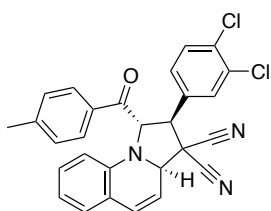


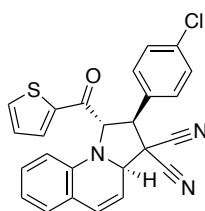
Supplementary Figure 3. 6994 analogs from the UPCMLD library

Active at 10 and 20 μ M



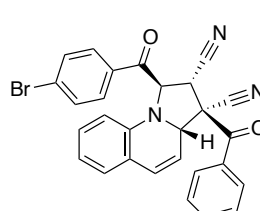
UPCMLDCBRC1000784

Chemical Formula: $C_{28}H_{19}Cl_2N_3O$
Molecular Weight: 484.38



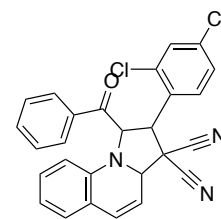
UPCMLDCBRC1000802

Chemical Formula: $C_{25}H_{16}ClN_3OS$
Molecular Weight: 441.93



UPCMLDCBRC1001299

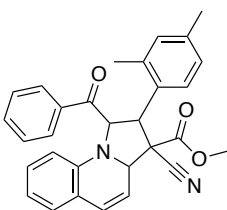
Chemical Formula: $C_{28}H_{18}BrN_3O_2$
Molecular Weight: 508.38



UPCMLDCBRC1033229

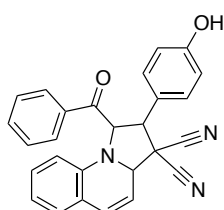
Chemical Formula: $C_{27}H_{17}Cl_2N_3O$
Molecular Weight: 470.35

Inactive at 10 and 20 μ M



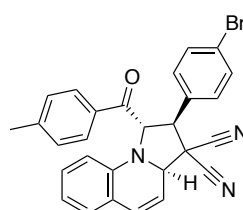
UPCMLDCBRC1002602

Chemical Formula: $C_{30}H_{26}N_2O_3$
Molecular Weight: 462.55



UPCMLDCBRC1004885

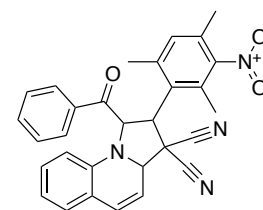
Chemical Formula: $C_{27}H_{19}N_3O_2$
Molecular Weight: 417.47



UPCMLDCBRC1038747

Chemical Formula: $C_{28}H_{20}BrN_3O$
Molecular Weight: 494.39

Autofluorescent

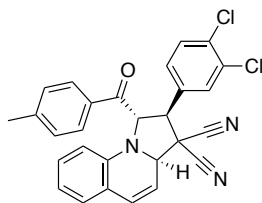


UPCMLDCBRC1033038

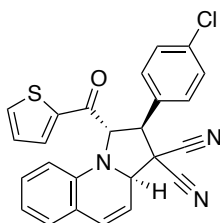
Chemical Formula: $C_{30}H_{24}N_4O_3$
Molecular Weight: 488.55

HPLC and HRMS Data:

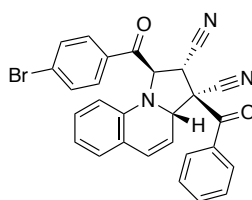
HPLC data were obtained on a Thermo Scientific Accela HPLC system using 3 μ L injections on a 2.1 x 50 mm 3.5 μ m Waters XTerra C_{18} column eluting with MeCN/ H_2O /MeOH containing 0.1% formic acid (flow rate of 500 μ L/min from 3:92:5 at 0-0.5 min to 93:2:5 at 4.0 min, back to 3:92:5 from 6.0 to 7.5 min). Absorbance was monitored at 210, 220, and 254 nm. HRMS data were obtained on a Thermo Scientific Exactive HRMS (ESI-). Samples were dissolved in MeCN and 5 μ L aliquots were direct-injected into the probe head (-60 V, 350 $^{\circ}$ C). Mass accuracy was determined with Thermo Xcalibur software.



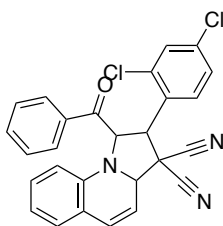
UPCMLDCBRC1000784. HPLC retention time 6.43 min. HRMS (HESI) m/z calcd for $C_{28}H_{18}N_3O_2Cl_2$ $[M-H]^-$ 482.0821, found 482.0841.



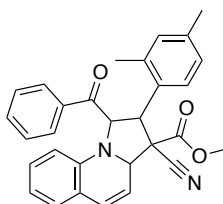
UPCMLDCBRC1000802. HPLC retention time 5.16 min. HRMS (HESI) m/z calcd for $C_{25}H_{15}N_3OClS$ $[M-H]^-$ 440.0619, found 440.0637.



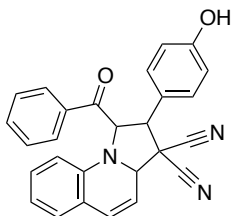
UPCMLDCBRC1001299. HPLC retention time 5.89 min. HRMS (HESI) m/z calcd for $C_{28}H_{17}N_3O_2Br$ $[M-H]^-$ 506.0499, found 506.0526.



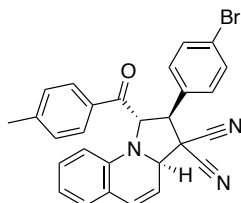
UPCMLDCBRC1033229. HPLC retention time 5.46 min. HRMS (HESI) m/z calcd for $C_{27}H_{16}N_3OCl_2$ $[M-H]^-$ 468.0665, found 468.0684.



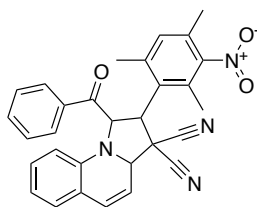
UPCMLDCBRC1002602. HPLC retention time 5.81 min. HRMS (HESI) m/z calcd for $C_{30}H_{25}N_2O_3$ $[M-H]^-$ 461.1860, found 461.1872.



UPCMLDCBRC1004885. HPLC retention time 4.90 min. HRMS (HESI) m/z calcd for $C_{27}H_{18}N_3O_2$ $[M-H]^-$ 416.1394, found 416.1408.

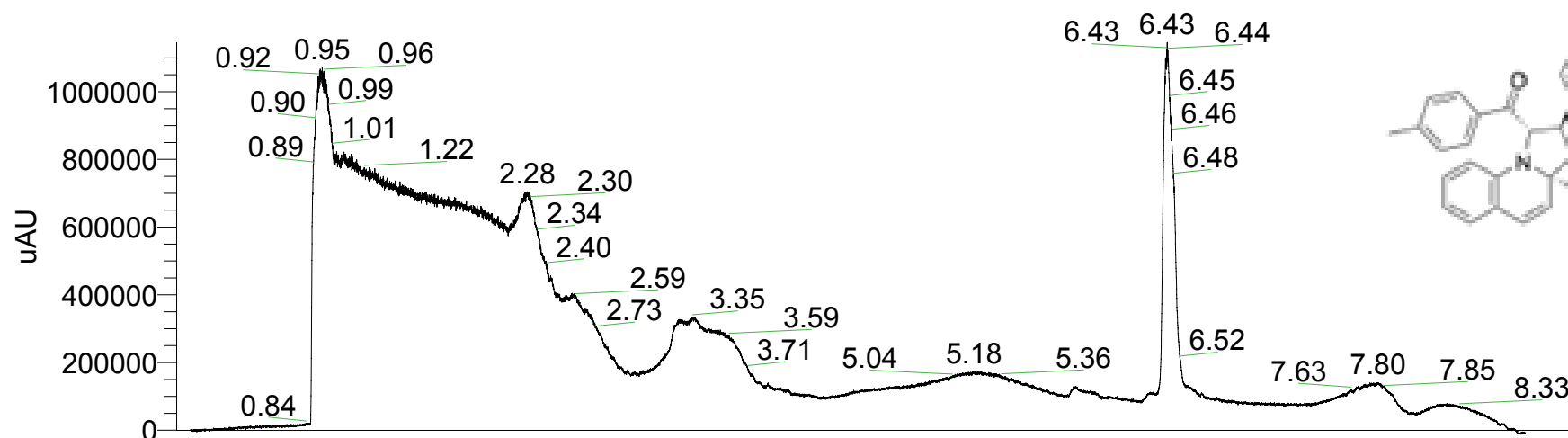


UPCMLDCBRC1038747. HPLC retention time 5.45 min. HRMS (HESI) m/z calcd for $C_{28}H_{19}N_3OBr$ $[M-H]^-$ 492.0706, found 492.0724.

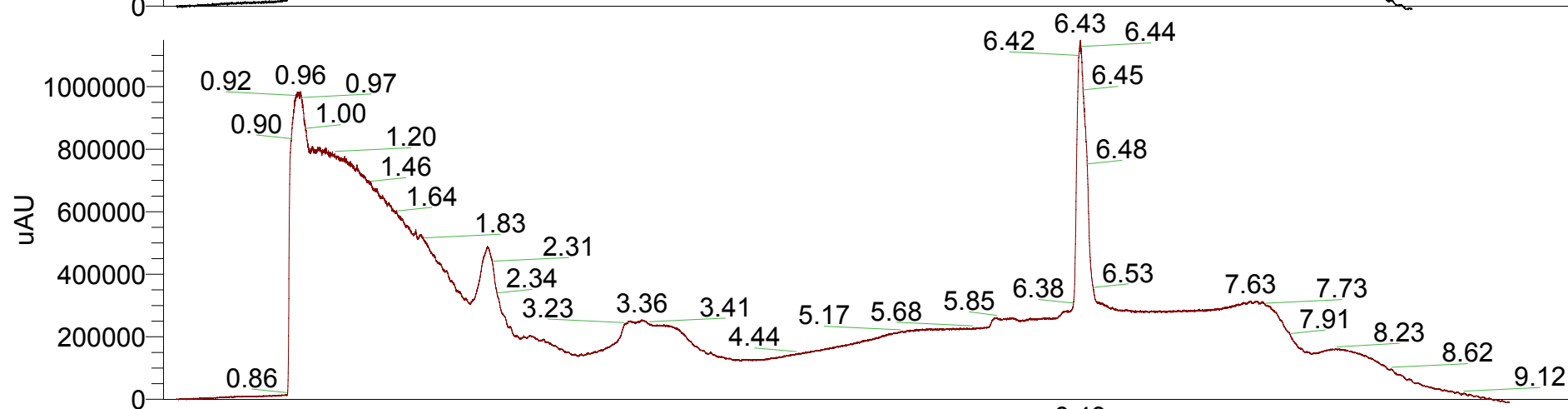


UPCMLDCBRC1033038. HPLC retention time 5.30 min. HRMS (HESI) m/z calcd for $C_{30}H_{23}N_4O_3$ $[M-H]^-$ 487.1765, found 487.1778.

