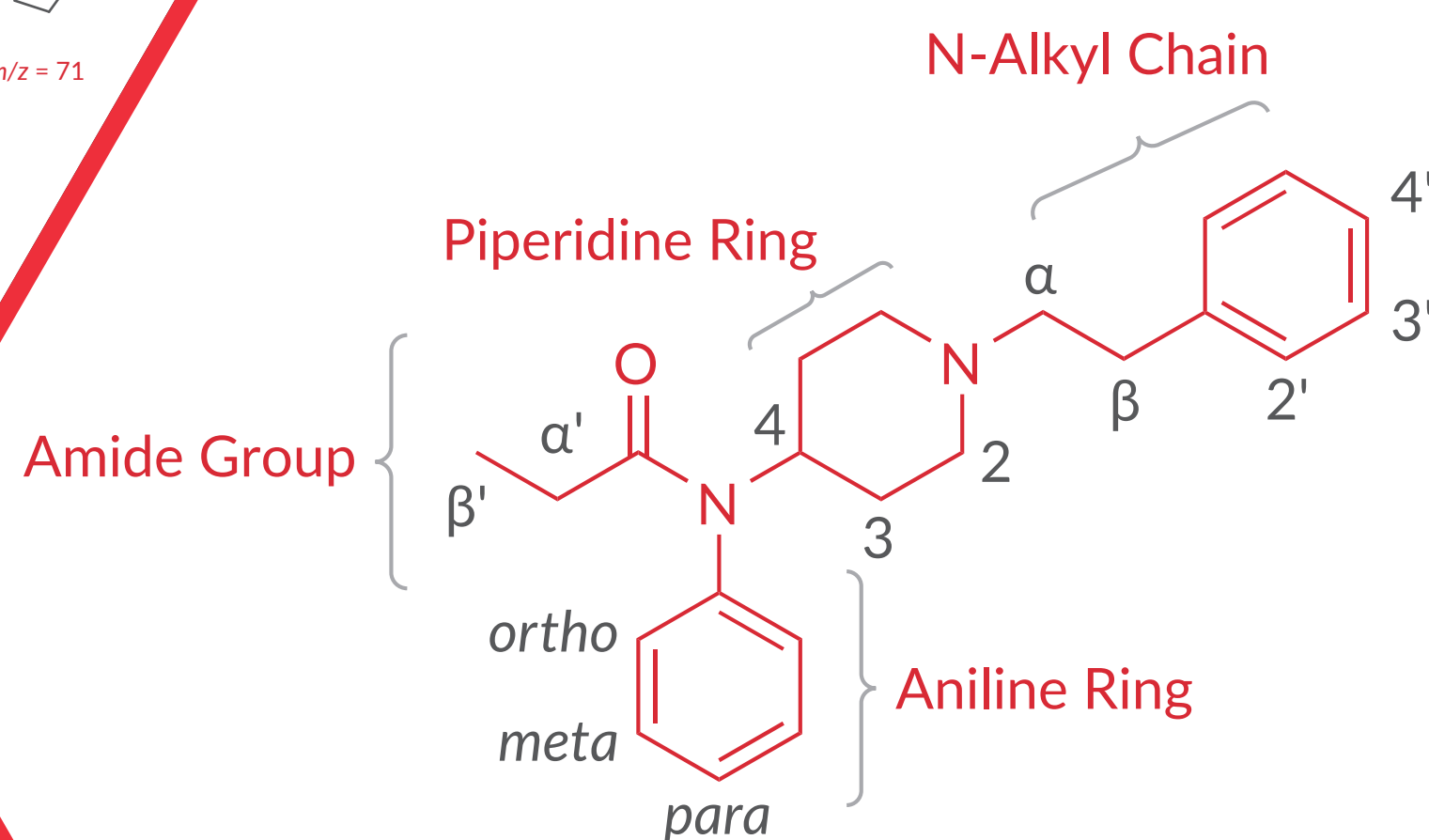
- If $R_1 = CH_3$, the m/z is +14
- If $R_1 = F$, the m/z is +18
- If $R_1 = OCH_3$, the m/z is +30
- If $R_1 = Cl$, the m/z is +34
- If $R_1 = CH(CH_3)_2$, the m/z is +42
- If $R_1 = Br$, the m/z is +78

R_2 (piperidine ring):

