**Application of Fentanyl Analog Screening Kit for Identification of Emerging Synthetic Opioids in Human Plasma and Urine by LC-QTOF**

Logan C. Krajewski1, Kenneth D. Swanson2, William A Bragg2, Rebecca L. Shaner2\*, Craig Seymour2, Melissa D. Carter2, Elizabeth I. Hamelin2, Rudolph C. Johnson2

1. Battelle at the Centers for Disease Control and Prevention, Atlanta, GA 30341
2. Division of Laboratory Sciences, National Center for Environmental Health, CDC, Atlanta, GA 30341

\*Correspondence to: E. I. Hamelin, Division of Laboratory Sciences, Centers for Disease Control and Prevention, 4770 Buford Hwy NE, MS-F44, Atlanta, GA 30341, USA. Email [elizabeth.hamelin@cdc.hhs.gov](mailto:elizabeth.hamelin@cdc.hhs.gov)

**Supplemental Information**

**Table S1.** List of all 174 compounds and their retention time in in-house personal compound database/library (PCDL).

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| --- | --- | --- | --- |
| **Name** | **Formula** | **Mass (Da)** | **Retention Time (Min)** |
| (±)-cis-3-methyl butyryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.21 |
| (±)-cis-3-methyl fentanyl (hydrochloride) | C23H30N2O | 350.2358 | 7.78 |
| (±)-cis-3-methyl thiofentanyl (hydrochloride) | C21H28N2OS | 356.1922 | 6.63 |
| (±)-trans-3-methyl fentanyl (hydrochloride) | C23H30N2O | 350.2358 | 7.15 |
| (±)-trans-3-methyl thiofentanyl (hydrochloride) | C21H28N2OS | 356.1922 | 6.02 |
| 2,2,3,3-tetramethyl-cyclopropylfentanyl (hydrochloride) | C27H36N2O | 404.2828 | 13.51 |
| 2,3-seco-fentanyl (hydrochloride) | C22H30N2O | 338.2358 | 10.19 |
| 2-fluoro MT-45 (hydrochloride) | C24H31FN2 | 366.2471 | 13.07 |
| 2'-fluoro ortho-fluorofentanyl (hydrochloride) | C22H26F2N2O | 372.2013 | 6.91 |
| 3-furanylfentanyl-D5 | C24H21D5N2O2 | 379.2308 | 8.35 |
| 3-methylfentanyl | C23H30N2O | 350.2358 | 8.06 |
| 4-ANPP | C19H24N2 | 280.194 | 5.74 |
| 4'-fluoro, para-fluoro (±)-trans-3-methyl fentanyl | C23H28F2N2O | 386.217 | 8.58 |
| 4'-fluorofentanyl (hydrochloride) | C22H27FN2O | 354.2107 | 5.99 |
| 4'-methyl acetylfentanyl (hydrochloride) | C22H28N2O | 336.2202 | 5.41 |
| 4'-methylfentanyl (hydrochloride) | C23H30N2O | 350.2358 | 8.52 |
| **Name** | **Formula** | **Mass (Da)** | **Retention Time (Min)** |
| 4-phenylfentanyl (hydrochloride) | C28H32N2O | 412.2515 | 12.91 |
| 6-MAM | C19H21NO4 | 327.1471 | 0.93 |
| Acetyl norfentanyl (hydrochloride) | C13H18N2O | 218.1419 | 0.85 |
| Acetylfentanyl | C21H26N2O | 322.2045 | 3.36 |
| Acetylfentanyl-13C6 | C15[13C]6H26N2O | 328.2246 | 3.42 |
| Acrylfentanyl | C22H26N2O | 334.2045 | 5.2 |
| Acrylfentanyl-D5 | C22H21D5N2O | 339.2359 | 5.21 |