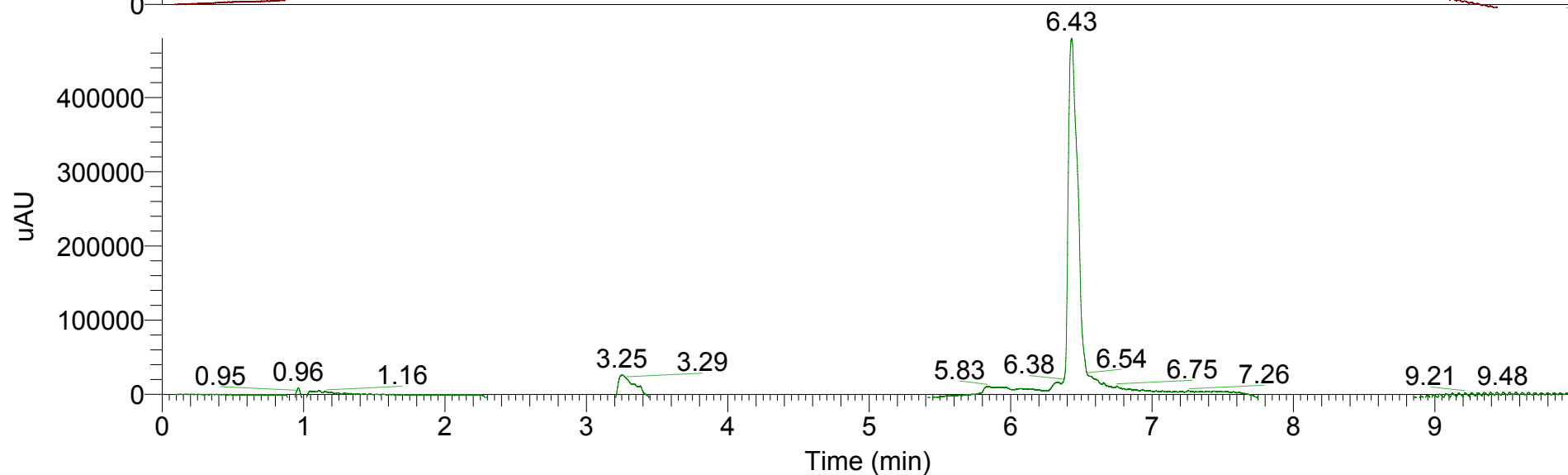
RT: 0.00 - 9.98



NL:
1.15E6
Channel A
UV
C1000784_
1

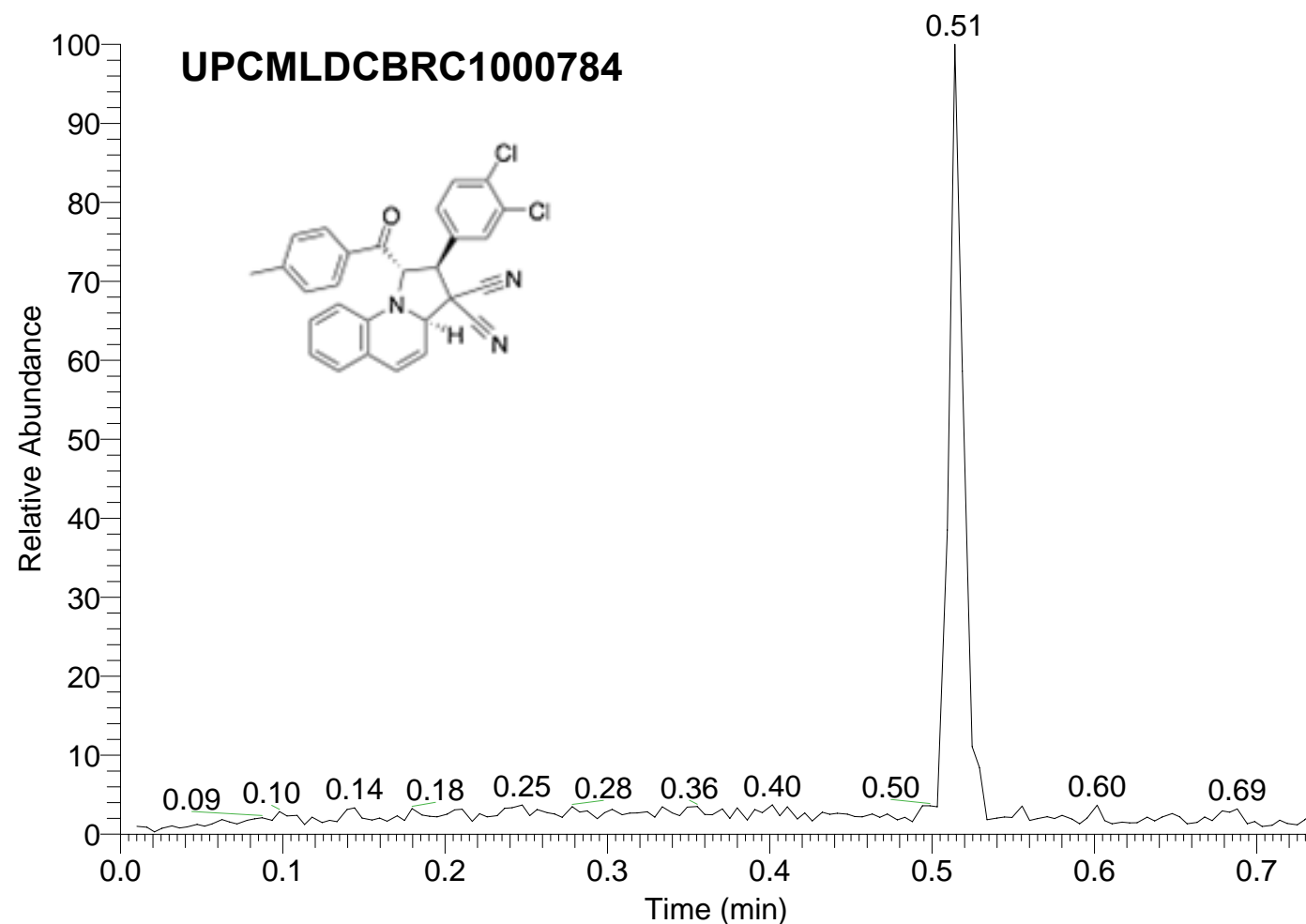


NL:
1.15E6
Channel B
UV
C1000784_
1



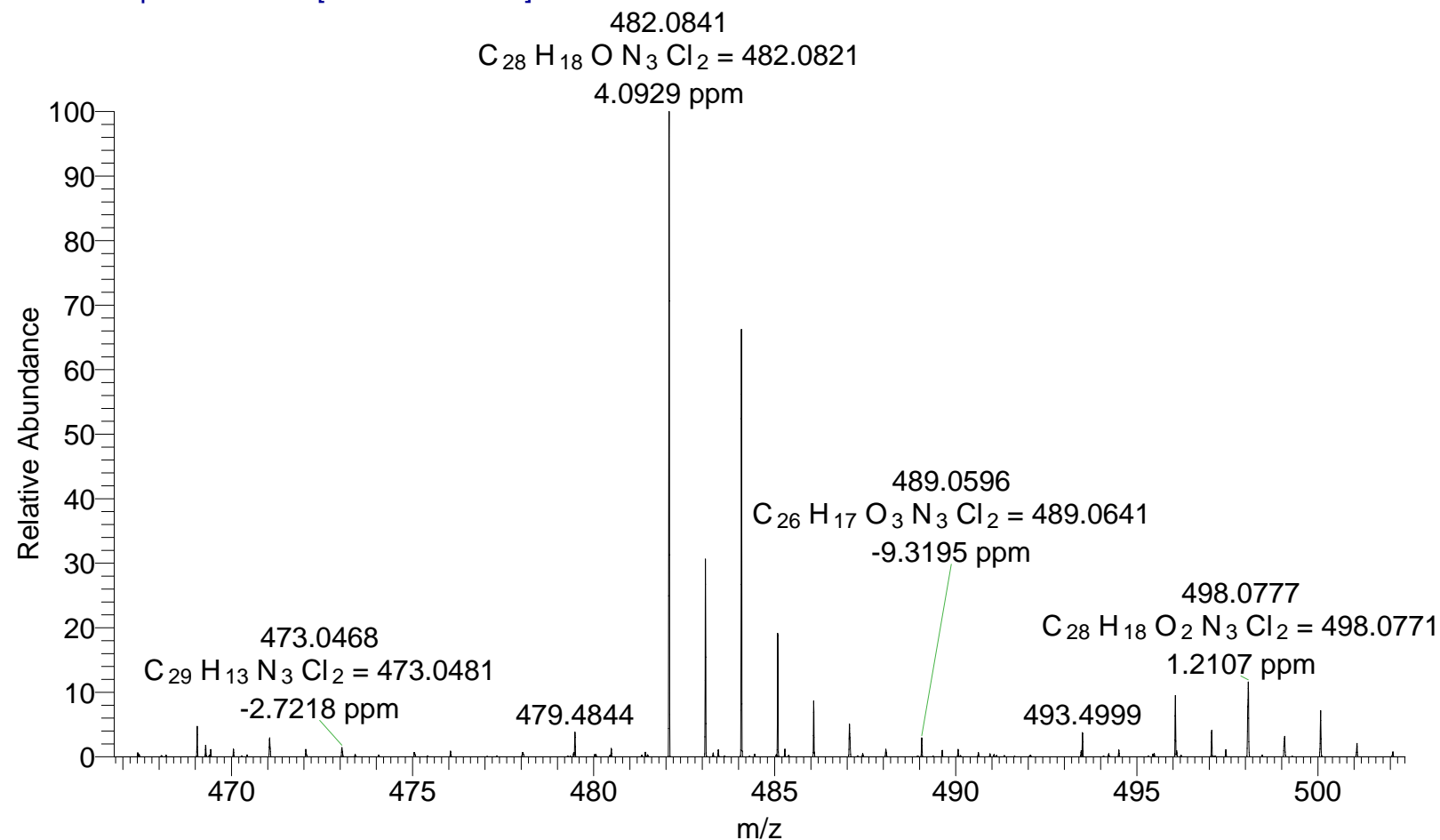
NL:
4.80E5
Channel C
UV
C1000784_
1

RT: 0.00 - 0.73

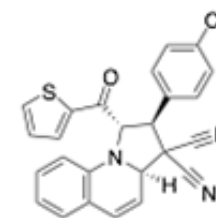
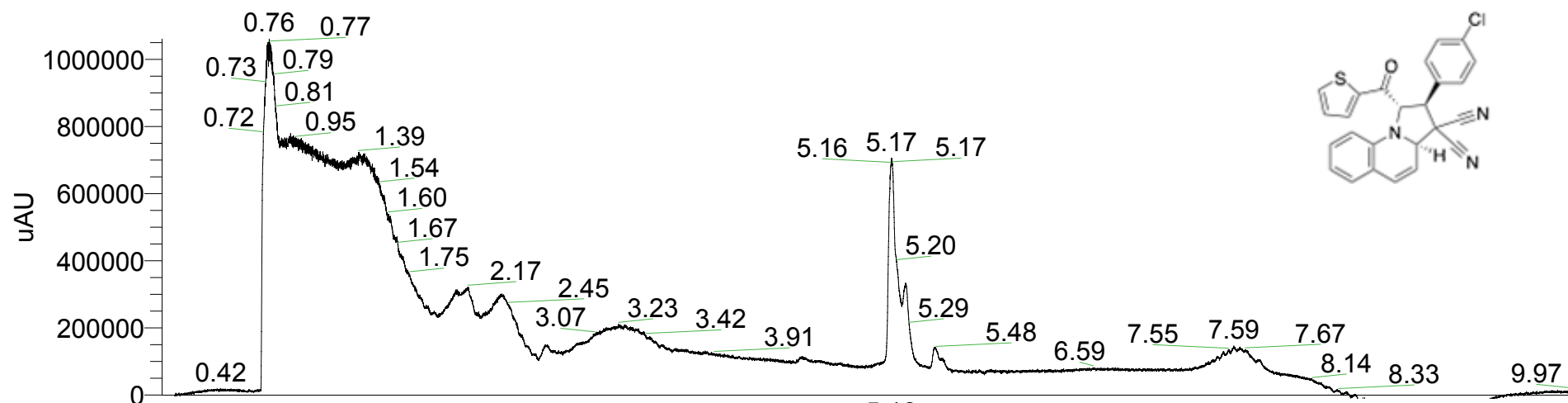


NL:
8.73E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1000784_DI

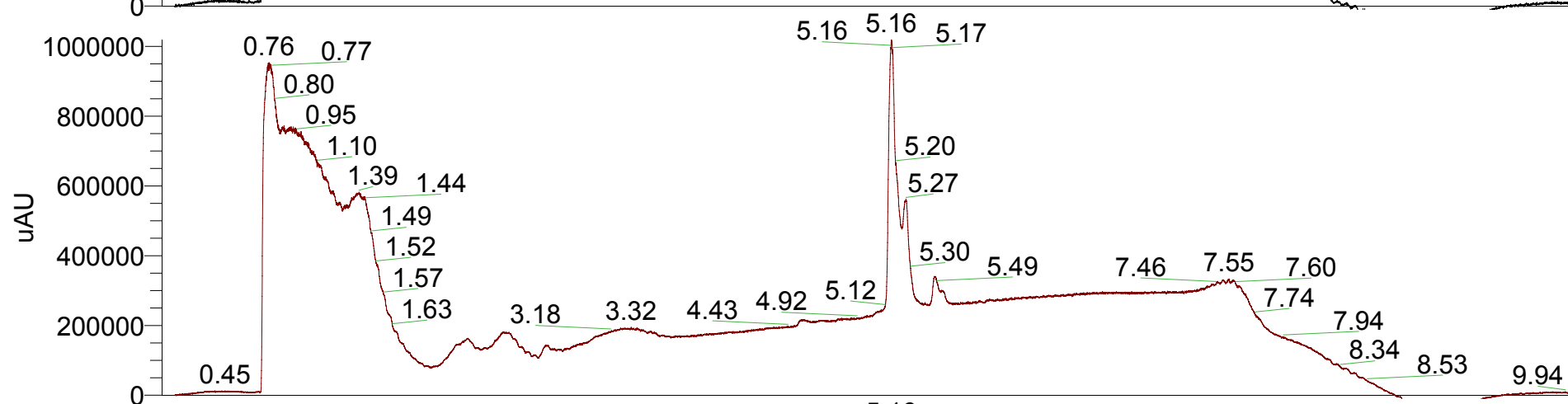
C1000784_DI #98-101 RT: 0.51-0.52 AV: 4 NL: 6.70E5
T: FTMS - p ESI Full ms [150.00-2000.00]