- If $R_2 = CH_3$, the m/z is +14
- If $R_2 = F$, the m/z is +18

Laboratory Guide for FENTANYL Identification, Naming, and Metabolism

Standardized Naming of Substituted Fentanyls

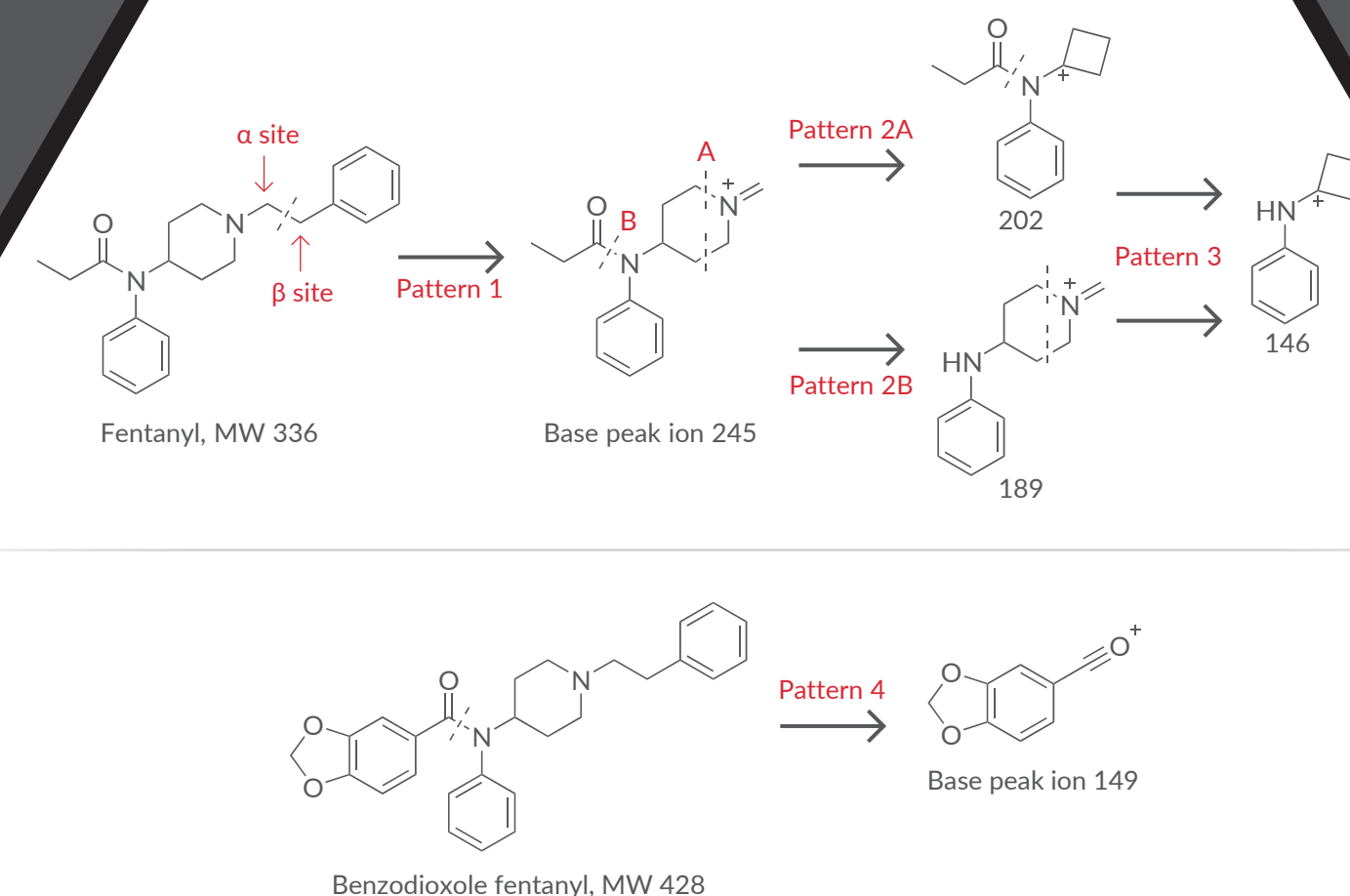


Simple substituents on the fentanyl skeleton (by region):

- **Amide group** substituents occur at either the α' or β' 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.
- **N-alkyl chain** substituents occur at either the α or β 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



Pattern 1: Fentanyl-like compounds cleave between the α and β 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 the loss of H_2O .

