

# CARFENTANIL STRUCTURAL ANALOGS FOUND IN STREET DRUGS BY PAPER SPRAY MASS SPECTROMETRY AND THEIR CHARACTERIZATION BY HIGH-RESOLUTION MASS SPECTROMETRY

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## BACKGROUND

Carfentanil has been appearing in the illicit drug supply and has been linked to fatal overdose events. Carfentanil is a synthetic opioid with an estimated potency 20-100 times that of fentanyl. Incomplete synthesis or incomplete purification is fairly common in the clandestine manufacture of drugs such as carfentanil, meaning the presence of side products and intermediates may be helpful in determining the synthetic pathway or drug origin. Two unidentified compounds began to appear in street drug samples containing carfentanil submitted to Substance.

## METHODS

The two unidentified compounds were first identified using Paper Spray-Mass Spectrometry then structurally characterized using high-resolution accurate mass spectrometry (HRAM). These compounds were also identified using HRAM in samples collected by Toronto's drug checking service, showing they may be present in other areas of North America.

$\mu$ -Opioid receptor binding modeling of these compounds was calculated using AutoDock Vina v.1.2.3 and found similar binding poses and binding energies to carfentanil.

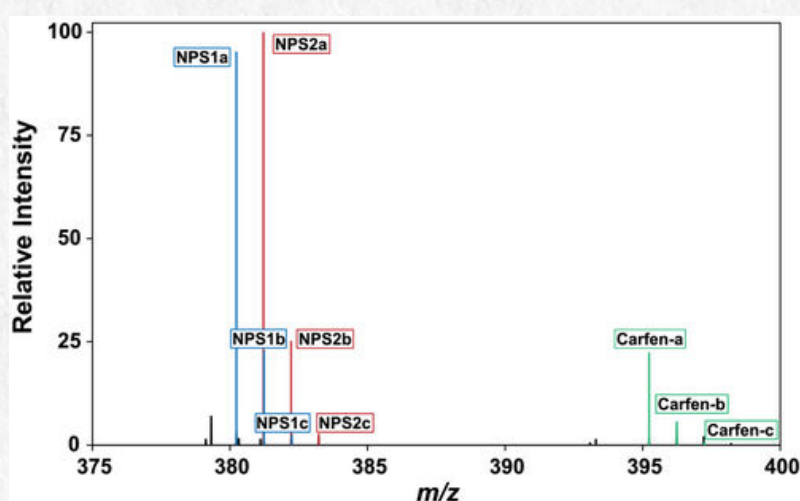
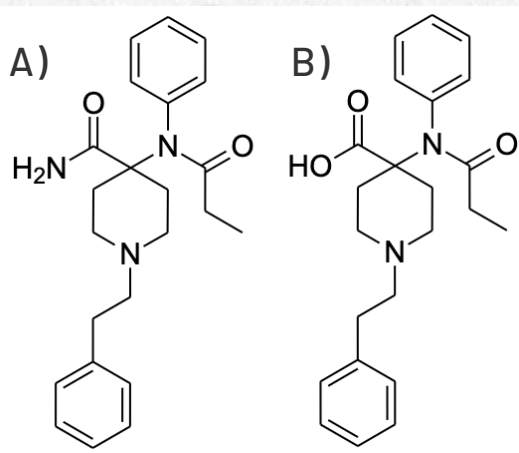


Fig. 1. HRAM of a carfentanil-containing drug sample. Two New Psychoactive Substances (NPS) NPS1a and NPS2a appeared alongside carfentanil in 31 out of 59 carfentanil-containing drug samples.

## RESULTS

The two compounds were identified to be desmethylcarfentanil amide and desmethylcarfentanil acid with binding energy calculations of 0.544 kJ/mol and -0.171 kJ/mol respectively.

These data suggest these compounds may share similar potencies to carfentanil itself. PSMS and HRAM analyses of a carfentanil standard were absent of these compounds, confirming that these were present in only the 31 street drug samples and not as a result of MS fragmentation of carfentanil.



## CONCLUSIONS

Desmethylcarfentanil amide (A) and desmethylcarfentanil acid (B) were identified and structurally characterized from 53% of street drug samples containing carfentanil.

More research is needed to determine whether these compounds are purposefully introduced or accidental byproducts of carfentanil synthesis. Toxicology studies should also be undertaken to assess their potential contribution to fatal overdose events.



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