| AH7921 | C16H22Cl2N2O | 328.1109 | 5.11 |
| AH7921-D3 | C16H19D3Cl2N2O | 331.1298 | 5.05 |
| Alfentanil | C21H32N6O3 | 416.2536 | 4.71 |
| α'-methoxy fentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 3.69 |
| α-methyl acetylfentanyl (hydrochloride) | C22H28N2O | 336.2202 | 4.31 |
| α'-methyl butyryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 10.76 |
| α-methyl butyryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 10.02 |
| α-methyl fentanyl (hydrochloride) | C23H30N2O | 350.2358 | 6.85 |
| α-methyl thiofentanyl (hydrochloride) | C21H28N2OS | 356.1922 | 5.72 |
| Benzodioxole fentanyl | C27H28N2O3 | 428.21 | 11.5 |
| Benzyl acrylfentanyl (hydrochloride) | C21H24N2O | 320.1889 | 3.96 |
| Benzyl carfentanil (hydrochloride) | C23H28N2O3 | 380.21 | 5.82 |
| Benzyl fentanyl (hydrochloride) | C21H26N2O | 322.2045 | 4.13 |
| Butyryl norfentanyl (hydrochloride) | C15H22N2O | 246.1732 | 1.69 |
| Butyrylfentanyl | C23H30N2O | 350.2358 | 8.1 |
| Carfentanil | C24H30N2O3 | 394.2256 | 7.94 |
| Carfentanyl-D5 | C24H25D5N2O3 | 399.257 | 7.78 |
| Crotonyl fentanyl | C23H28N2O | 348.2202 | 7.35 |
| Cyclobutyl fentanyl (hydrochloride) | C24H30N2O | 362.2358 | 10.41 |
| Cyclohexyl fentanyl (hydrochloride) | C26H34N2O | 390.2671 | 12.53 |
| Cyclopentenyl fentanyl (hydrochloride) | C25H30N2O | 374.2358 | 11.31 |
| Cyclopentyl fentanyl (hydrochloride) | C25H32N2O | 376.2515 | 12.02 |
| Cyclopropylfentanyl | C23H28N2O | 348.2202 | 7.09 |
| Cyclopropylfentanyl-D5 | C23H23D5N2O | 353.2516 | 7.21 |
| Ethoxyacetyl fentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 4.32 |
| Fentanyl | C22H28N2O | 336.2202 | 5.36 |
| Fentanyl carbamate | C22H28N2O2 | 352.2151 | 7.68 |
| Fentanyl methylcarbamate | C21H26N2O2 | 338.1994 | 5.13 |
| Fentanyl-D5 | C22H23D5N2O | 341.2516 | 5.46 |
| Fluoroisobutyrylfentanyl | C23H29FN2O | 368.2264 | 8.27 |
| Furanyl fentanyl 3-furancarboxamide isomer (hydrochloride) | C24H26N2O2 | 374.1994 | 8.28 |
| Furanyl norfentanyl (hydrochloride) | C16H18N2O2 | 270.1368 | 1.44 |
| Furanylethyl fentanyl (hydrochloride) | C20H26N2O2 | 326.1994 | 3.226 |
| Furanylfentanyl | C24H26N2O2 | 374.1994 | 7.35 |
| **Name** | **Formula** | **Mass (Da)** | **Retention Time (Min)** |
| Heptanoyl fentanyl (hydrochloride) | C26H36N2O | 392.2828 | 13.48 |
| Hexanoyl fentanyl (hydrochloride) | C25H34N2O | 378.2671 | 12.65 |
| Isobutyryl fentanyl (hydrochloride) | C23H30N2O | 350.2358 | 7.5 |
| Isobutyrylfentanyl-D5 | C23H25D5N2O | 355.2672 | 7.62 |
| Isopropyl U-47700 | C18H26Cl2N2O | 356.1422 | 9.22 |
| Isovaleryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.14 |
