

# A compound suspected of being a Fentanyl

## The search gives no hint – best MF 568 – no interesting substructures

NIST MS Search 2.3 - [Quick, Presearch Default - InLib = -1589, 100 spectra]

4. Unknown Possibly Fentanyl

(M) 1,2,3,4-Tetrahydro-1 $\beta$ , 2 $\alpha$ , 3 $\alpha$ , 4- $\beta$ -...  
568 594R 12.4P

(M) Cephalotaxine, 3-deoxy-3,11-epoxy-...  
568 570R 12.4P

(M) 6-Ethyl-2-[(4-fluorophenyl)carbonyl]-5-me...  
558 562R 8.72P

(M) 1-Benzyl-4-(4-chlorobenzyl)pyrrolidin-2,5-...  
551 598R 6.68P

(M) Morphinan, 7,8-didehydro-4,5-epoxy-3,6-...  
546 548R 5.38P 2465R1

(M) 4-Androsten-3,17-dione dimethoxime  
544 549R 4.96P 2608R1

(M) Pregni-4-ene-3,20-dione, 17,21-dihydrox...  
536 537R 3.70P

(M) 1,2,4-Triazole-3(2H)-thione, 5-(3,4-dimeth...  
535 549R 3.56P

(M) 1-[1-(2-Chloro-benzyl)-5-hydroxy-2-methyl...  
534 541R 3.42P

(M) 1-[3-(4-Dichlorophenyl)-3-[4-methyl-6-[1-p...  
527 574R 2.62P

(M) Tricyclo[4.2.1.1(2,5)]dec-3-ene, 10-met...  
527 529R 2.62P

(M) 1-Isopropenyl-4,5-dimethylbicyclo[4.3.0]...  
522 525R 2.11P

Unknown Possibly Fentanyl  
Head to Tail MF=568 RMF=594  
Difference Head to Tail Side by Side Subtraction  
568 594R 12.4P

Plot of Hit

Name: 1,2,3,4-tetrahydro-1 $\beta$ , 2 $\alpha$ , 3 $\alpha$ , 4- $\beta$ -4-aminophenanthrene-1  
Formula: C<sub>25</sub>H<sub>27</sub>NO<sub>6</sub>  
MW: 557 Exact Mass: 557.183838 CAS#: 160290-33-5 NIST#: 1304  
Other DBs: None  
Contributor: LAC, NIDDK, NIH, Bethesda, MD 20892  
InChIKey: WBESAMXWJNNFL-UHFFFAOYSA-N Non-steroid  
10 largest peaks:  
105 999 | 313 654 | 77 293 | 208 197 | 314 180 |  
83 138 | 184 133 | 180 83 | 85 82 | 106 72 |  
Synonyms:  
1,4-Amino-2,3-bis(benzoyloxy)-1,2,3,4-tetrahydro-1-phenanthrenyl ben  
Estimated non-polar retention index (n-alkane scale):  
Value: 4626 iu  
Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Lib. Search Other Search Names Compare Librarian MSMS Quick Quick

# If we do a hybrid search we do not get much more information

NIST MS Search 2.3 - [Hybrid precursor = 0, Presearch Default - 100 spectra]

3. Unknown Possibly Fentanyl

(M) 11-Deoxycortisol, bis(O-methylxime) 662 662R -2DM

(M) Glutaric acid, cyclohexylmethyl dodec-9... 648 772R 2927RI 10DM

(M) 3-Cyclopentylpropionic acid, 4-pentade... 647 768R 50DM

(M) 3-Cyclopentylpropionic acid, 3-pentade... 642 761R 50DM

(M) Glutaric acid, hex-5-en-1-yl tridec-2-yn-1... 640 786R 10DM

(M) 3,17-Dimethoxypregna-2,4-dien-20-one 637 638R 2960RI 44DM

(M) 3-Cyclopentylpropionic acid, 3-tetradec... 636 756R 64DM

(M) Glutaric acid, hex-2-en-1-yl tridec-2-yn-1... 633 760R 2760RI 10DM

(M) Epitestosterone, trifluoroacetate, O-met... 628 631R -11DM

(M) Succinic acid, 2,2-dichloroethyl dodec-... 623 652R 2586RI 24DM

(M) 4-Androsten-3,17-dione dimethoxime 618 627R 2608RI 58DM

(M) Pregn-4-ene-3,20-dione, 17,21-di... 614 614R -2DM

Unknown Possibly Fentanyl Head to Tail MF=502 RMF=502 11-Deoxycortisol, bis(O-methylxime) 662 662R

