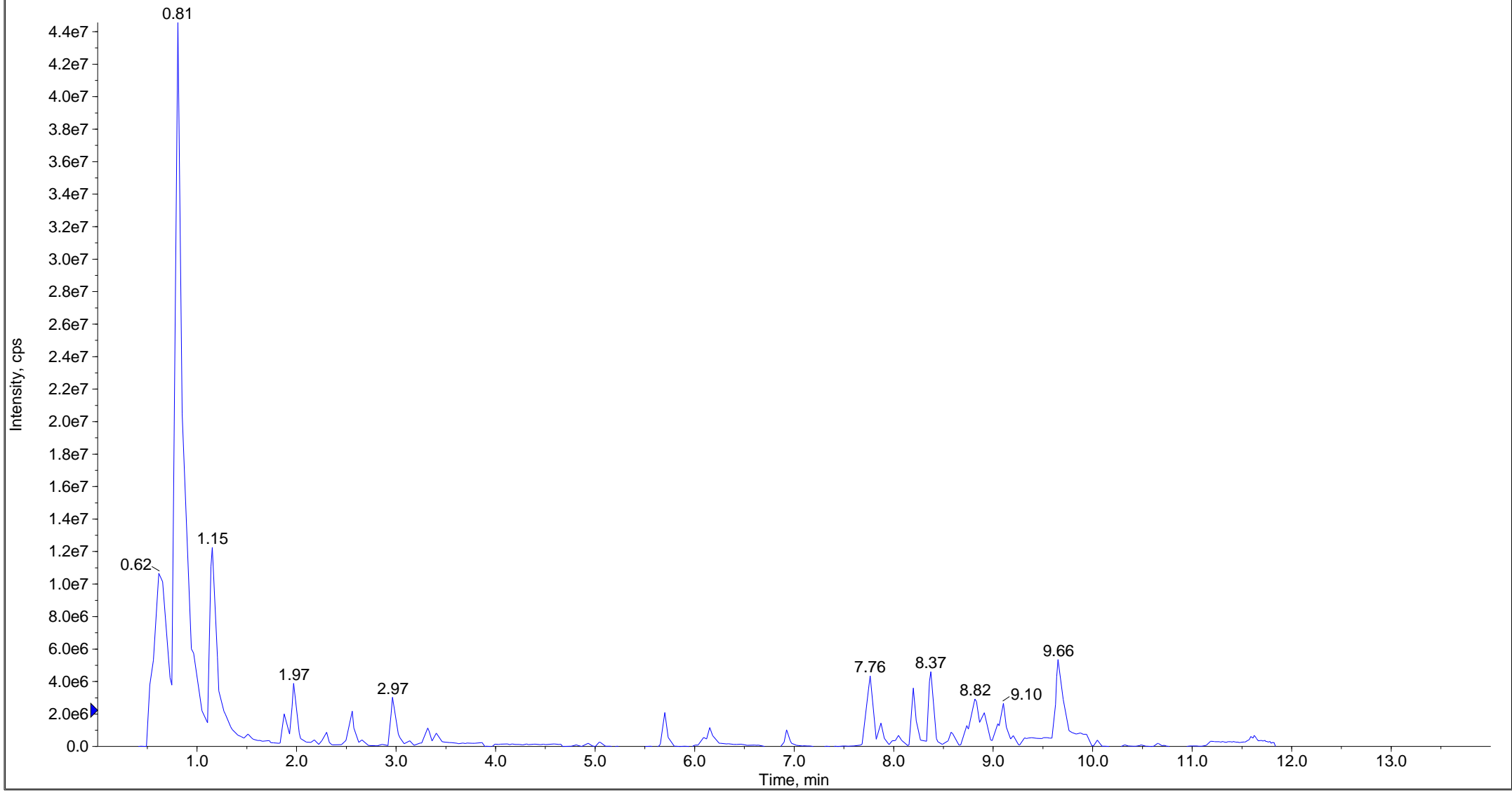


Supplementary Figure 1. Total ion chromatograms (TIC) of mass spectrometry detection of randomly selected 48 metabolites as an example.