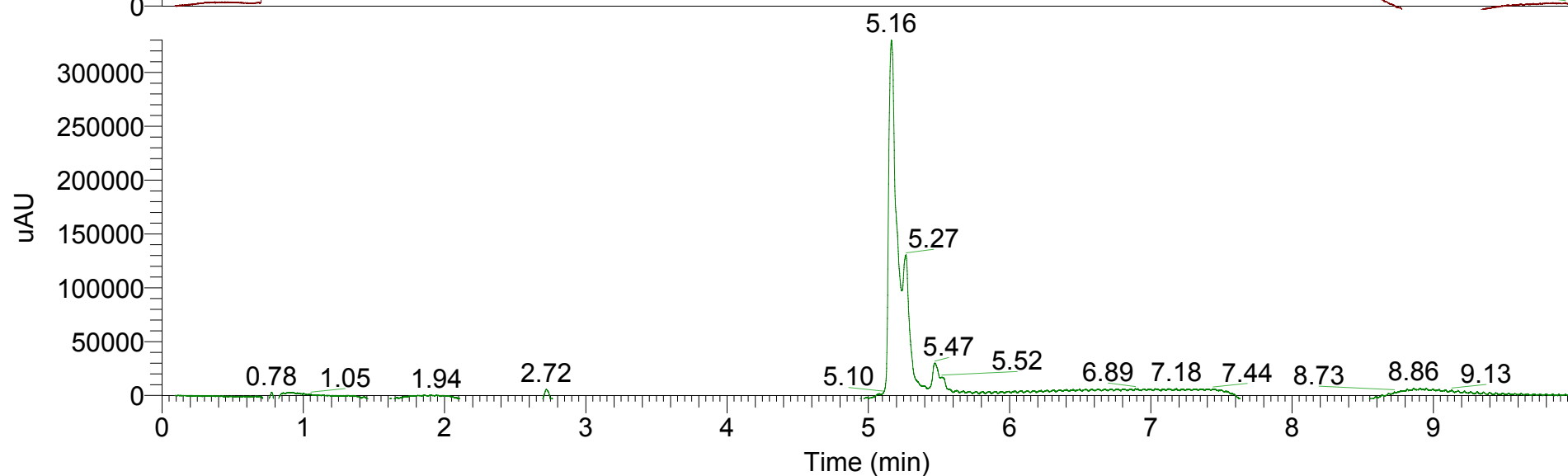
RT: 0.00 - 9.98



NL:
1.06E6
Channel A
UV
C1000802_
1_1806050
95823

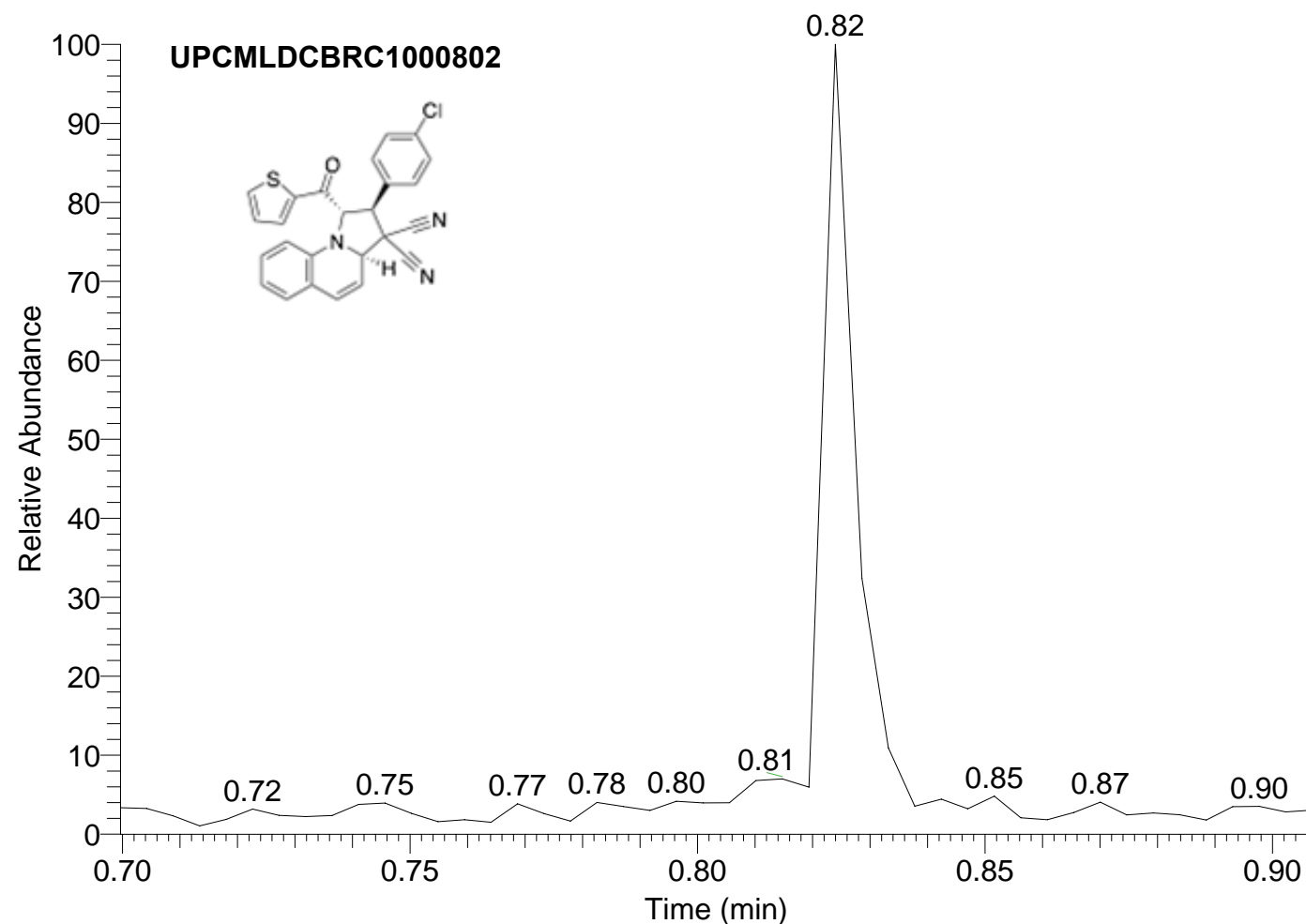


NL:
1.02E6
Channel B
UV
C1000802_
1_1806050
95823



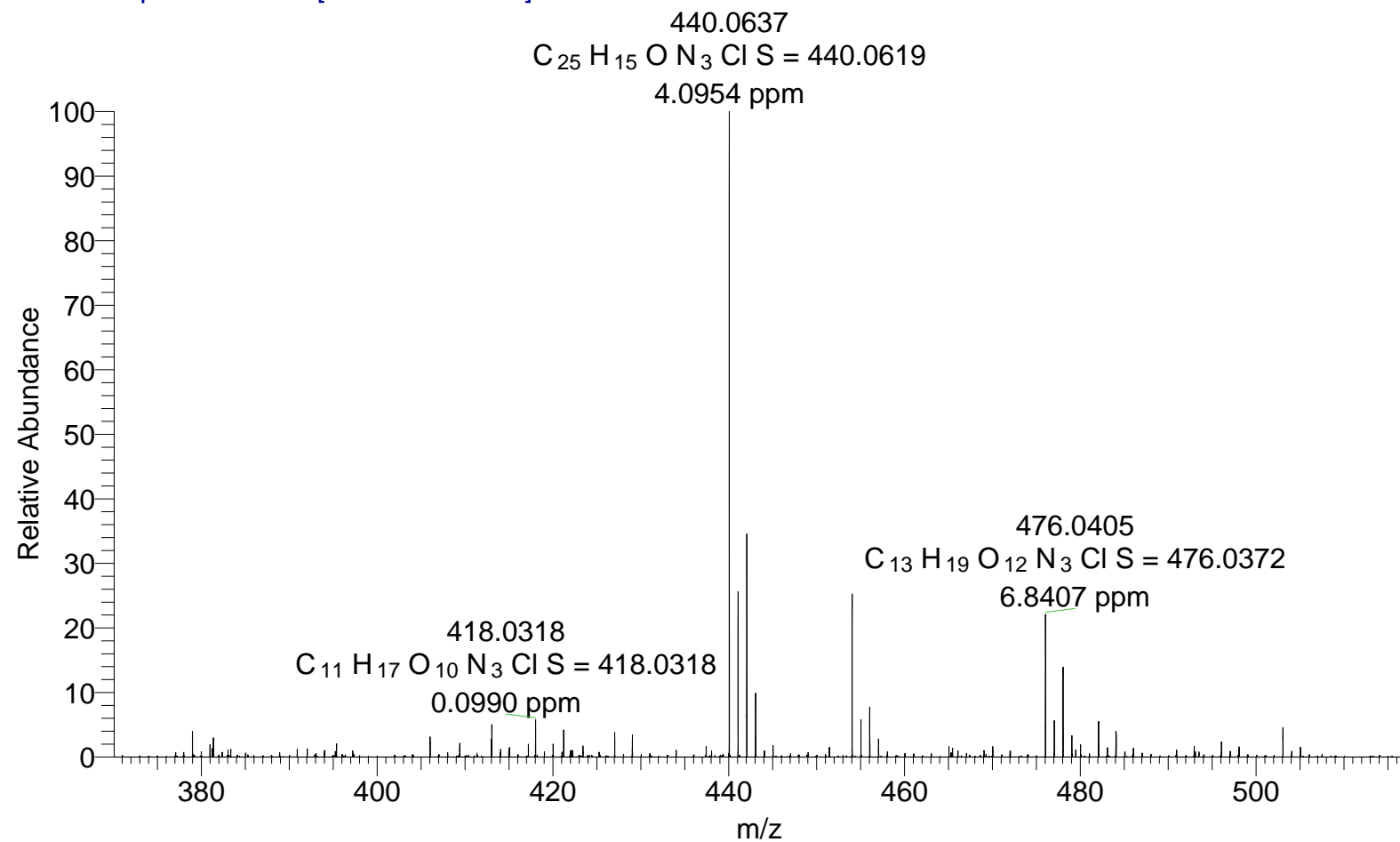
NL:
3.30E5
Channel C
UV
C1000802_
1_1806050
95823

RT: 0.70 - 0.91

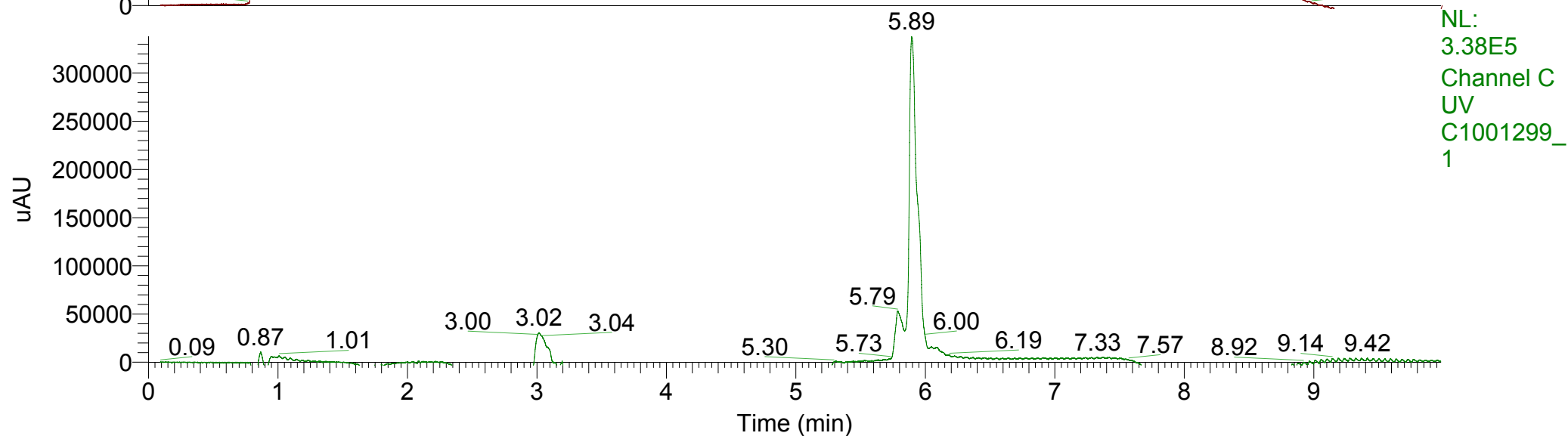
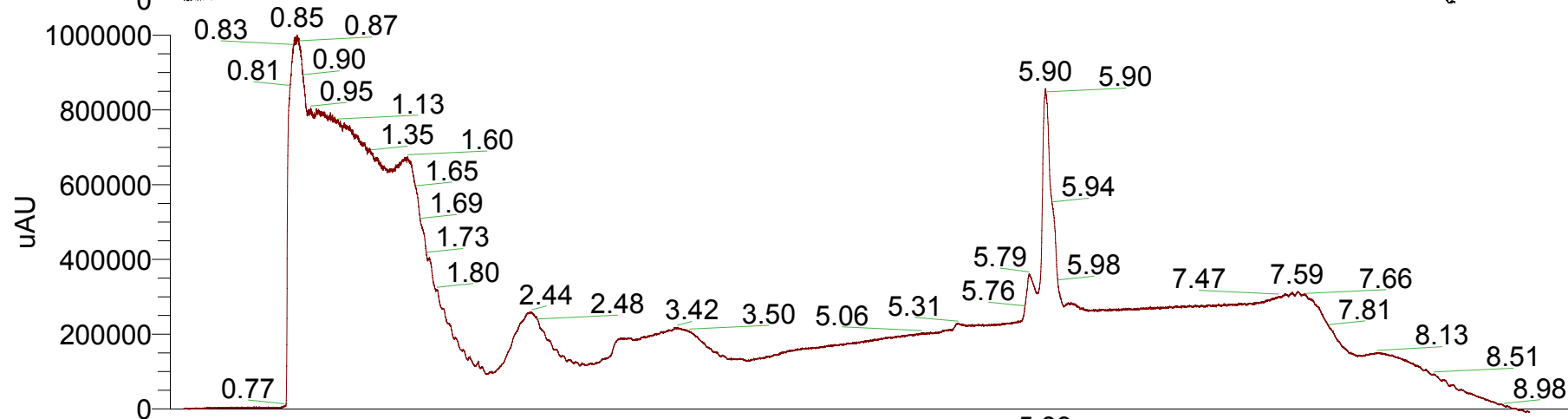
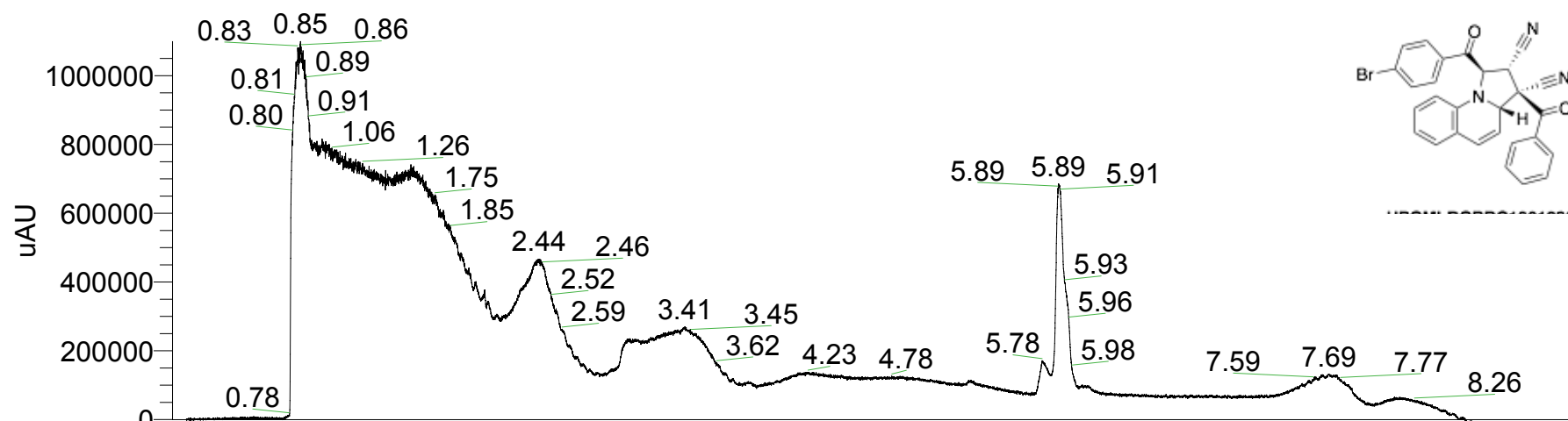


