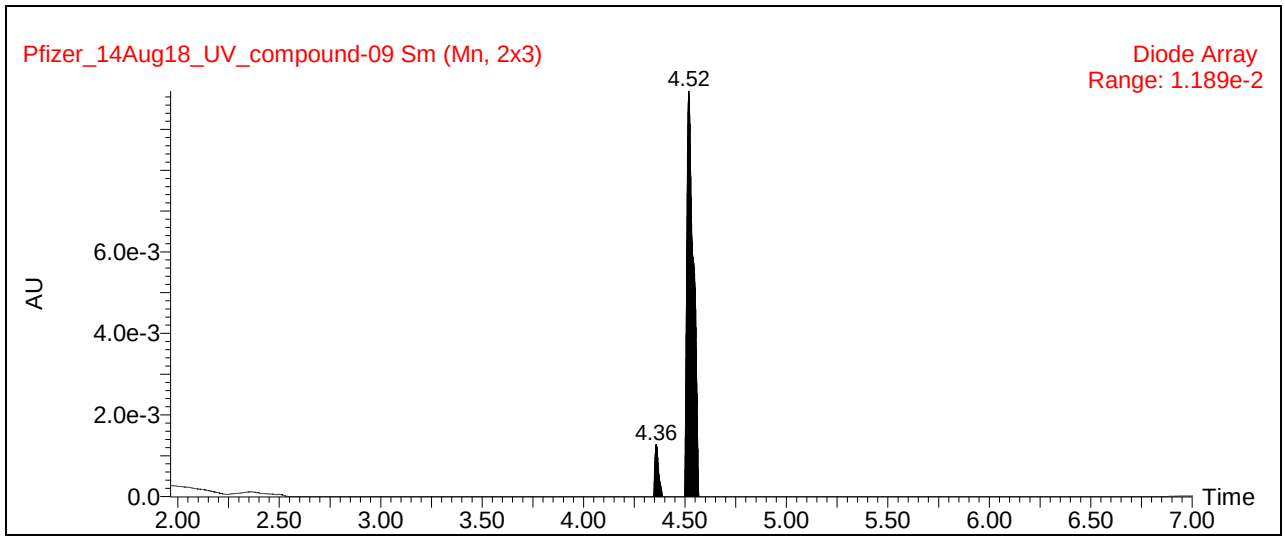
NovaBioAssays

# Qualitative Compound Report

| | | | |
|---|---|---|---|
| **Data File:** | UV: Pfizer 14Aug18 Sample 09<br>MS: pfizer_14Aug18_MS_compound_9 | **Sample Name:** | 00712940-0087-001 |
| **Sample Type:** | Sample | **Position:** | 1:9 |
| **Instrument Name:** | Waters UPLC with TUV and Thermo Q Exactive MS | **User Name:** | Birlandy Pérez |
| **LC Method:** | pfizer_TUV_7min_400ulmin_sep17 | **Calibration Status:** | |
| **MS Method:** | pfizer_pos_full-ms_compound_7min_15may2017 | **Comment:** | |




**User Chromatogram Peak List**

| Compound Name | Compound Formula | Area | RT | Purity |
|---|---|---|---|---|
| | | 12.191 | 3.528 | |
| | | 36.578 | 3.836 | |
| | | 20.953 | 4.058 | |
| | | 11.975 | 4.164 | |
| | | 18.856 | 4.24 | |
| | | 123.753 | 4.358 | |
| Cpd-09-4.5 | C23H27NO5 | 507.752 | 4.518 | 68% |
| | | 12.313 | 4.947 | |

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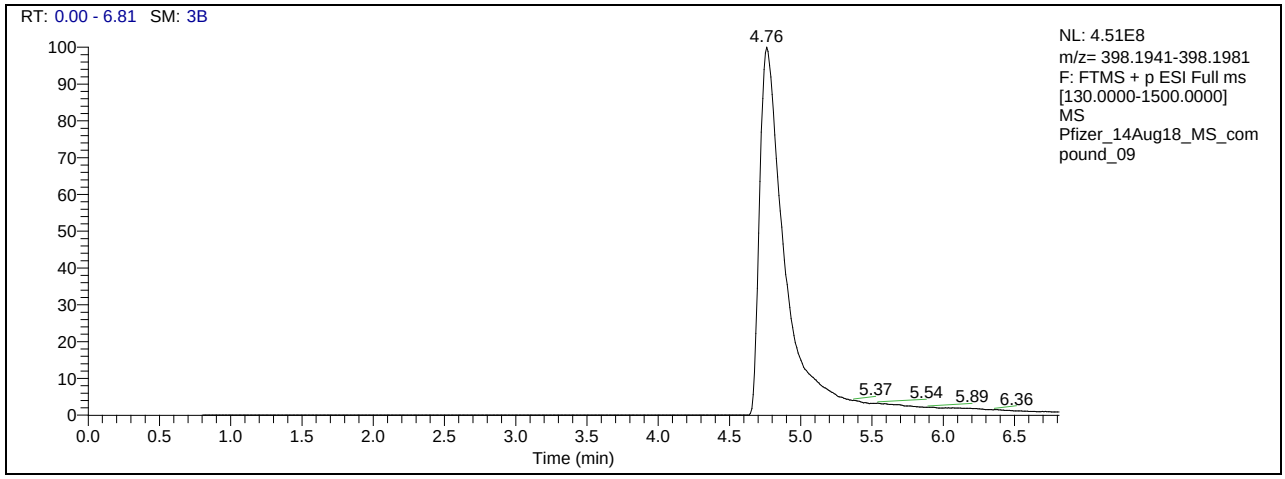
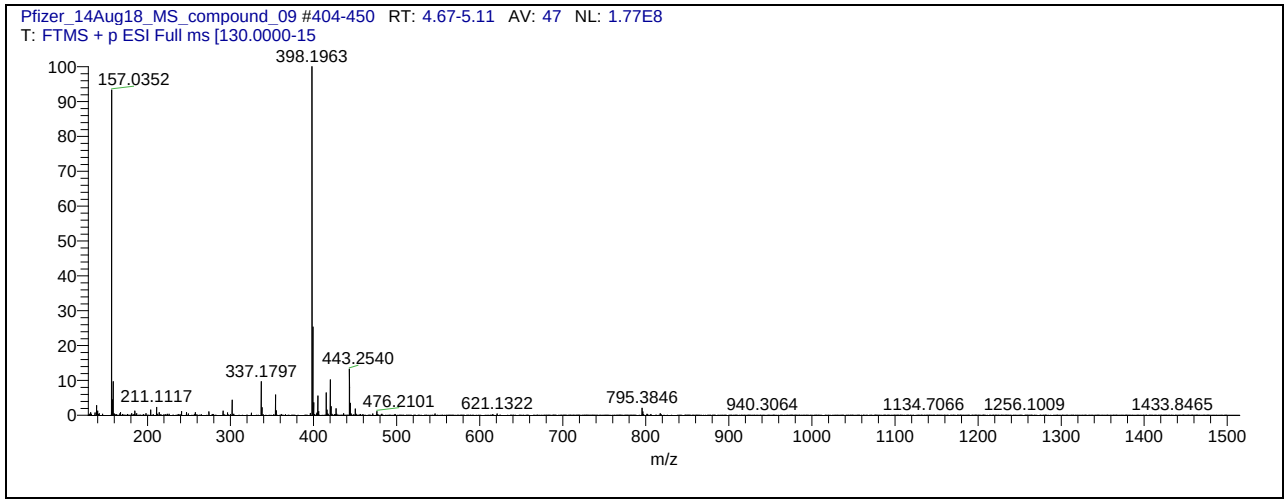