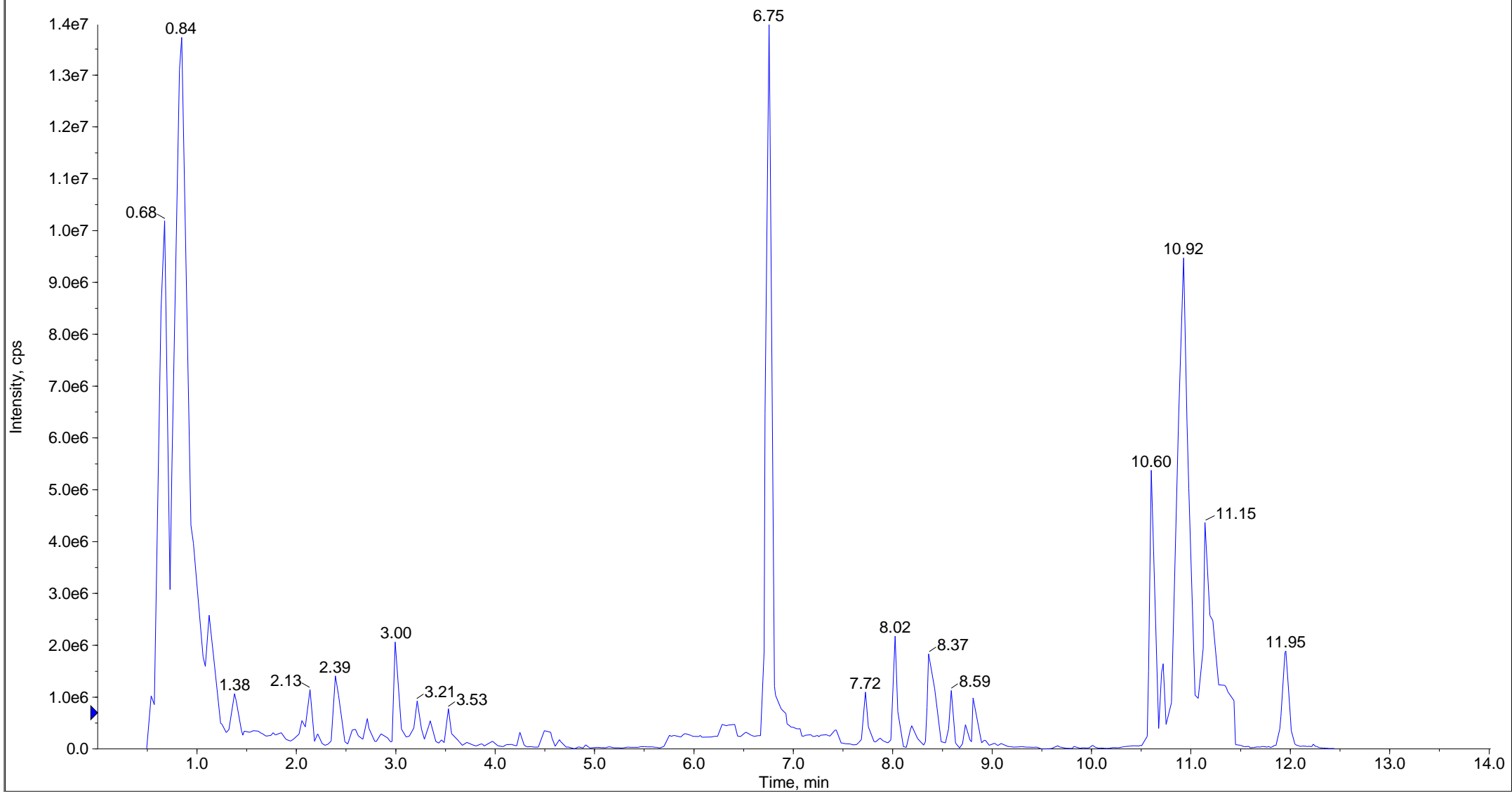
TIC of +MRM (625 pairs): from Sample 10 (A20106281a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.5e7 cps.



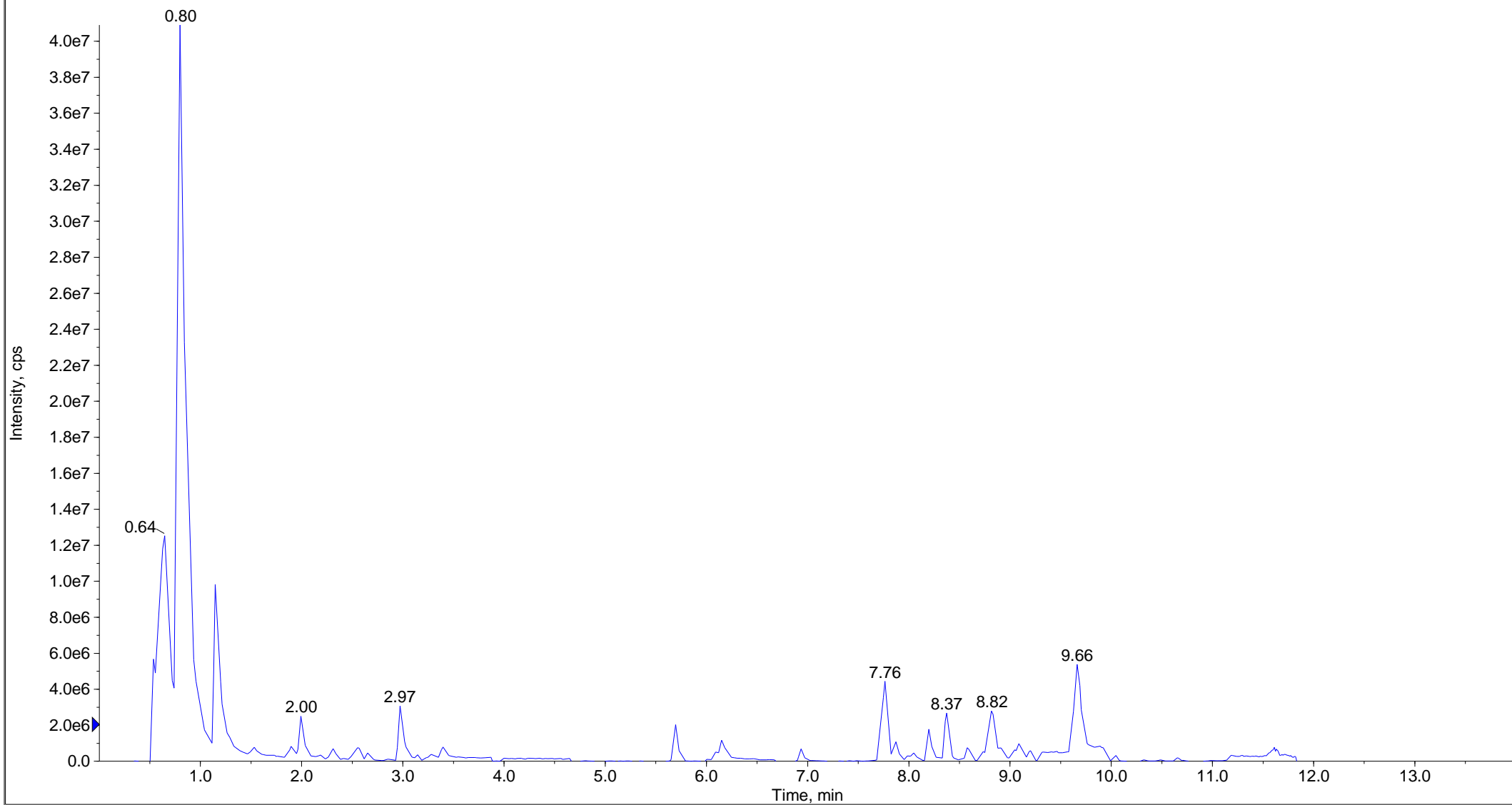
TIC of -MRM (791 pairs): from Sample 