NL:
5.06E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1000802_DI

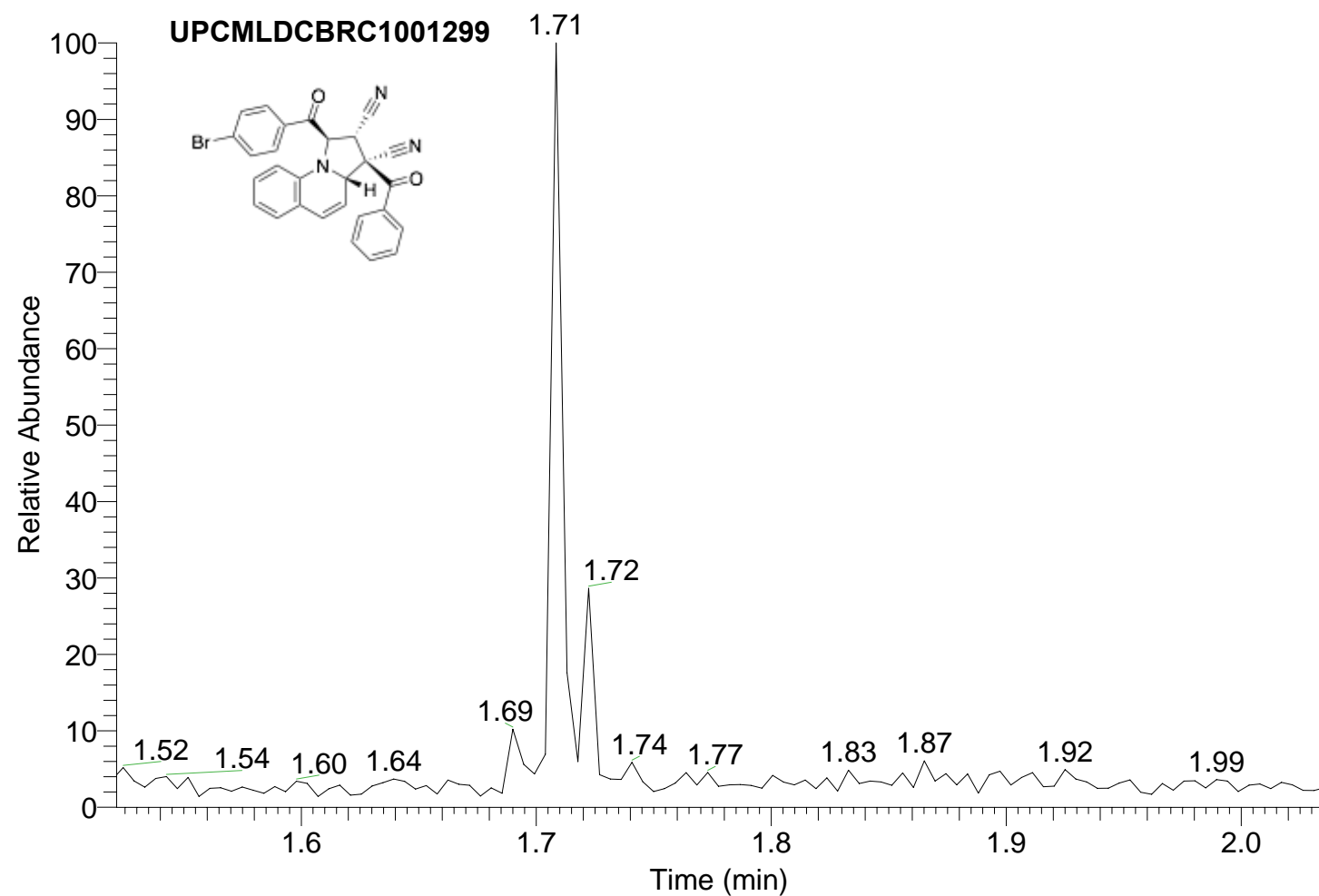
C1000802_DI #177-180 RT: 0.82-0.83 AV: 4 NL: 5.03E5
T: FTMS - p ESI Full ms [150.00-2000.00]



NL:
1.10E6
Channel A
UV
C1001299_
1

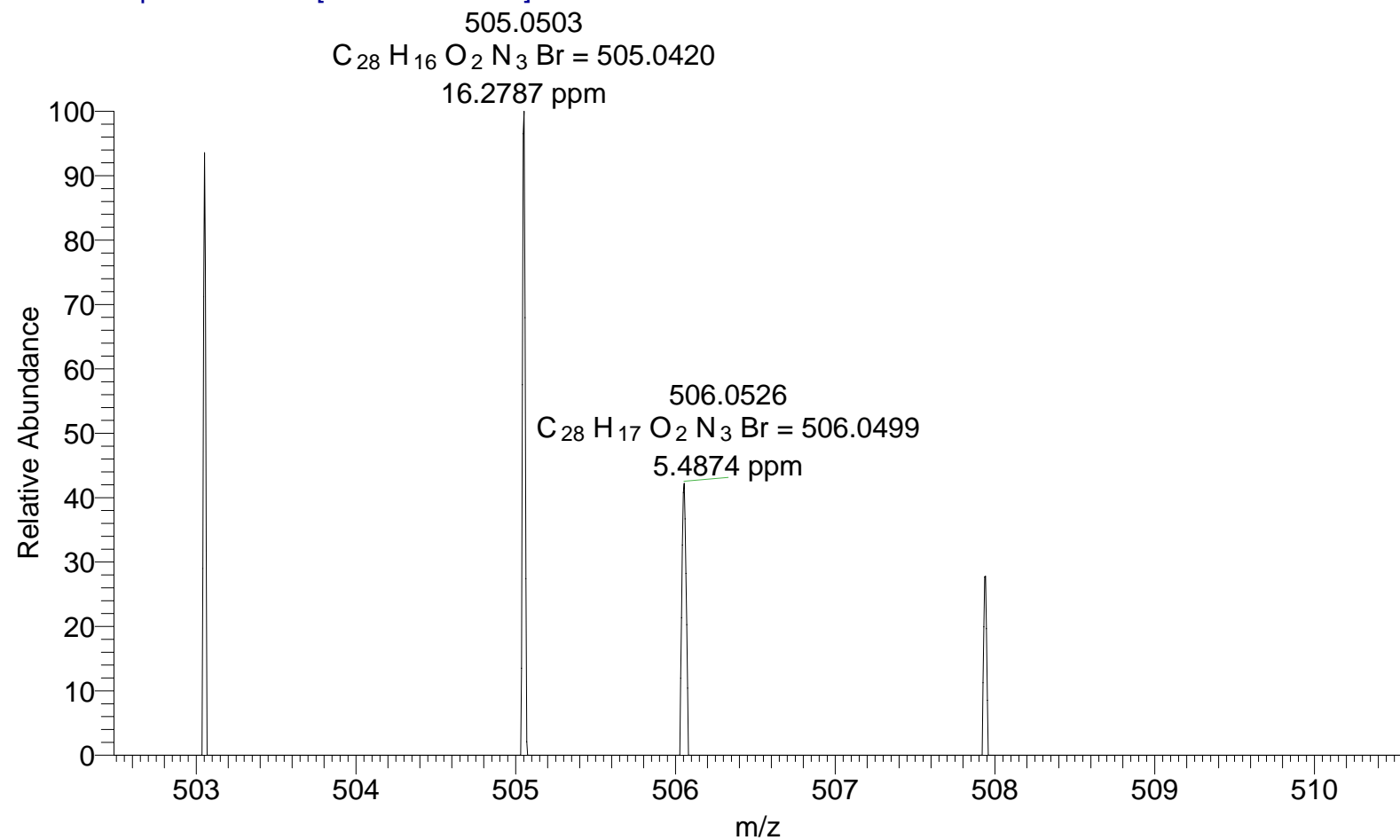


RT: 1.52 - 2.03

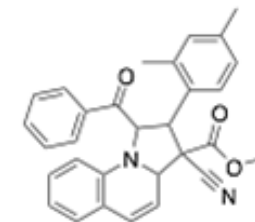
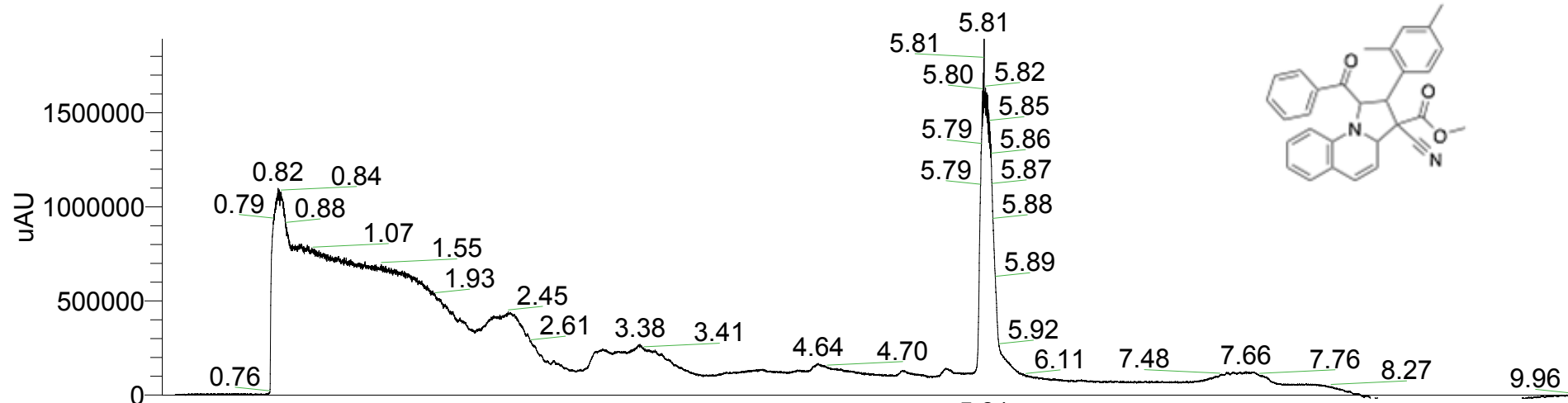


NL:
5.09E7
TIC MS
C1001299_
DI

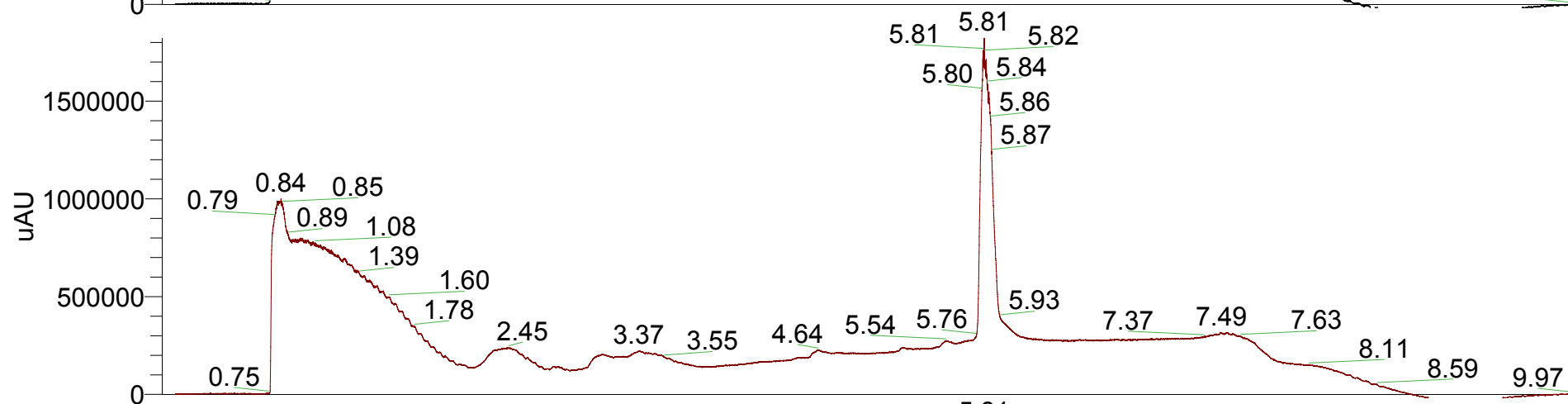
C1001299_DI #369 RT: 1.70 AV: 1 NL: 4.85E3
T: FTMS - p ESI Full ms [150.00-2000.00]