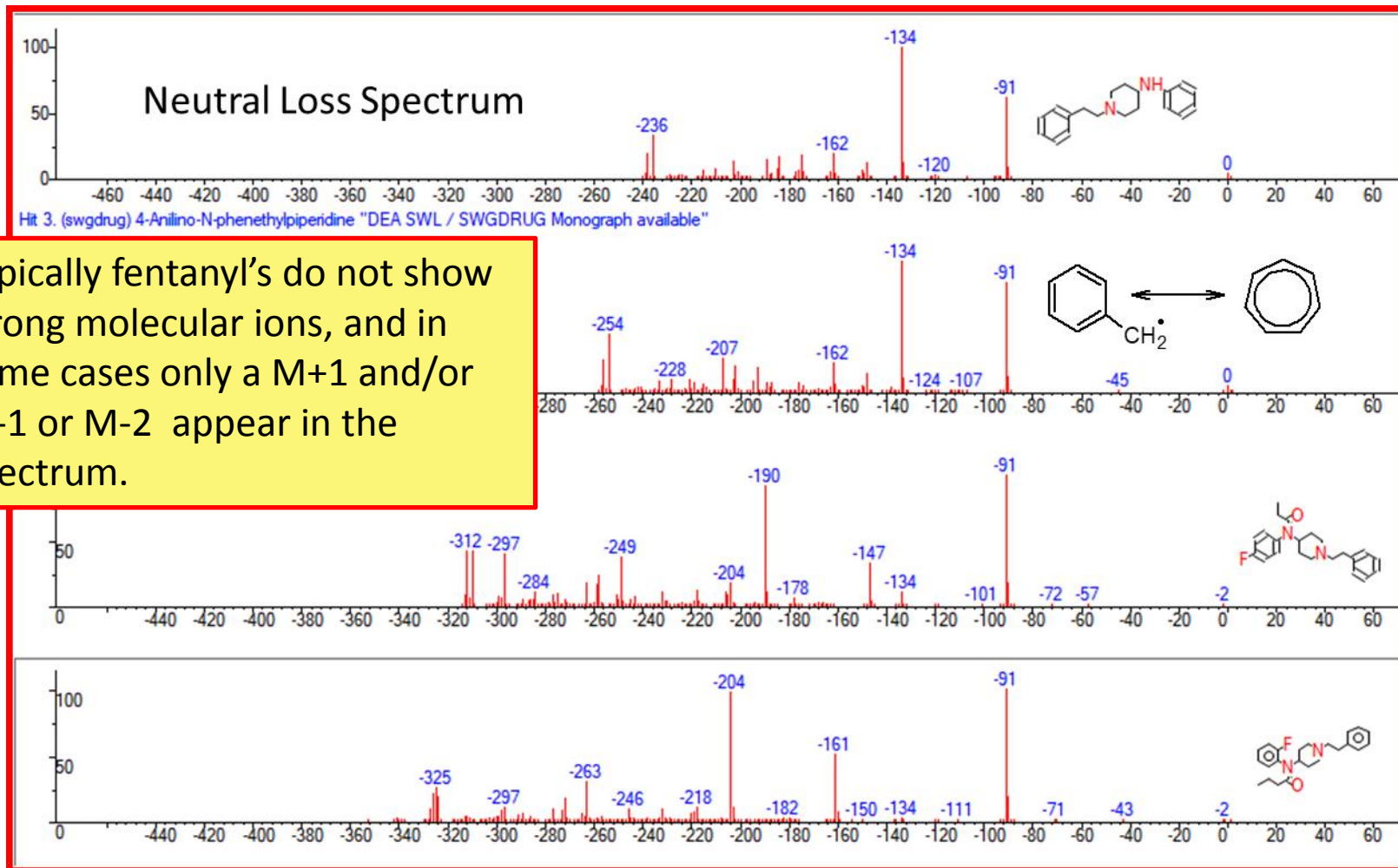
Name: 11-Deoxycortisol, bis(O-methylxime)  
Formula: C<sub>23</sub>H<sub>36</sub>N<sub>2</sub>O<sub>4</sub>  
MW: 404 Exact Mass: 404.267508 NIST#: 394517 ID#: 119899 DB:  
Contributor: NIST Mass Spectrometry Data Center, 2012  
CAS#: 74129-11-1 UNII: 7Z6P-0YVCSA FSA-N