| Lofentanil | C25H32N2O3 | 408.2413 | 9.82 |
| meta-fluoro methoxyacetyl fentanyl (hydrochloride) | C22H27FN2O2 | 370.2057 | 3.43 |
| meta-fluorobutyryl fentanyl (hydrochloride) | C23H29FN2O | 368.2264 | 9.07 |
| meta-fluorofentanyl (hydrochloride) | C22H27FN2O | 354.2107 | 6.12 |
| meta-fluoroisobutyryl fentanyl (hydrochloride) | C23H29FN2O | 368.2264 | 8.34 |
| meta-methyl cyclopropylfentanyl (hydrochloride) | C24H30N2O | 362.2358 | 10.66 |
| meta-methyl furanyl fentanyl (hydrochloride) | C25H28N2O2 | 388.2151 | 10.57 |
| meta-methyl methoxyacetyl fentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 4.62 |
| meta-methylfentanyl (hydrochloride) | C23H30N2O | 350.2358 | 8.13 |
| Methacrylfentanyl | C23H28N2O | 348.2202 | 6.01 |
| Methoxyacetylfentanyl | C22H28N2O2 | 352.2151 | 2.85 |
| Methoxyacetylfentanyl-D5 | C22H23D5N2O2 | 357.2465 | 2.98 |
| Morphine | C17H19NO3 | 285.1365 | 0.73 |
| Morphine-3-glucuronide | C23H27NO9 | 461.1686 | 0.69 |
| MT45 | C24H32N2 | 348.2566 | 12.81 |
| N-(3-ethylindole) norfentanyl | C24H29N3O | 375.2311 | 7.65 |
| N,N-dimethylamido-despropionyl fentanyl | C22H29N3O | 351.2311 | 6.75 |
| Naloxone | C19H21NO4 | 327.1471 | 0.82 |
| Naltrexone | C20H23NO4 | 341.1627 | 0.93 |
| N-benzyl furanyl norfentanyl (hydrochloride) | C23H24N2O2 | 360.1838 | 5.67 |
| N-methyl cyclopropyl norfentanyl (hydrochloride) | C16H22N2O | 258.1732 | 1.46 |
| N-methyl norcarfentanil (hydrochloride) | C17H24N2O3 | 304.1787 | 1.38 |
| Norcarfentanil | C16H22N2O3 | 290.163 | 1.42 |
| Norcarfentanil-D5 | C16H17D5N2O3 | 295.1944 | 1.39 |
| Norfentanyl | C14H20N2O | 232.1576 | 1.17 |
| Norfentanyl-D5 | C14H15D5N2O | 237.189 | 1.14 |
| Norlofentanil | C17H24N2O3 | 304.1787 | 1.75 |
| Norsufentanil | C16H24N2O2 | 276.1838 | 1.95 |
| Ocfentanil | C22H27FN2O2 | 370.2057 | 3.32 |
| Ocfentanil-D5 | C22H22D5FN2O2 | 375.237 | 3.34 |
| ortho-fluoro acrylfentanyl (hydrochloride) | C22H25FN2O | 352.1951 | 5.64 |
| ortho-fluoro furanyl fentanyl (hydrochloride) | C24H25FN2O2 | 392.19 | 8.02 |
| ortho-fluorobutyryl fentanyl (hydrochloride) | C23H29FN2O | 368.2264 | 9.25 |
| ortho-fluorofentanyl (hydrochloride) | C22H27FN2O | 354.2107 | 6.23 |
| ortho-fluoroisobutyryl fentanyl (hydrochloride) | C23H29FN2O | 368.2264 | 8.75 |
| ortho-isopropyl furanyl fentanyl | C27H32N2O2 | 416.2464 | 12.52 |
| **Name** | **Formula** | **Mass (Da)** | **Retention Time (Min)** |
| ortho-methoxy butyryl fentanyl (hydrochloride) | C24H32N2O2 | 380.2464 | 10.48 |
| ortho-methoxy furanyl fentanyl | C25H28N2O3 | 404.21 | 8.73 |
| ortho-methyl acetylfentanyl (hydrochloride) | C22H28N2O | 336.2202 | 4.66 |