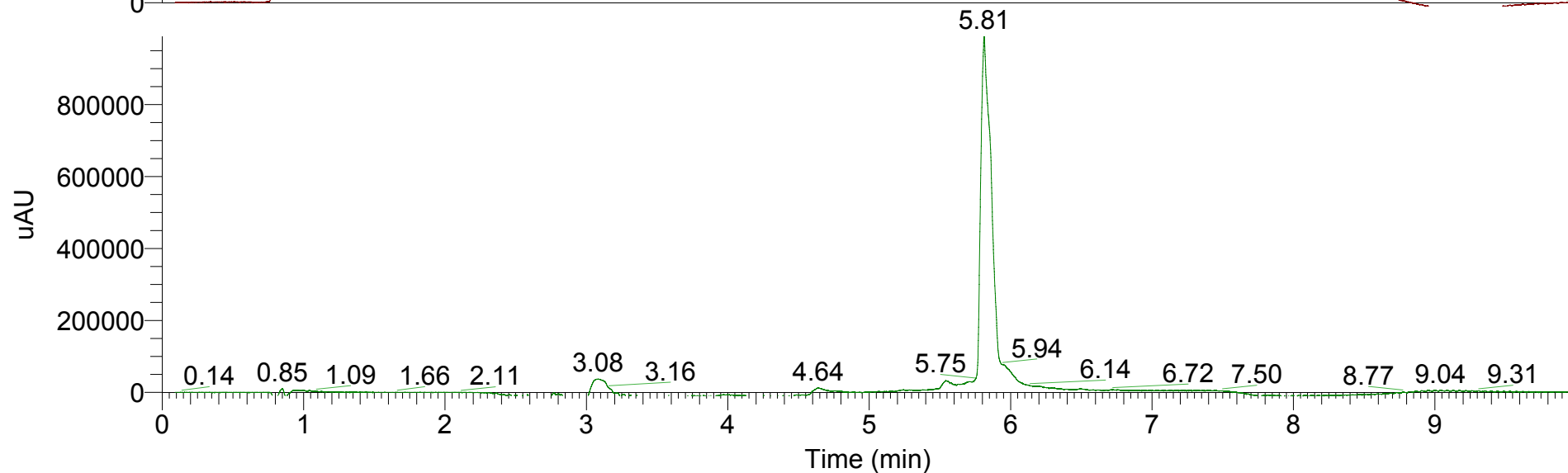
RT: 0.00 - 9.98



NL:
1.89E6
Channel A
UV
C1002602_
1

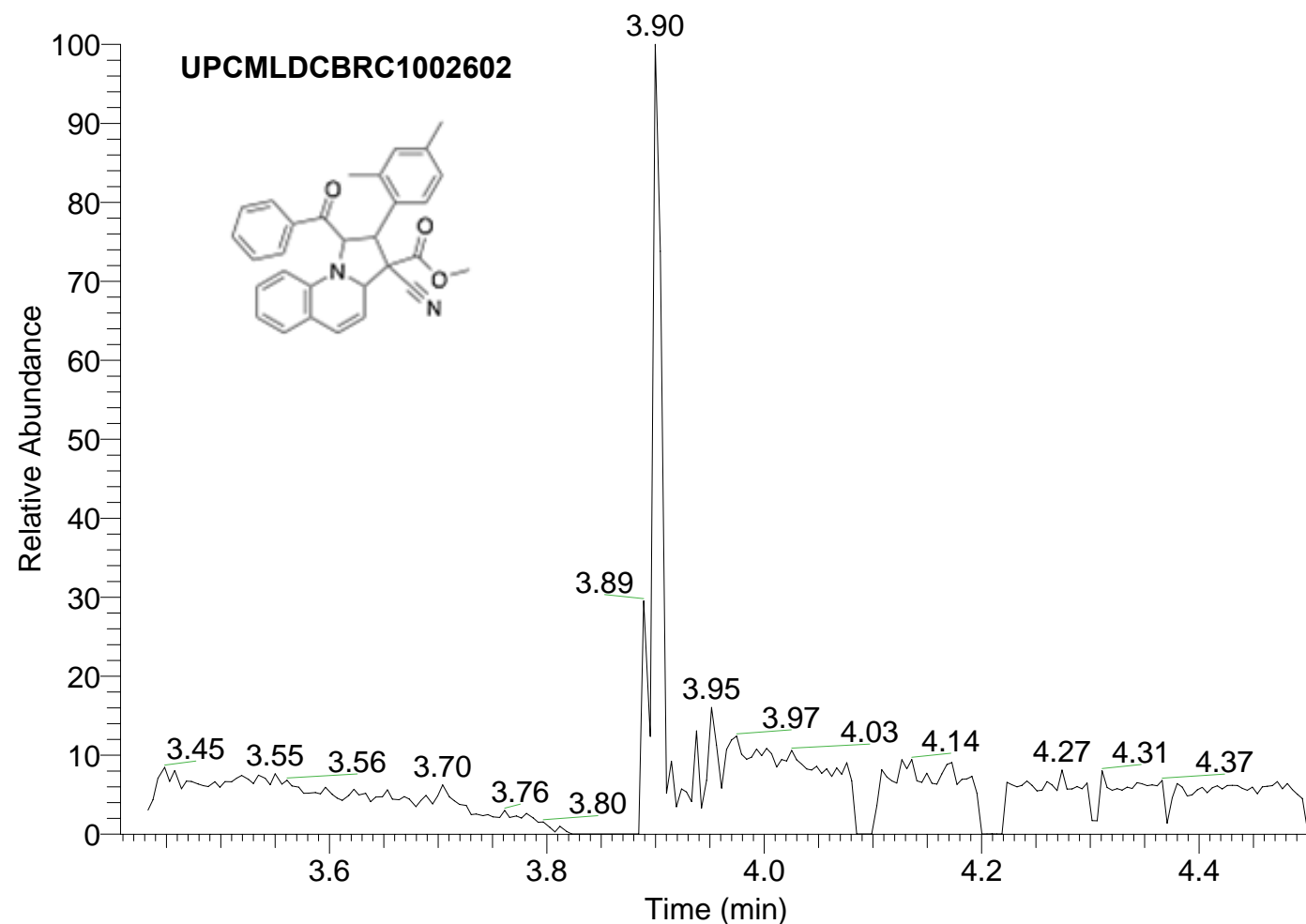


NL:
1.82E6
Channel B
UV
C1002602_
1



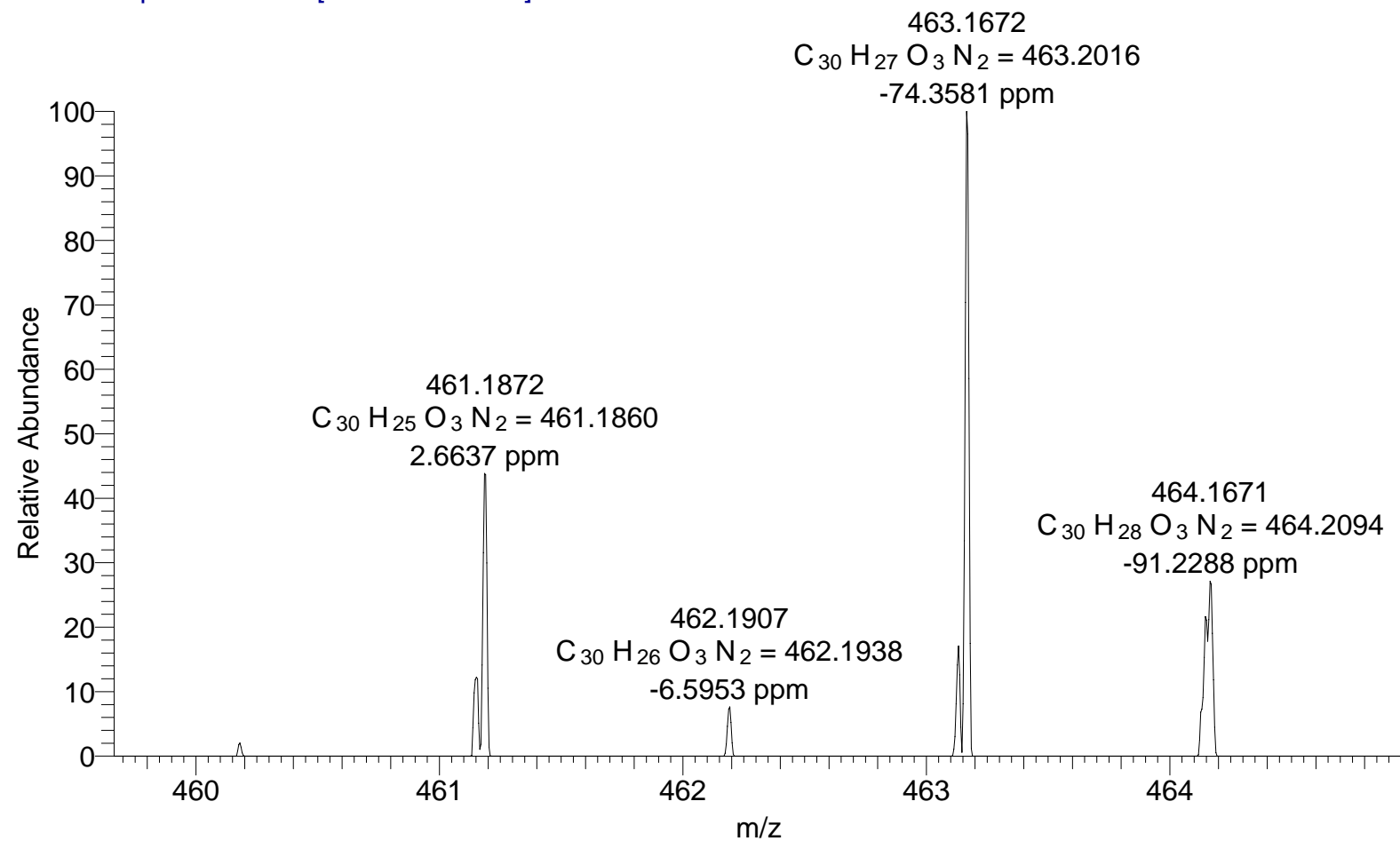
NL:
9.89E5
Channel C
UV
C1002602_
1

RT: 3.41 - 4.50

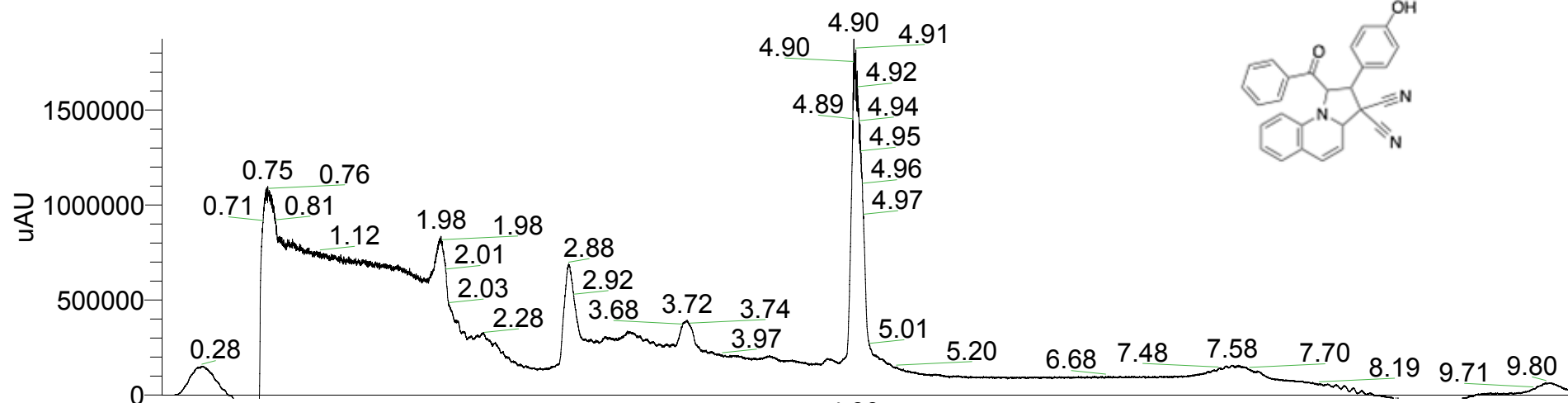


NL:
8.53E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1002602_DI

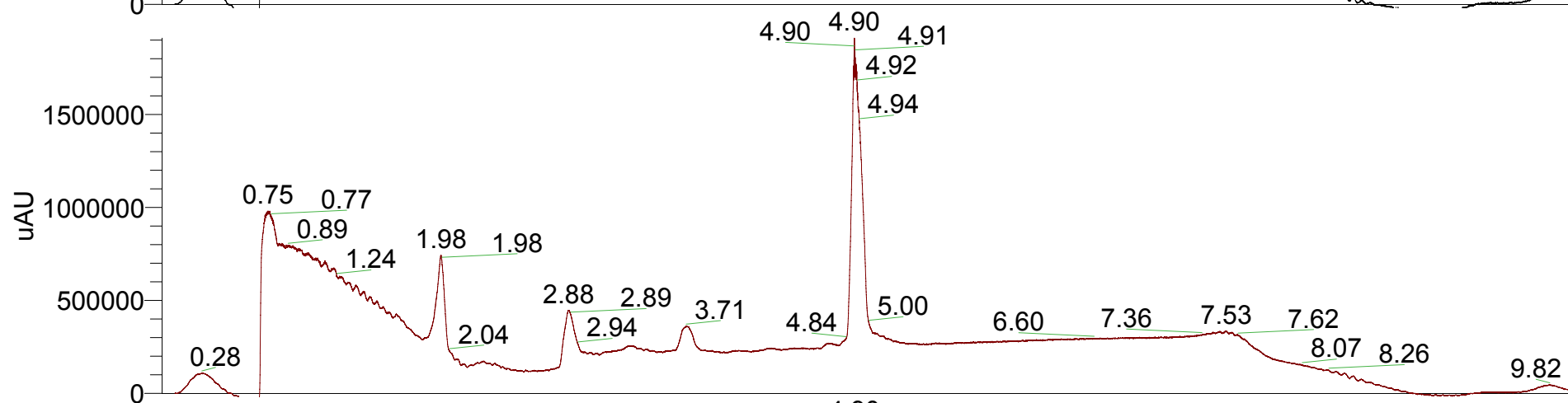
C1002602_DI #823-828 RT: 3.89-3.91 AV: 6 NL: 2.72E4
T: FTMS - p ESI Full ms [150.00-2000.00]