41 (A20106282a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.4e7 cps.



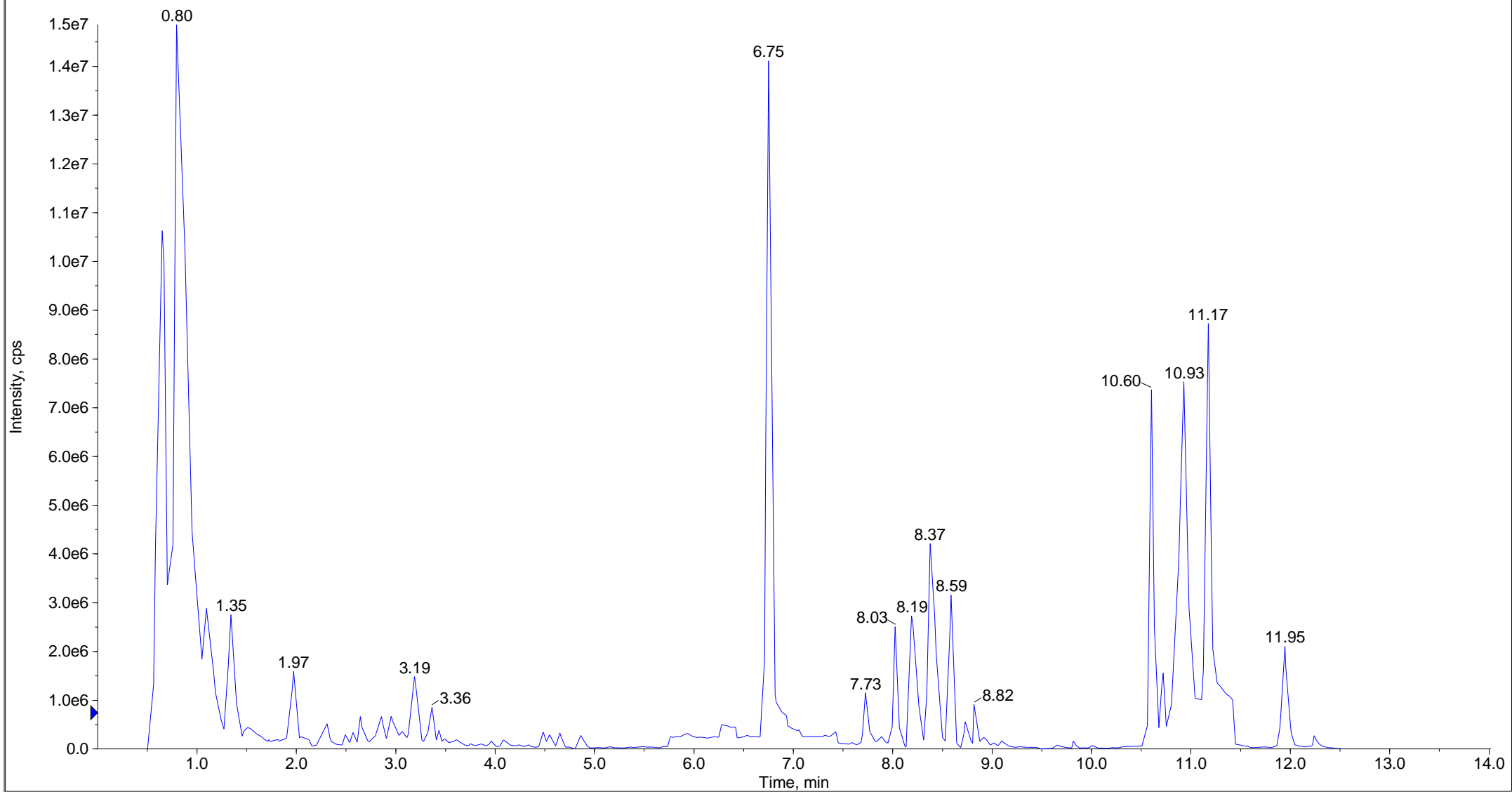
TIC of +MRM (625 pairs): from Sample 11 (A20106282a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.1e7 cps.