| ortho-methyl acrylfentanyl (hydrochloride) | C23H28N2O | 348.2202 | 7.23 |
| ortho-methyl cyclopropylfentanyl (hydrochloride) | C24H30N2O | 362.2358 | 9.73 |
| ortho-methyl furanyl fentanyl (hydrochloride) | C25H28N2O2 | 388.2151 | 9.74 |
| ortho-methyl methoxyacetyl fentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 4.17 |
| ortho-methyl phenyl fentanyl (hydrochloride) | C27H30N2O | 398.2358 | 12.26 |
| ortho-methylfentanyl (hydrochloride) | C23H30N2O | 350.2358 | 7.66 |
| para-chloro acrylfentanyl (hydrochloride) | C22H25ClN2O | 368.1655 | 9.23 |
| para-chloro cyclobutyl fentanyl (hydrochloride) | C24H29ClN2O | 396.1968 | 12.39 |
| para-chloro cyclopentyl fentanyl (hydrochloride) | C25H31ClN2O | 410.2125 | 13.02 |
| para-chloro cyclopropyl fentanyl (hydrochloride) | C23H27ClN2O | 382.1812 | 11.47 |
| para-chloro furanyl fentanyl | C24H25ClN2O2 | 408.1605 | 11.68 |
| para-chloro methoxyacetyl fentanyl (hydrochloride) | C22H27ClN2O2 | 386.1761 | 5.45 |
| para-chloro valeryl fentanyl (hydrochloride) | C24H31ClN2O | 398.2125 | 12.72 |
| para-chlorobutyryl fentanyl (hydrochloride) | C23H29ClN2O | 384.1968 | 11.97 |
| para-chlorofentanyl (hydrochloride) | C22H27ClN2O | 370.1812 | 9.61 |
| para-chloroisobutyryl fentanyl (hydrochloride) | C23H29ClN2O | 384.1968 | 11.81 |
| para-fluoro acrylfentanyl | C22H25FN2O | 352.1951 | 5.66 |
| para-fluoro crotonyl fentanyl | C23H27FN2O | 366.2107 | 7.87 |
| para-fluoro cyclopentyl fentanyl (hydrochloride) | C25H31FN2O | 394.242 | 12.18 |
| para-fluoro cyclopropyl fentanyl (hydrochloride) | C23H27FN2O | 366.2107 | 7.69 |
| para-fluoro furanyl fentanyl (hydrochloride) | C24H25FN2O2 | 392.19 | 8.09 |
| para-fluoro furanyl fentanyl 3-furancarboxamide | C24H25FN2O2 | 392.19 | 8.71 |
| para-fluoro methoxyacetyl fentanyl (hydrochloride) | C22H27FN2O2 | 370.2057 | 3.38 |
| para-fluoro tetrahydrofuran fentanyl (hydrochloride) | C24H29FN2O2 | 396.2213 | 4.8 |
| para-fluoro valeryl fentanyl (hydrochloride) | C24H31FN2O | 382.242 | 11.94 |
| para-fluoroacetyl fentanyl (hydrochloride) | C21H25FN2O | 340.1951 | 3.77 |
| para-fluorobutyryl fentanyl (hydrochloride) | C23H29FN2O | 368.2264 | 8.86 |
| para-fluorofentanyl (hydrochloride) | C22H27FN2O | 354.2107 | 6.07 |
| para-methoxy acetylfentanyl (hydrochloride) | C22H28N2O2 | 352.2151 | 4.2 |
| para-methoxy acrylfentanyl (hydrochloride) | C23H28N2O2 | 364.2151 | 6.39 |
| para-methoxy butyryl fentanyl (hydrochloride) | C24H32N2O2 | 380.2464 | 9.66 |
| para-methoxy furanyl fentanyl (hydrochloride) | C25H28N2O3 | 404.21 | 8.64 |
| para-methoxy methoxyacetyl fentanyl (hydrochloride) | C23H30N2O3 | 382.2256 | 3.83 |