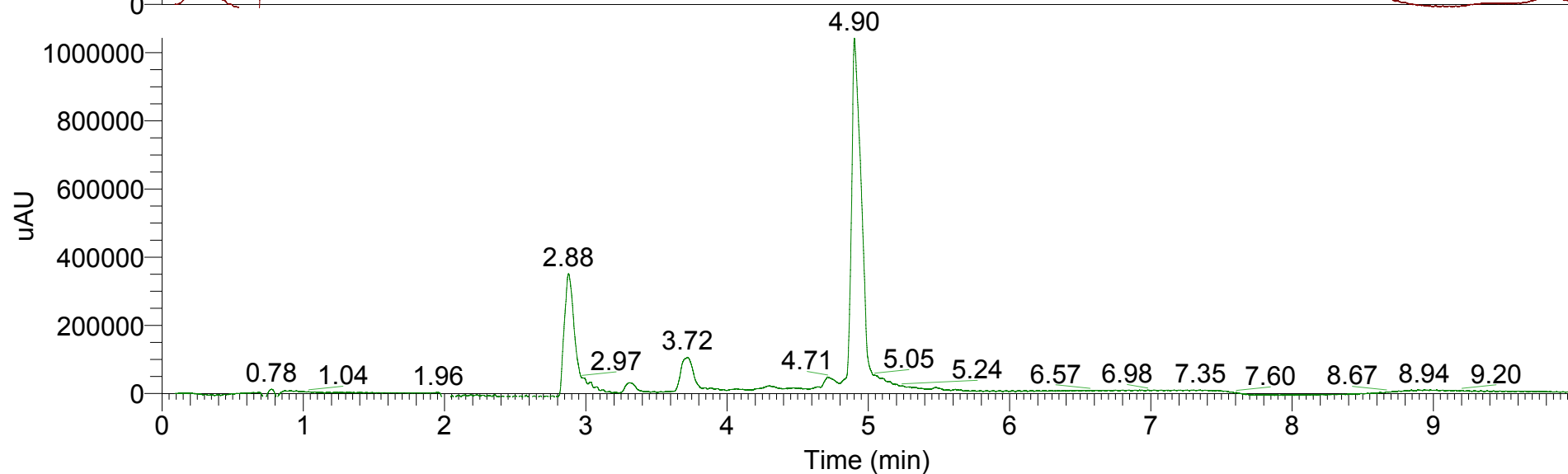
RT: 0.00 - 9.98



NL:
1.87E6
Channel A
UV
C1004885_
1

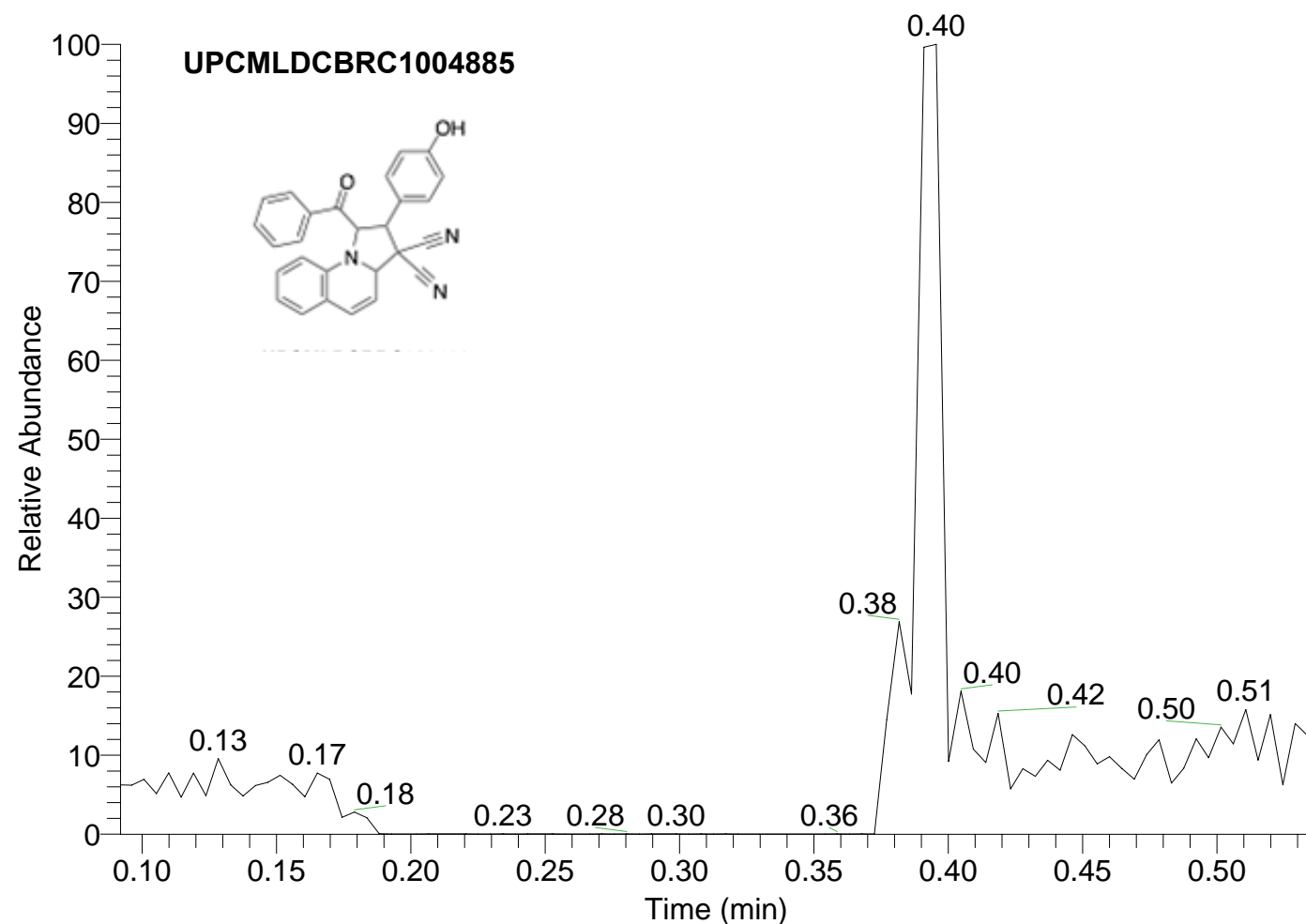


NL:
1.91E6
Channel B
UV
C1004885_
1



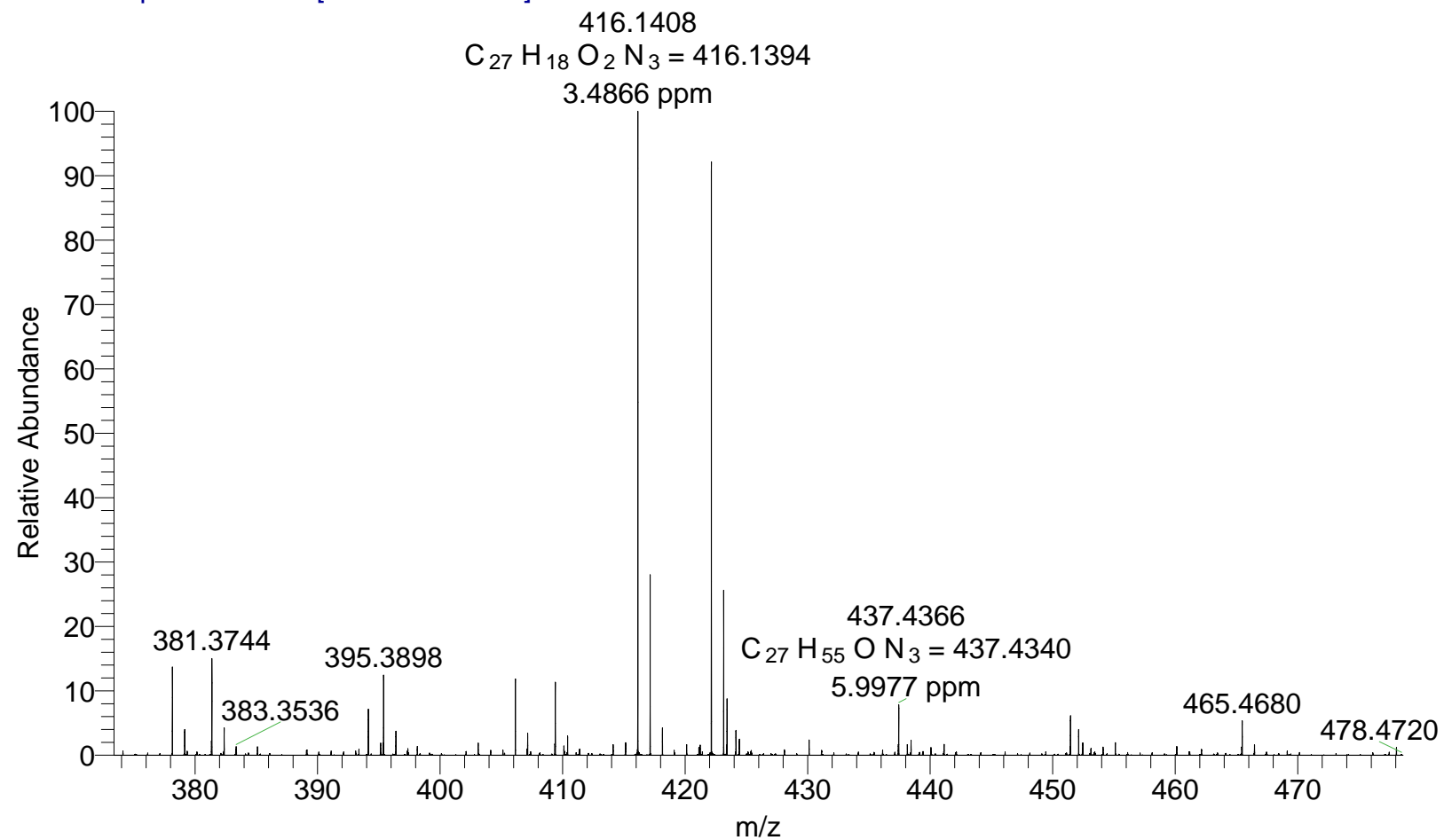
NL:
1.04E6
Channel C
UV
C1004885_
1

RT: 0.09 - 0.54

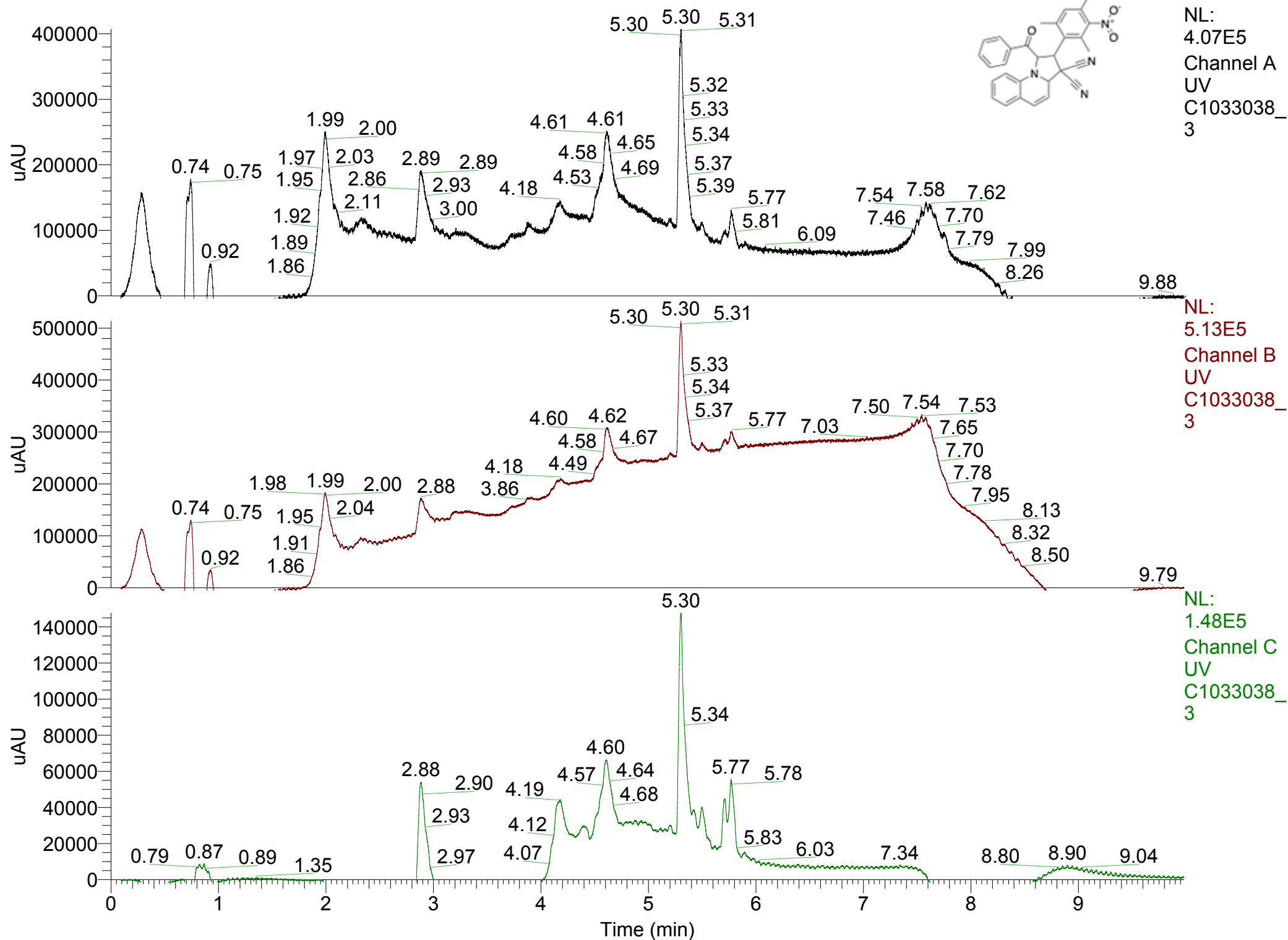


NL:
5.42E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1004885_DI

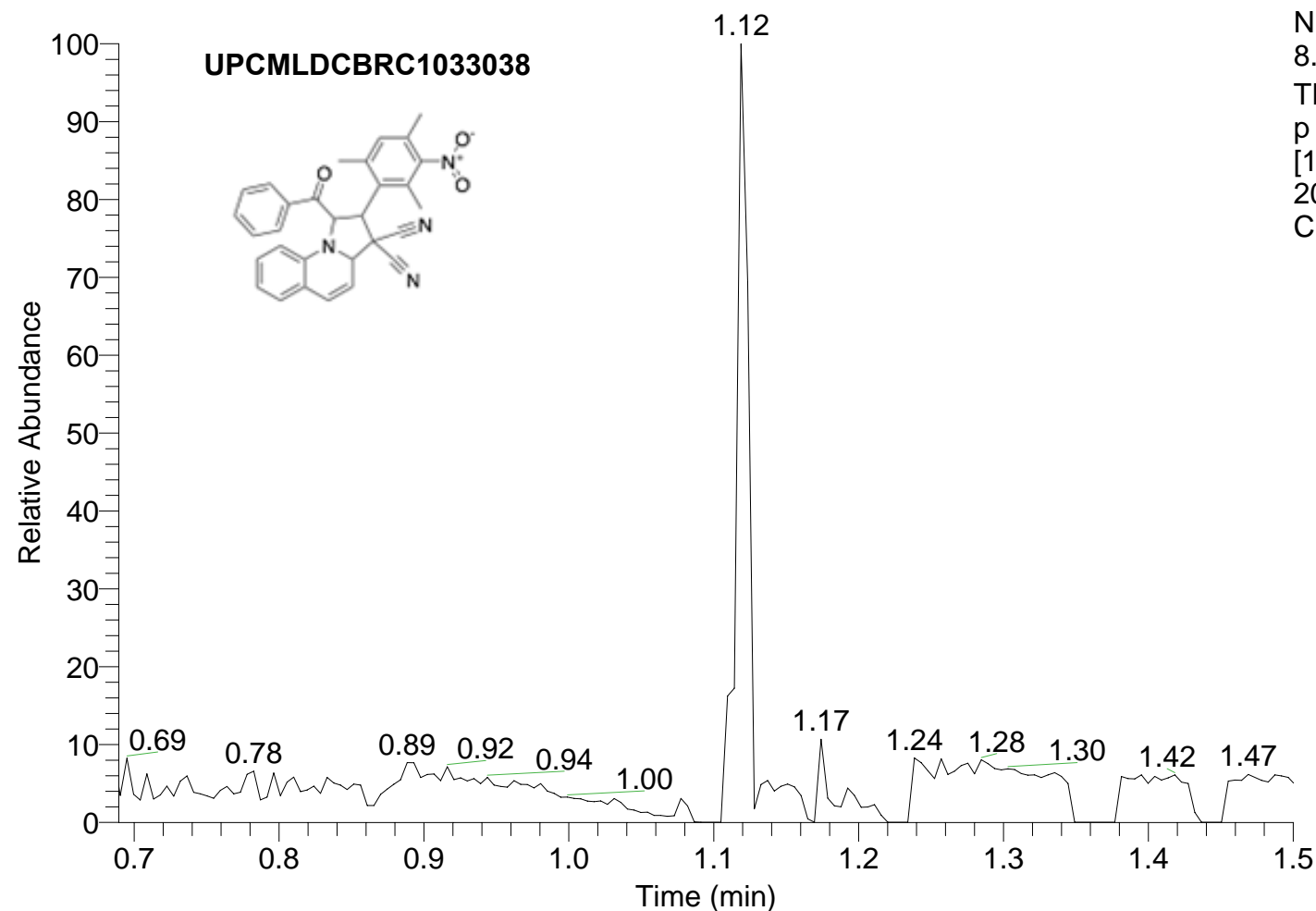
C1004885_DI #83-85 RT: 0.39-0.40 AV: 3 NL: 1.98E6
T: FTMS - p ESI Full ms [150.00-2000.00]