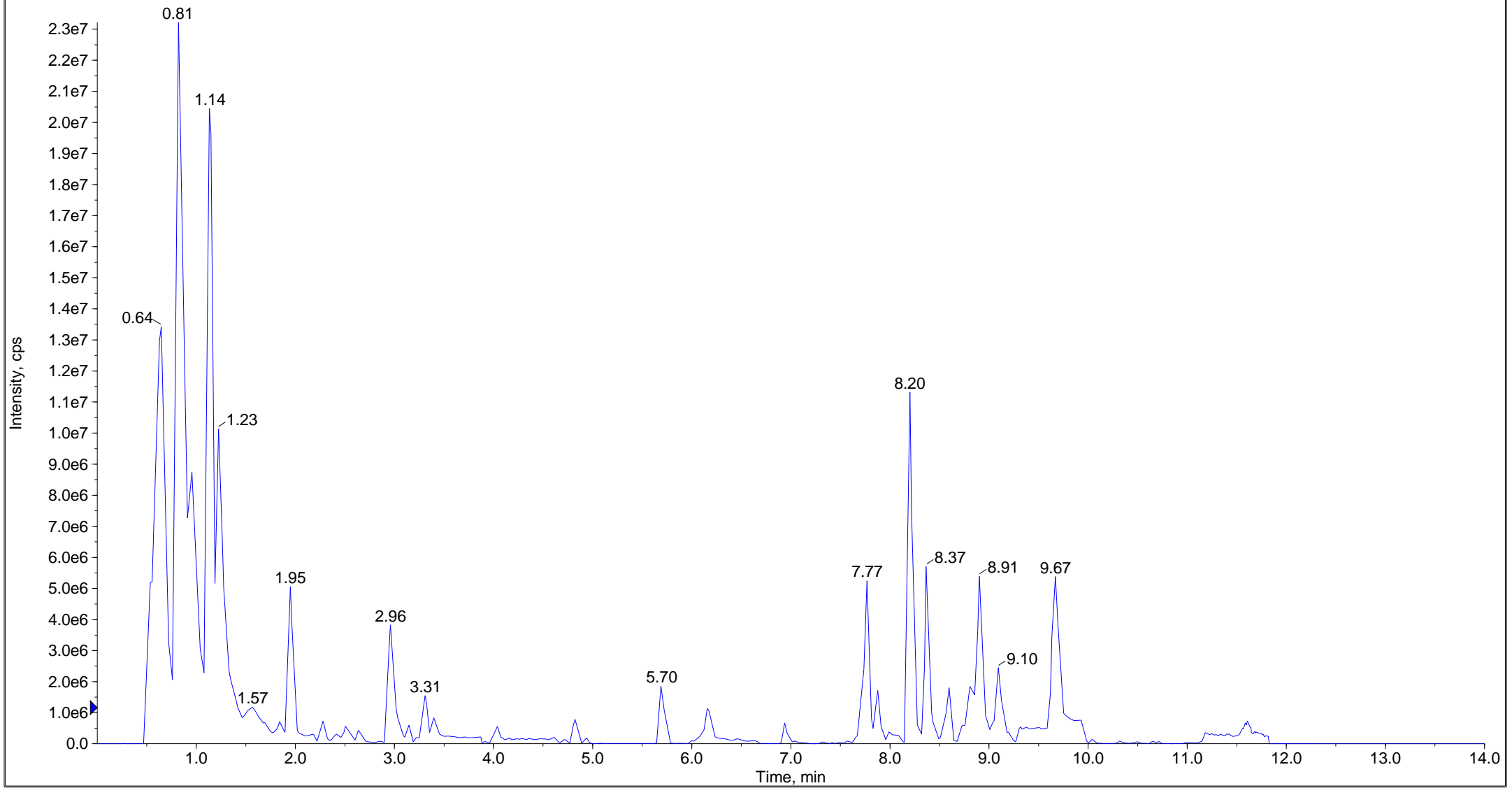
TIC of -MRM (791 pairs): from Sample 42 (A20106283a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.5e7 cps.