## Mass Spectrum



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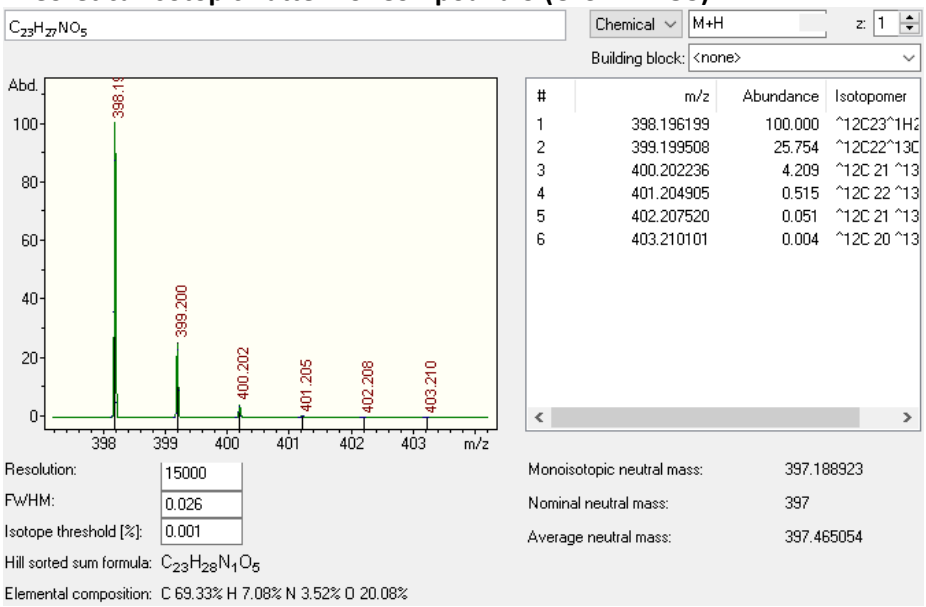
| m/z | Calc m/z | Diff (ppm) | z | Abund | Formula | Ion |
|---|---|---|---|---|---|---|
| 398.1033 | | | 1 | 25817.5 | | |
| 398.1047 | | | 1 | 25376 | | |
| 398.1857 | | | 1 | 445347.8 | | |
| 398.1963 | 398.196 | 0.2536438 | 1 | 1.78E+08 | C23H27NO5 | M[+H]+ |
| 398.287 | | | 1 | 32109.9 | | |
| 399.0166 | | | 1 | 32705.5 | | |
| 399.1889 | | | 1 | 28270.2 | | |
| 399.1993 | 399.2 | -0.521043 | 1 | 45103460 | C23H27NO5 | M[+H]+ |
| 399.2506 | | | 1 | 94972.3 | | |
| 400.1754 | | | 1 | 1696366 | | |
| 400.202 | 400.202 | -0.589702 | 1 | 6443561 | C23H27NO5 | M[+H]+ |
| 401.1786 | | | 1 | 371348.1 | | |
| 401.2046 | 401.205 | -0.76021 | 1 | 448181.1 | C23H27NO5 | M[+H]+ |
| 402.1819 | | | 1 | 32428.3 | | |
| 402.1884 | | | 1 | 20544.5 | | |
| 402.2064 | 402.208 | -2.784632 | 1 | 31646.6 | C23H27NO5 | M[+H]+ |
| 403.0947 | | | 1 | 29130.2 | | |
| 403.2025 | | | 1 | 85429.1 | | |
| 403.2222 | | | 1 | 23547.9 | | |
| 403.2325 | | | 1 | 190828.1 | | |

**Theoretical Isotopic Pattern of Compound-9 (C23H27NO5)**




**------End of Report------**