RT: 0.00 - 9.98

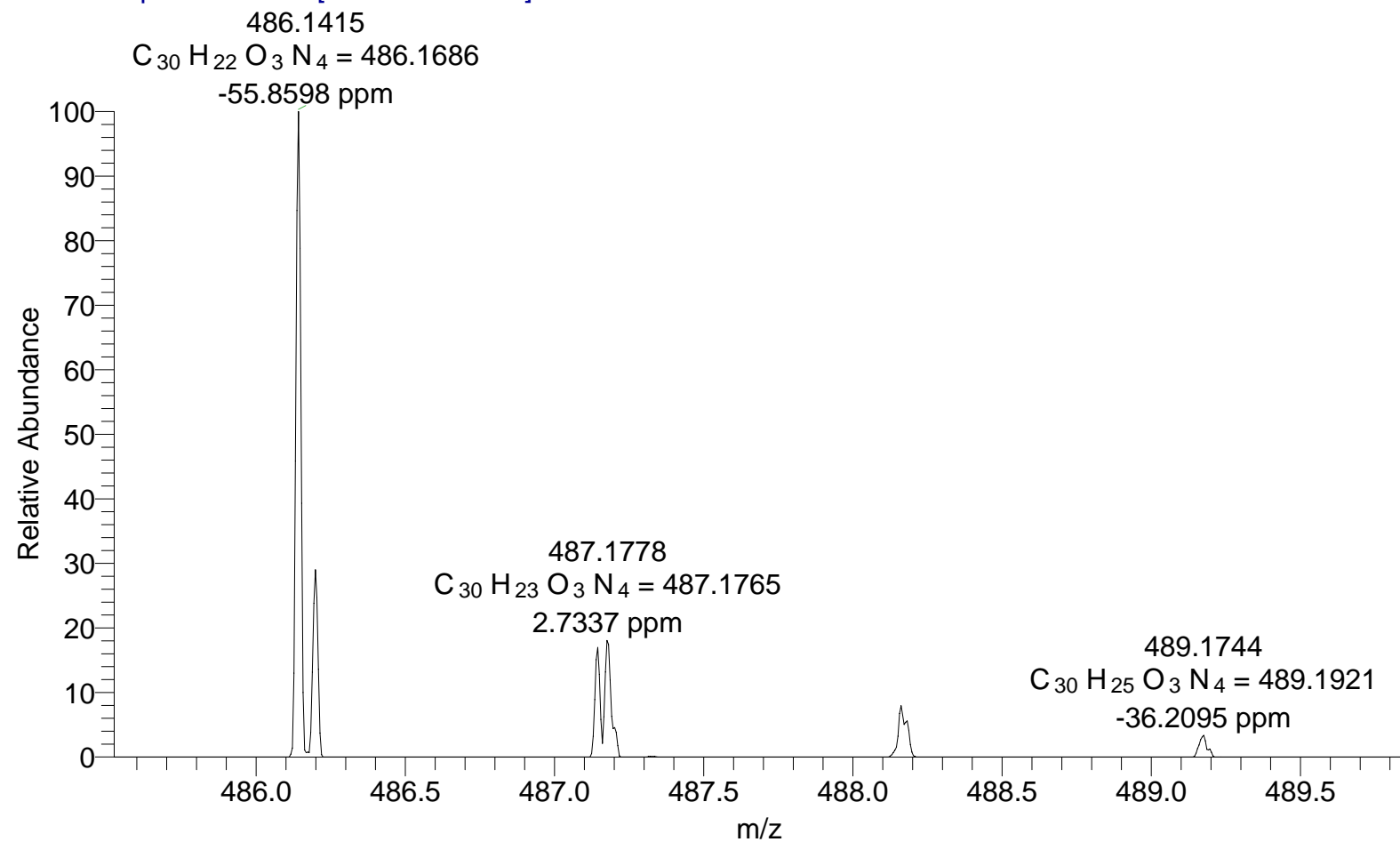


RT: 0.69 - 1.50

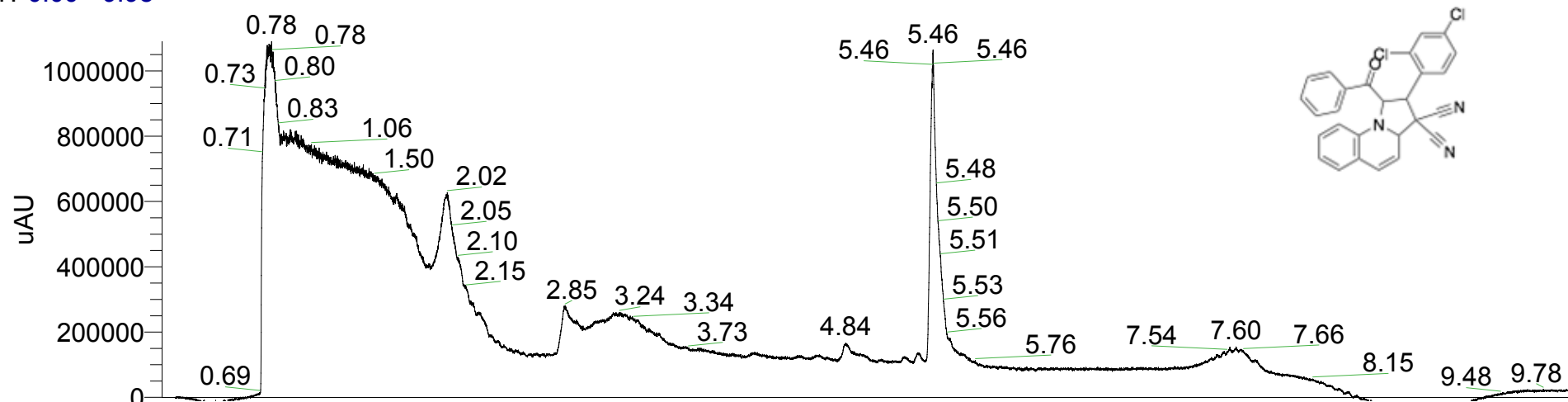


NL:
8.11E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1033038_DI

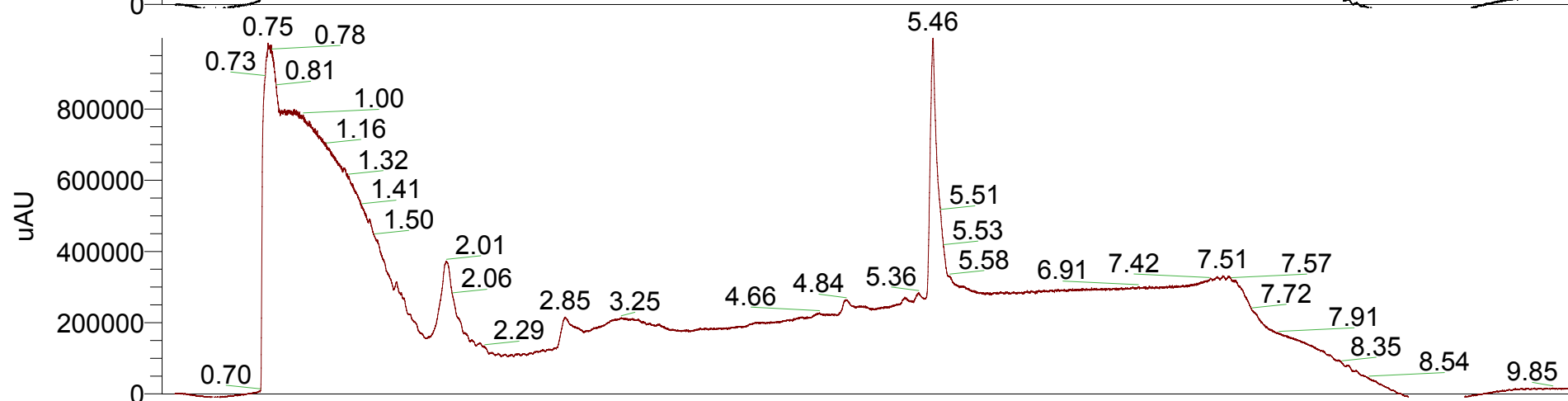
C1033038_DI #240-244 RT: 1.11-1.13 AV: 5 NL: 2.32E5
T: FTMS - p ESI Full ms [150.00-2000.00]