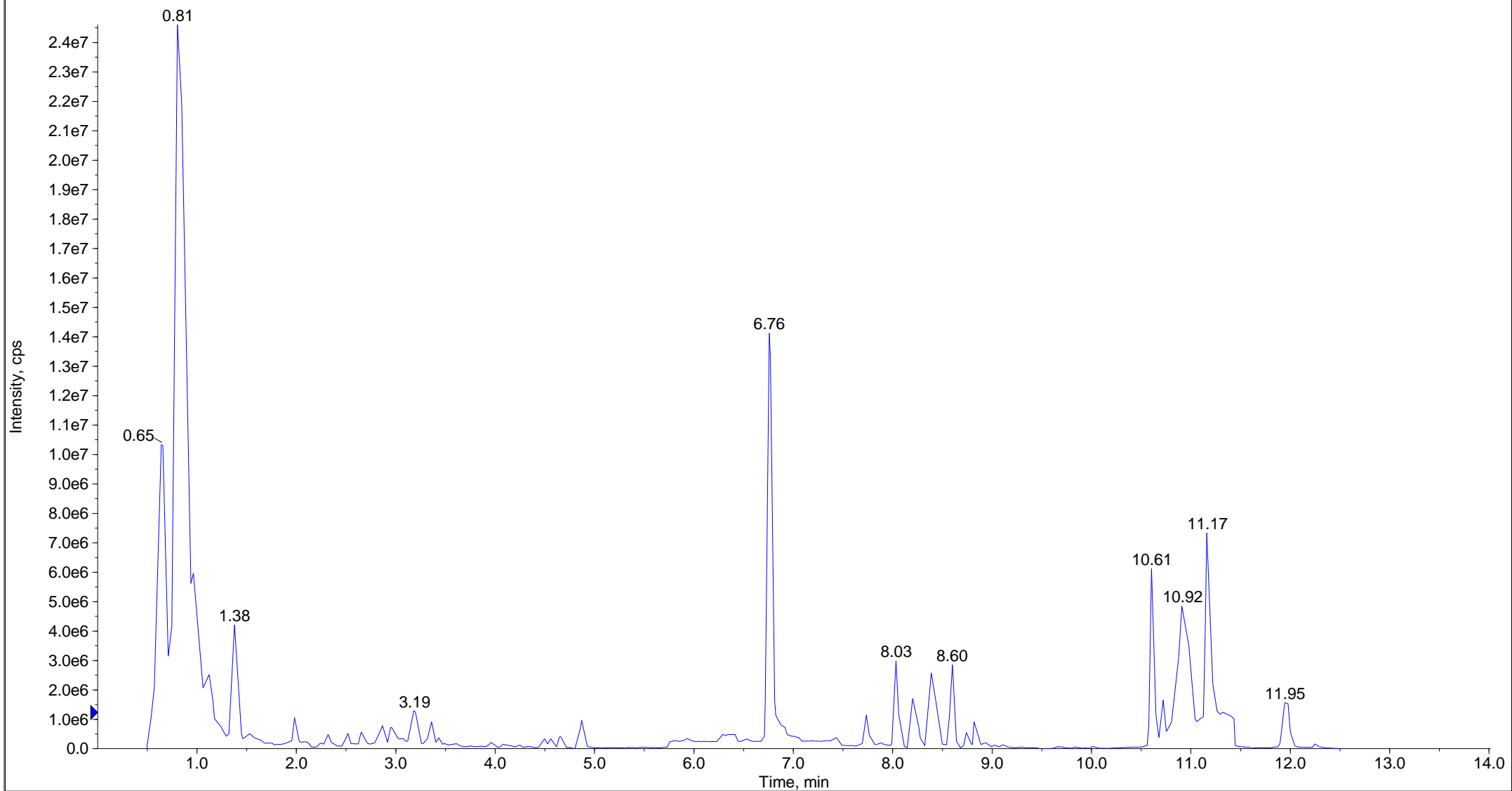
TIC of +MRM (625 pairs): from Sample 12 (A20106283a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.3e7 cps.