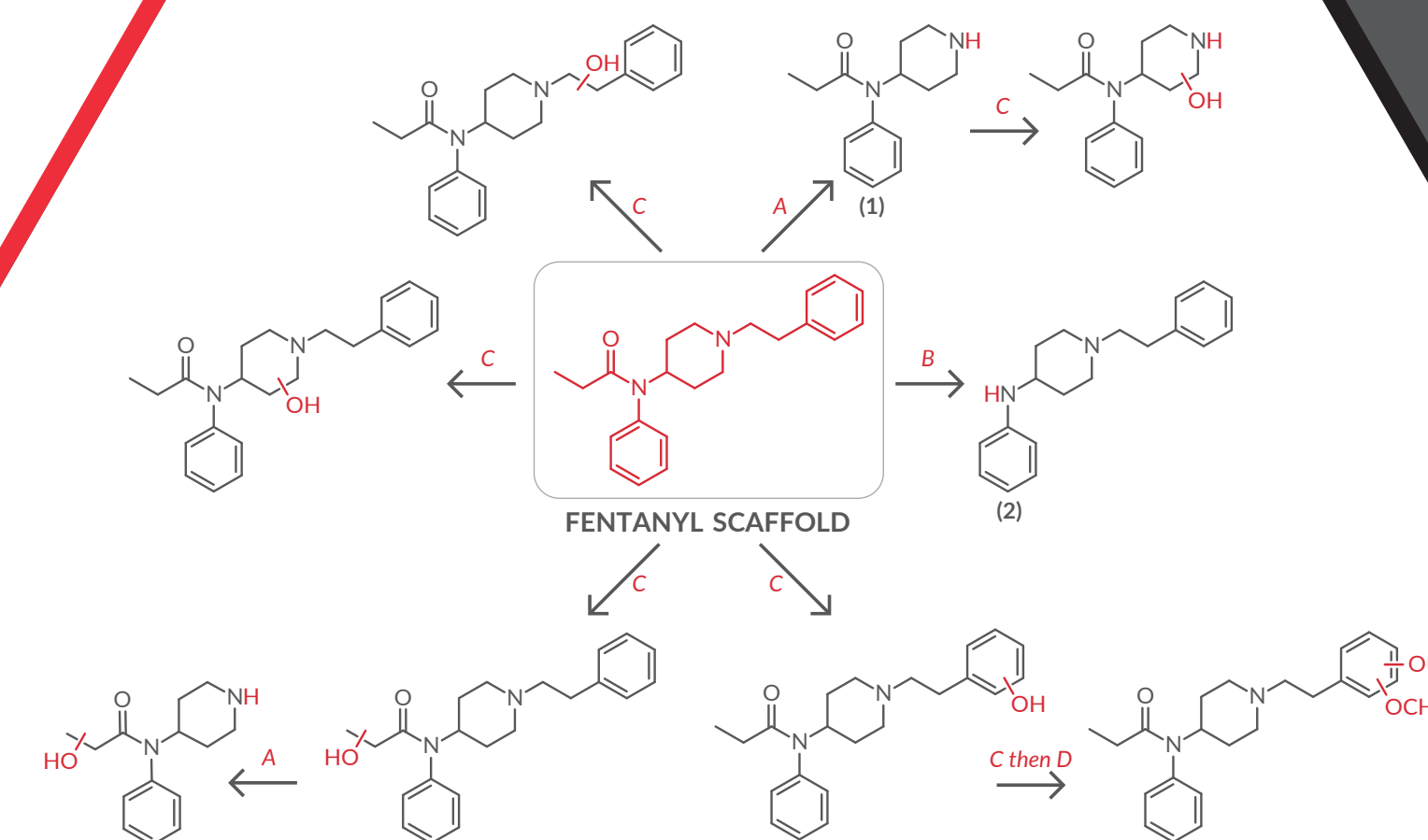
Pattern 2: Additional cleavage of the BP ion occurs along the piperidine ring and at the amide C-N bond.

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 identifying unknown fentanyls at www.caymanchem.com/fentanylpatterns

Fentanyl Metabolism: Typical Phase I Metabolites

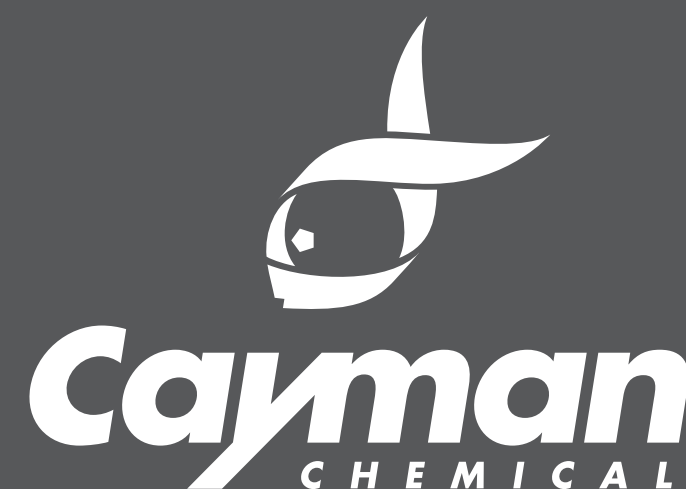


The known routes of fentanyl metabolism include N-dealkylation to form norfentanyl (1), hydrolysis to form 4-ANPP (2), and numerous sites for hydroxylation.

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 fentanyl metabolism at www.caymanchem.com/fentanylmetabolism



Search hundreds of fentanyl standards using the Cayman Spectral Library and GC-MS Search Tool at www.caymanchem.com/forensics