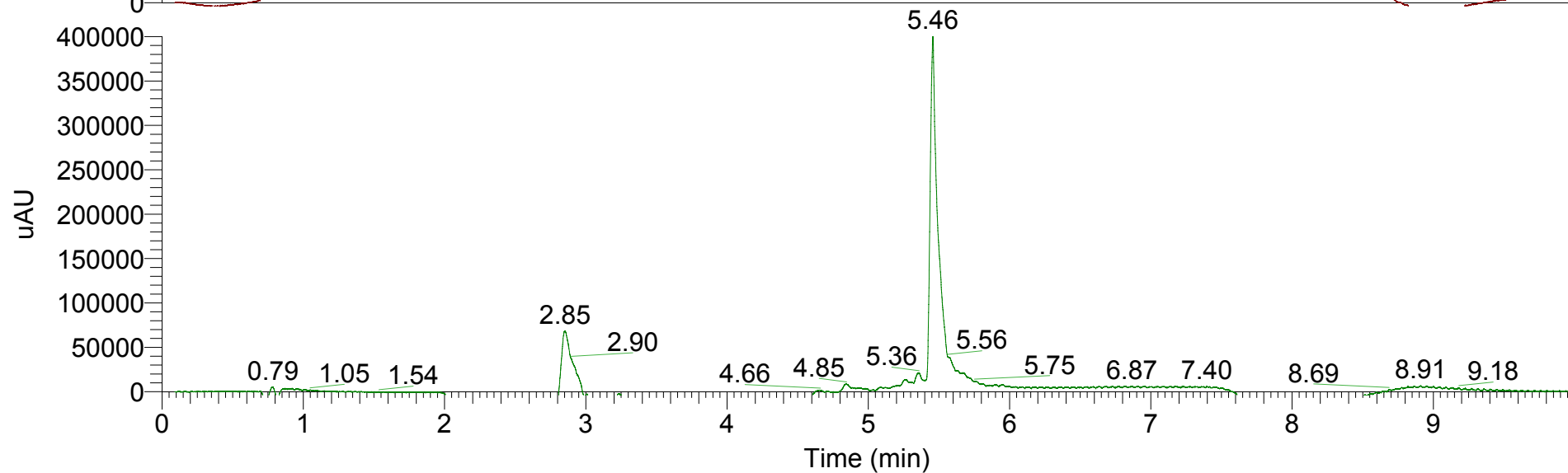
RT: 0.00 - 9.98



NL:
1.09E6
Channel A
UV
C1033229_
1

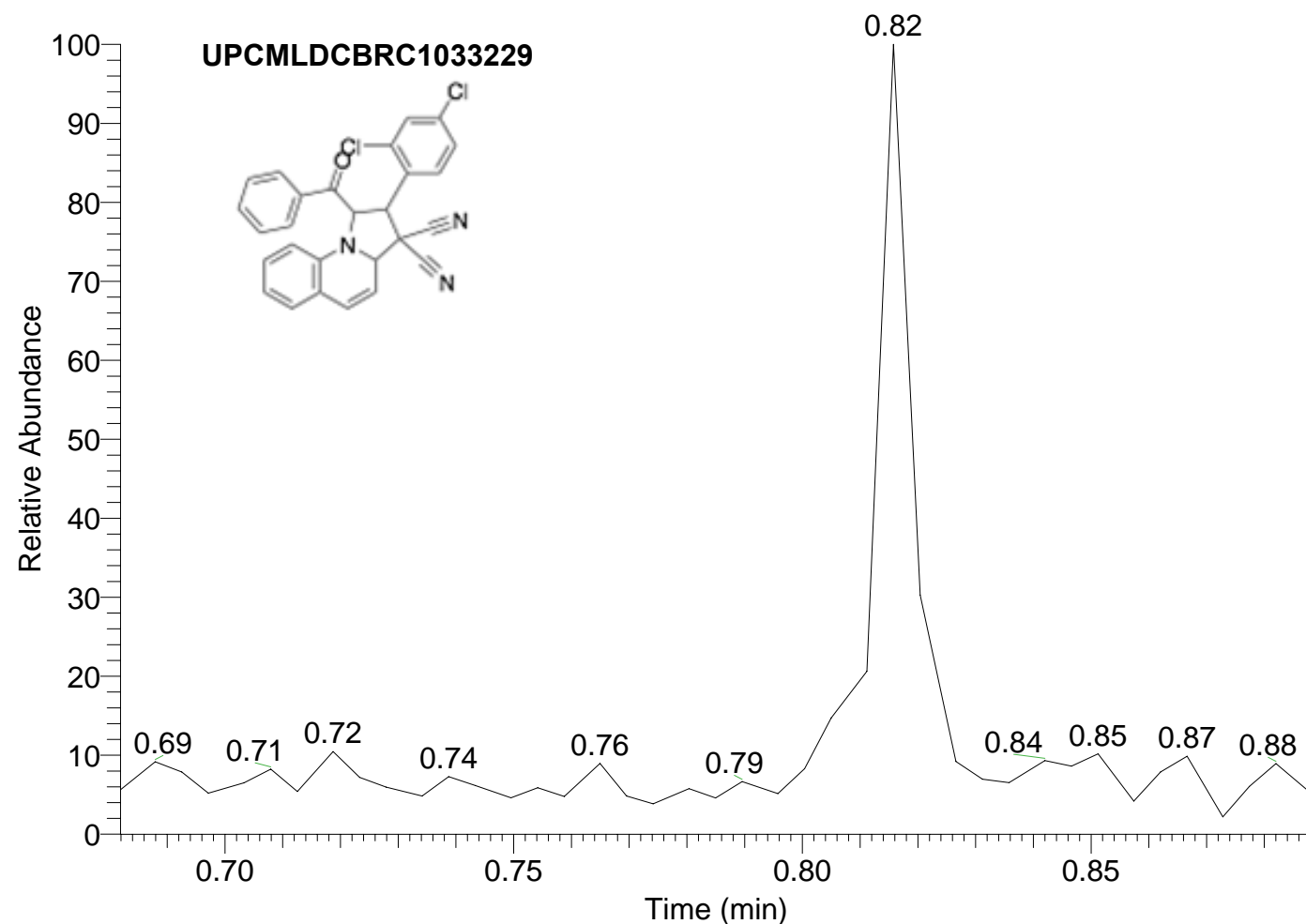


NL:
9.99E5
Channel B
UV
C1033229_
1



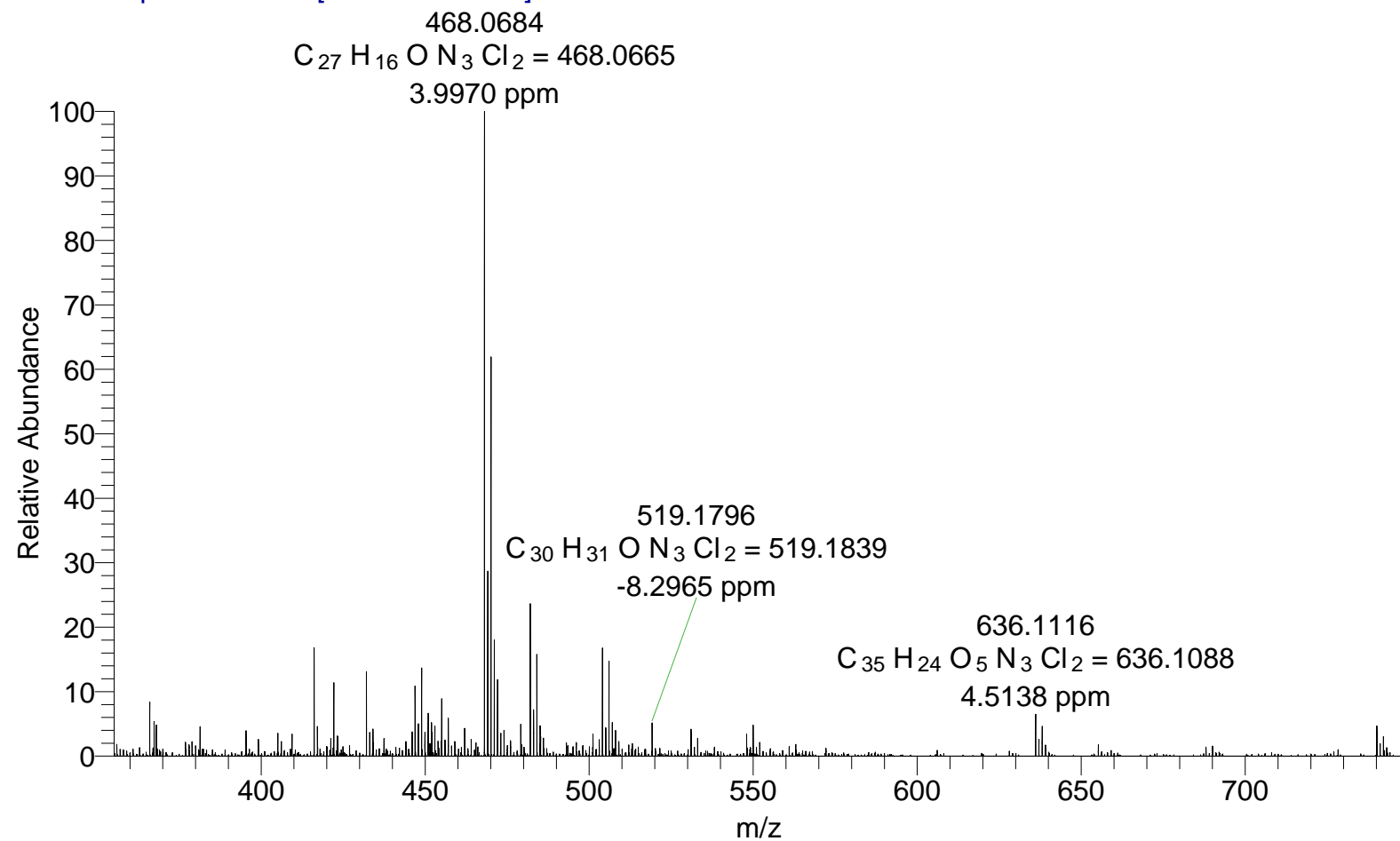
NL:
4.00E5
Channel C
UV
C1033229_
1

RT: 0.68 - 0.89

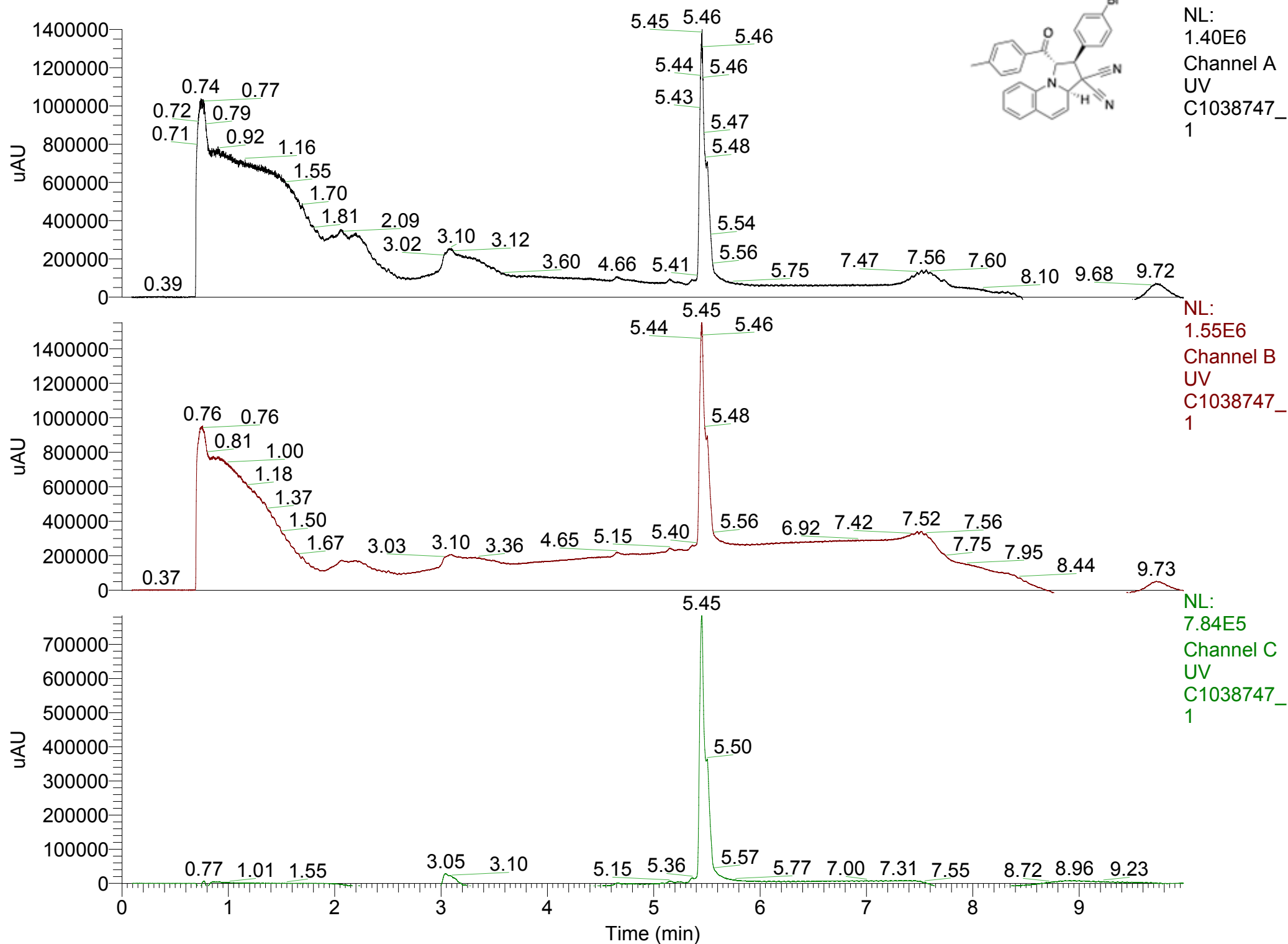


NL:
4.36E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1033229_DI

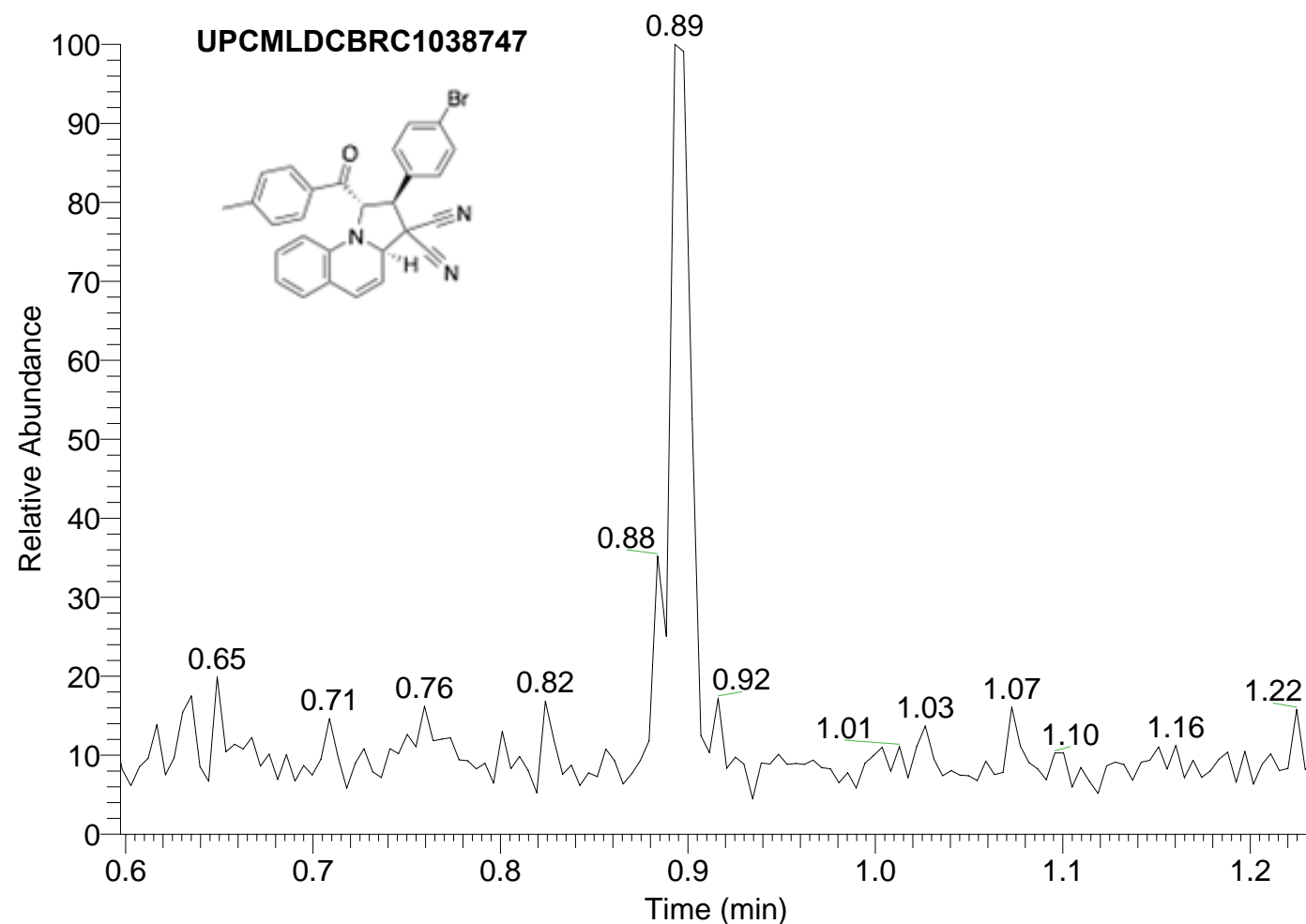
C1033229_DI #156-158 RT: 0.80-0.82 AV: 3 NL: 5.25E5
T: FTMS - p ESI Full ms [150.00-2000.00]



RT: 0.00 - 9.98



RT: 0.60 - 1.23



NL:
2.17E7
TIC F: FTMS -
p ESI Full ms
[150.00-
2000.00] MS
C1038747_DI

C1038747_DI #190-196 RT: 0.88-0.91 AV: 7 NL: 4.15E5
T: FTMS - p ESI Full ms [150.00-2000.00]