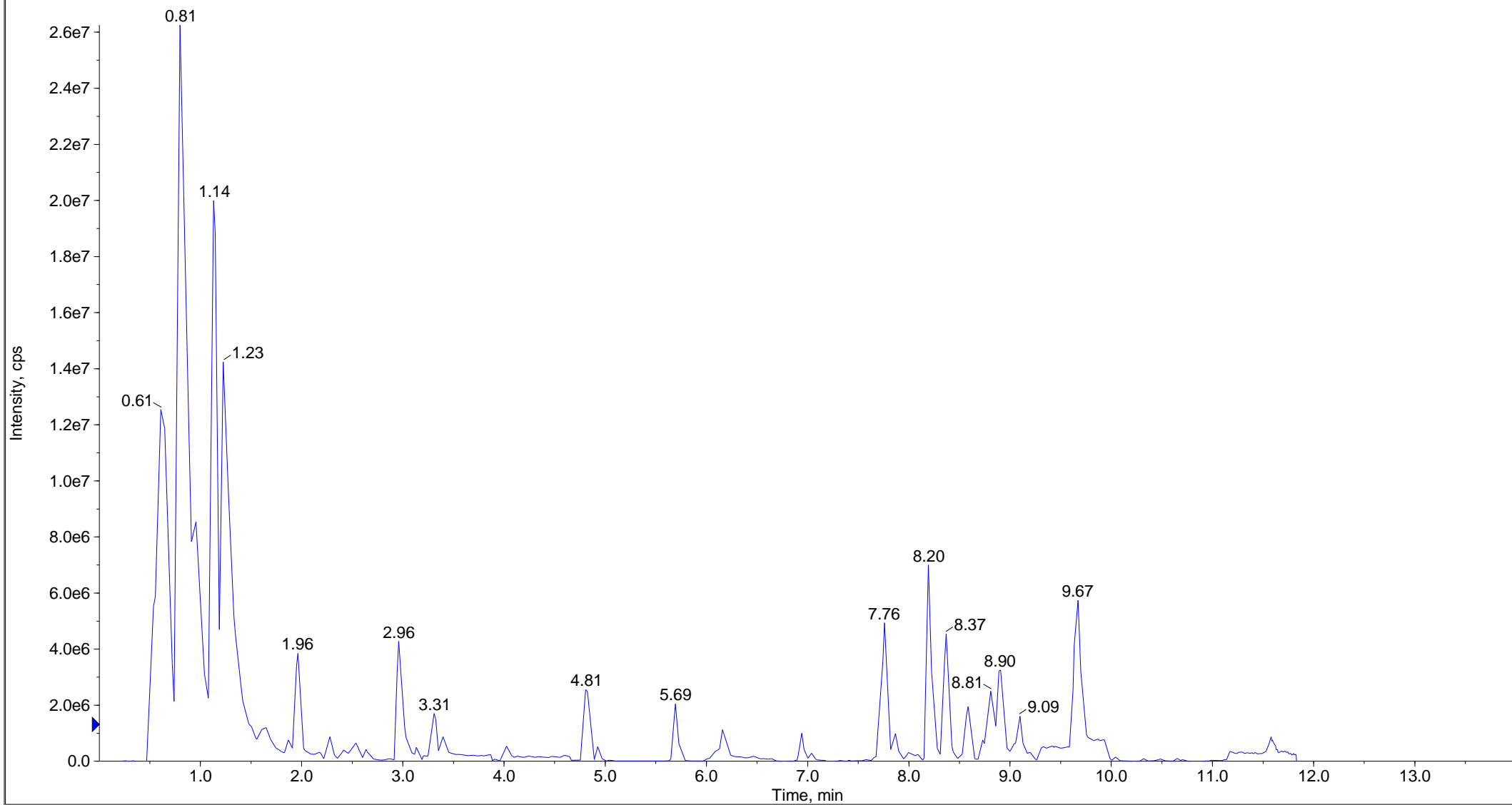
TIC of -MRM (791 pairs): from Sample 43 (A20106284a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.5e7 cps.



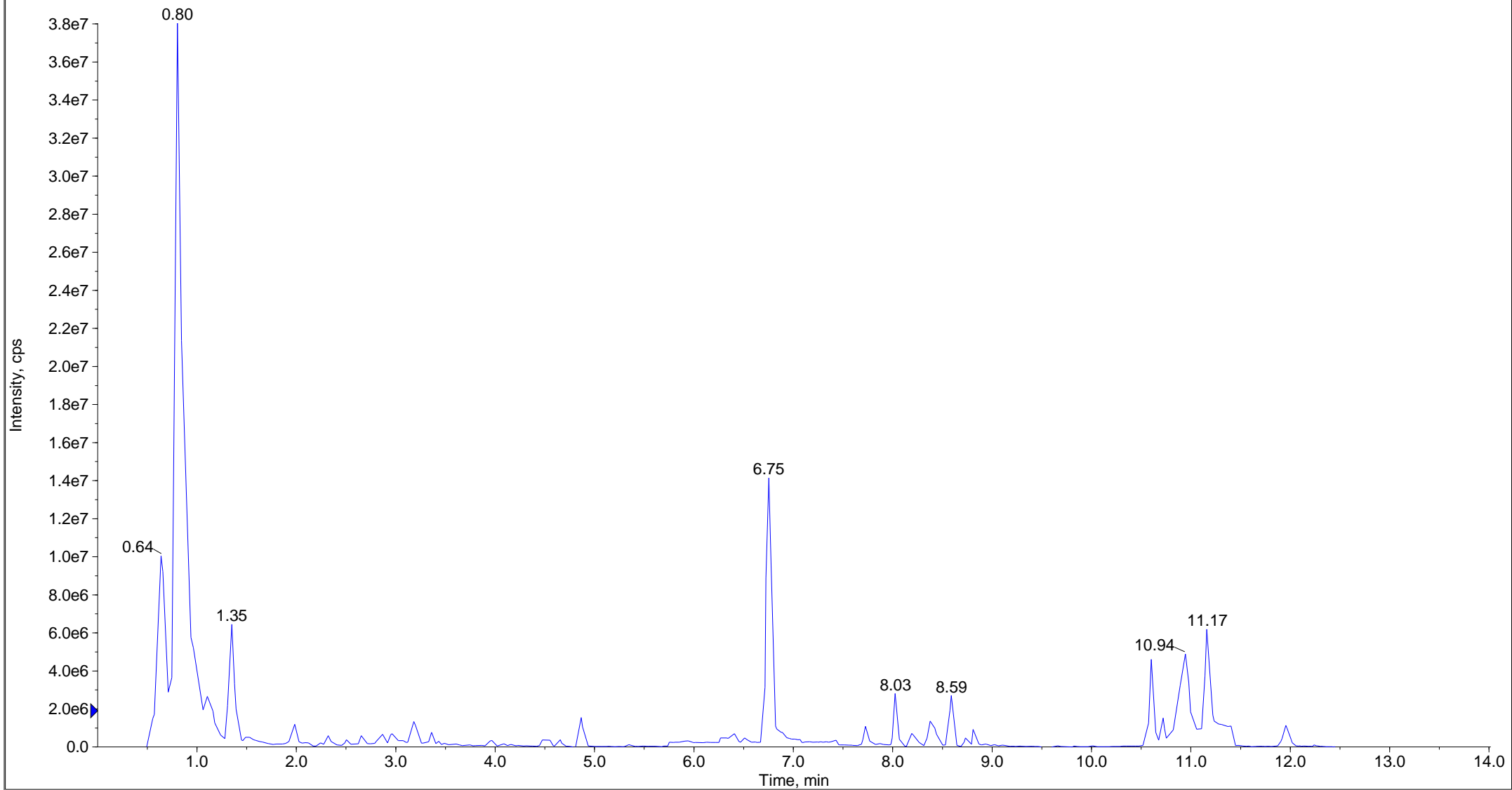