| para-methoxy tetrahydrofuran fentanyl (hydrochloride) | C25H32N2O3 | 408.2413 | 5.44 |
| para-methoxy valeryl fentanyl (hydrochloride) | C25H34N2O2 | 394.262 | 12.07 |
| para-methoxyfentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 6.61 |
| para-methyl acetylfentanyl (hydrochloride) | C22H28N2O | 336.2202 | 5.48 |
| para-methyl acrylfentanyl (hydrochloride) | C23H28N2O | 348.2202 | 8.19 |
| para-methyl butyryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.78 |
| **Name** | **Formula** | **Mass (Da)** | **Retention Time (Min)** |
| para-methyl cyclopentyl fentanyl (hydrochloride) | C26H34N2O | 390.2671 | 12.86 |
| para-methyl cyclopropyl fentanyl (hydrochloride) | C24H30N2O | 362.2358 | 10.85 |
| para-methyl furanyl fentanyl (hydrochloride) | C25H28N2O2 | 388.2151 | 10.77 |
| para-methyl isobutyryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.28 |
| para-methyl methoxyacetyl fentanyl (hydrochloride) | C23H30N2O2 | 366.2307 | 4.87 |
| para-methyl tetrahydrofuran fentanyl (hydrochloride) | C25H32N2O2 | 392.2464 | 6.91 |
| para-methylfentanyl (hydrochloride) | C23H30N2O | 350.2358 | 8.74 |
| Phenoxyacetyl fentanyl (hydrochloride) | C27H30N2O2 | 414.2307 | 12.12 |
| Phenyl fentanyl (hydrochloride) | C26H28N2O | 384.2202 | 10.79 |
| Phenylacetyl fentanyl (hydrochloride) | C27H30N2O | 398.2358 | 12.17 |
| Pivaloyl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.72 |
| Remifentanil (hydrochloride) | C20H28N2O5 | 376.1998 | 2.25 |
| Senecioylfentanyl | C24H30N2O | 362.2358 | 10.28 |
| ß-hydroxy fentanyl (hydrochloride) | C22H28N2O2 | 352.2151 | 3.55 |
| ß-Hydroxythioacetylfentanyl | C19H24N2O2S | 344.1558 | 1.84 |
| ß-Hydroxythiofentanyl | C20H26N2O2S | 358.1715 | 3 |
| ß-methyl acetylfentanyl (hydrochloride) | C22H28N2O | 336.2202 | 4.73 |
| ß-methyl fentanyl (hydrochloride) | C23H30N2O | 350.2358 | 7.59 |
| Sufentanil | C22H30N2O2S | 386.2028 | 9.92 |
| Sufentanil-D5 | C22H25D5N2O2S | 391.2342 | 9.98 |
| Tetrahydrofuran fentanyl (hydrochloride) | C24H30N2O2 | 378.2307 | 4.12 |
| Tetrahydrofuran fentanyl 3-tetrahydrofurancarboxamide | C24H30N2O2 | 378.2307 | 4.06 |
| Tetrahydrofuran fentanyl -D5 | C24H25D5N2O2 | 383.2621 | 4.36 |
| Thienyl fentanyl (hydrochloride) | C19H24N2OS | 328.1609 | 3.41 |
| Thiofentanyl (hydrochloride) | C20H26N2OS | 342.1766 | 4.51 |
| Thiophene fentanyl (hydrochloride) | C24H26N2OS | 390.1766 | 11.78 |
| U47700 | C16H22Cl2N2O | 328.1109 | 4.51 |
| U-48800 (hydrochloride) | C17H24Cl2N2O | 342.1266 | 6.11 |
| U-49900 | C18H26Cl2N2O | 356.1422 | 7.38 |
| U-50488 | C19H26Cl2N2O | 368.1422 | 9.58 |
| Valeryl fentanyl (hydrochloride) | C24H32N2O | 364.2515 | 11.77 |