MSMS

Hybrid

402

A very common (almost universal) neutral loss for fentanyl is the 91, so a good guess for a molecular ion is the highest mass major ion + 91



With the highest mass of our unknown (313) the 91 neutral loss gives 404 (not 402) as M+

The default condition is to allow the program to estimate a molecular mass if it is not in the spectrum

Library Search Options

Search MS/MS Libraries Automation Limits Constraints RI (GC)

Spectrum Search Type

Identity  Similarity

Hybrid

Precursor MW

Nom. Mass

Spectrum Search Options

Reverse Search  Penalize rare compounds

Match Ion Mode

Presearch

Default  Fast  Off  MW 1

InChIKey

blank = match search spectrum InChIKey

Other Options

Automation  Auto Report

Apply Limits  Use Constraints

Structure Similarity Search Options

Match Number of Rings  Show Homologues

OK Cancel Help

This works for most unknown spectra, but it is not foolproof.

When it does not work the results do not show the common structural elements that are expected if the search is working.

# The program's nominal mass calculation can be overridden.

Library Search Options

Search MS/MS Libraries Automation Limits Constraints RI (GC)

Spectrum Search Type  
 Identity  Similarity  
Hybrid

Precursor MW  
 Nom. Mass

Spectrum Search Options  
 Reverse Search  Penalize rare compounds  
 Match Ion Mode

Presearch  
 Default  Fast  Off  MW   
 InChIKey   
blank = match search spectrum InChIKey

Other Options  
 Automation  Auto Report  
 Apply Limits  Use Constraints

Structure Similarity Search Options  
 Match Number of Rings  Show Homologues

OK Cancel Help

Here we specify the molecular ion  $m/z$  value, here derived from the assumed loss of 91 from  $M+$  to yield the large 313 peak..

# With the M+ specified, the hybrid search yields a large number of fentanyls (all of the first 12 hits)

NIST MS Search 2.3 - [Hybrid precursor = 0, Presearch Default - 100 spectra]

2. Unknown Possibly Fentanyl

(M) Isobutyryl fentanyl  
821 823R 2797RI 54DM

(M) Furanylfentanyl  
813 814R 30DM

(sw) Fentanyl  
804 810R 68DM

(sw) Butyryl fentanyl  
801 806R 54DM

(M) Fentanyl  
799 815R 2744RI 68DM

(M) Cyclopentyl fentanyl  
797 802R 3145RI 28DM

(M) Acrylfentanyl  
787 795R 2830RI 70DM

(M) Valeryl fentanyl  
783 792R 2981RI 40DM

(M) Butyryl fentanyl  
781 787R 288

(M) N-Phenyl-1-(2-phenylethyl)-4-piperidin...  
755 760R 2485RI 52DM

(sw) 1-(2-phenethyl)-4-(N-acetanilido)piperidi...  
733 821R 82DM

(M) Acetanilide  
691 707R 275

125

313

41 55 105 146 189 207 230 253 279 346 369 392 415 439 462 486 509 533 557 580

41 69 77 97 132 146 160 189 217 242 335 363 402

600

2R 3145RI

243511

ereo

5%) iu

(mainlib) Cyclopentyl fentanyl

Plot/Text of Hit / Plot of Hit

Lib. Search Other Search Names Compare Librarian MSMS

Hybrid Hybrid 404

For Help, press F1

The spectrum from the latest Cayman library  
2,2,3,3-tetramethylcyclopropyl fentanyl

CC1(C)C(C)(C)C1C(=O)N2CCN(CC2)CC3=CC=CC=C3