TIC of +MRM (625 pairs): from Sample 13 (A20106284a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.6e7 cps.



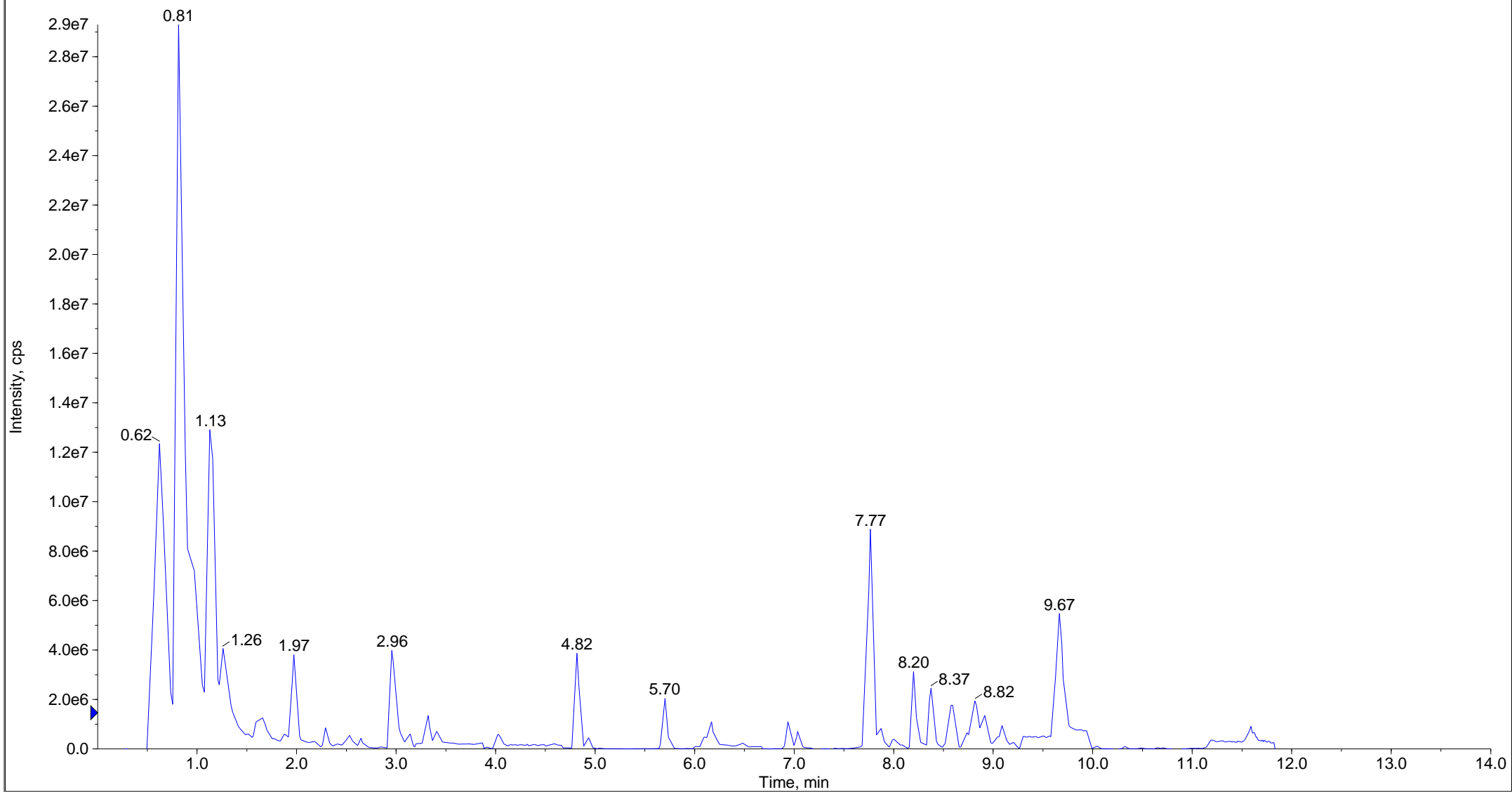
TIC of -MRM (791 pairs): from Sample 44 (A20106285a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.8e7 cps.



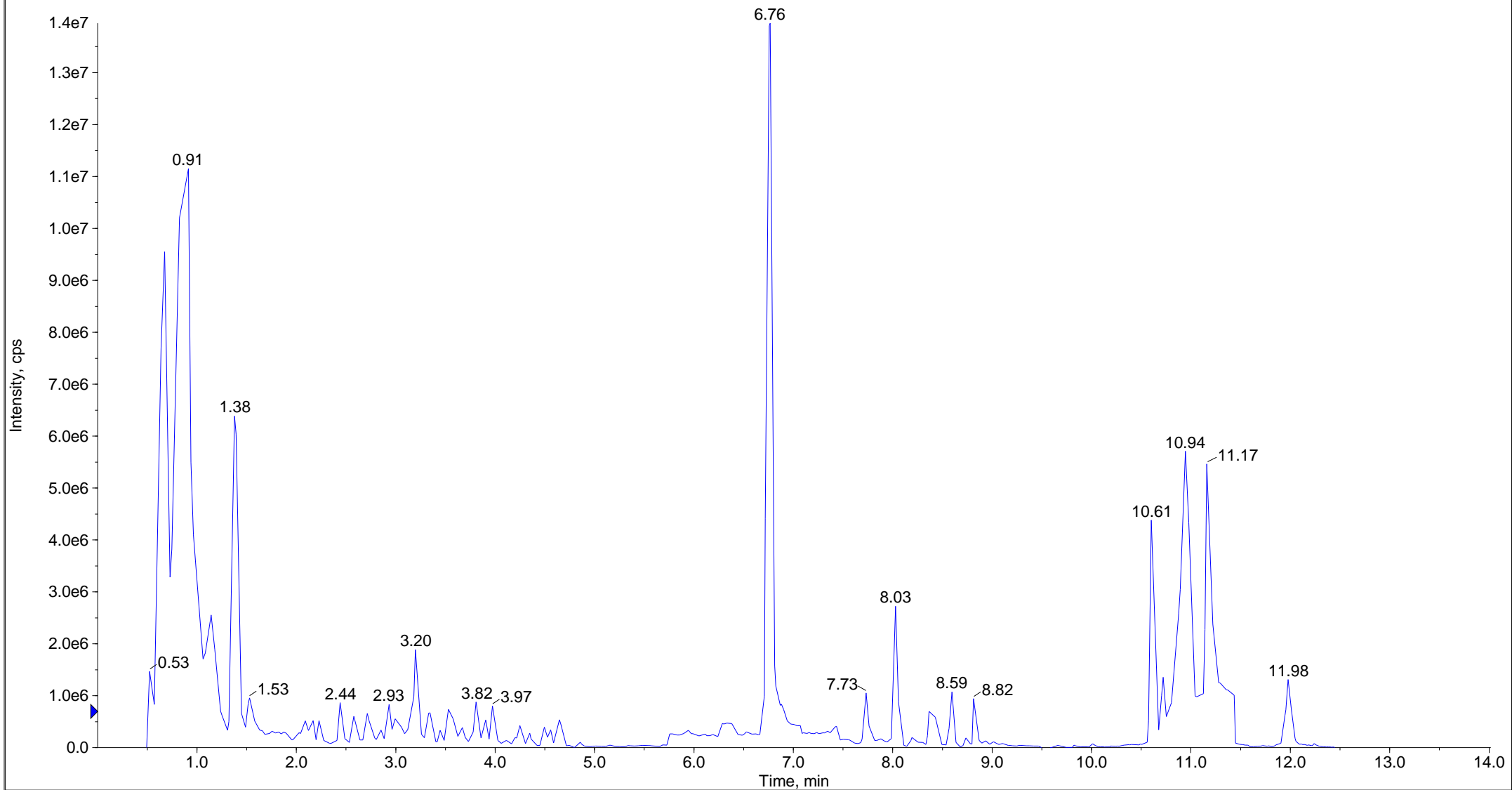
TIC of +MRM (625 pairs): from Sample 14 (A20106285a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.9e7 cps.



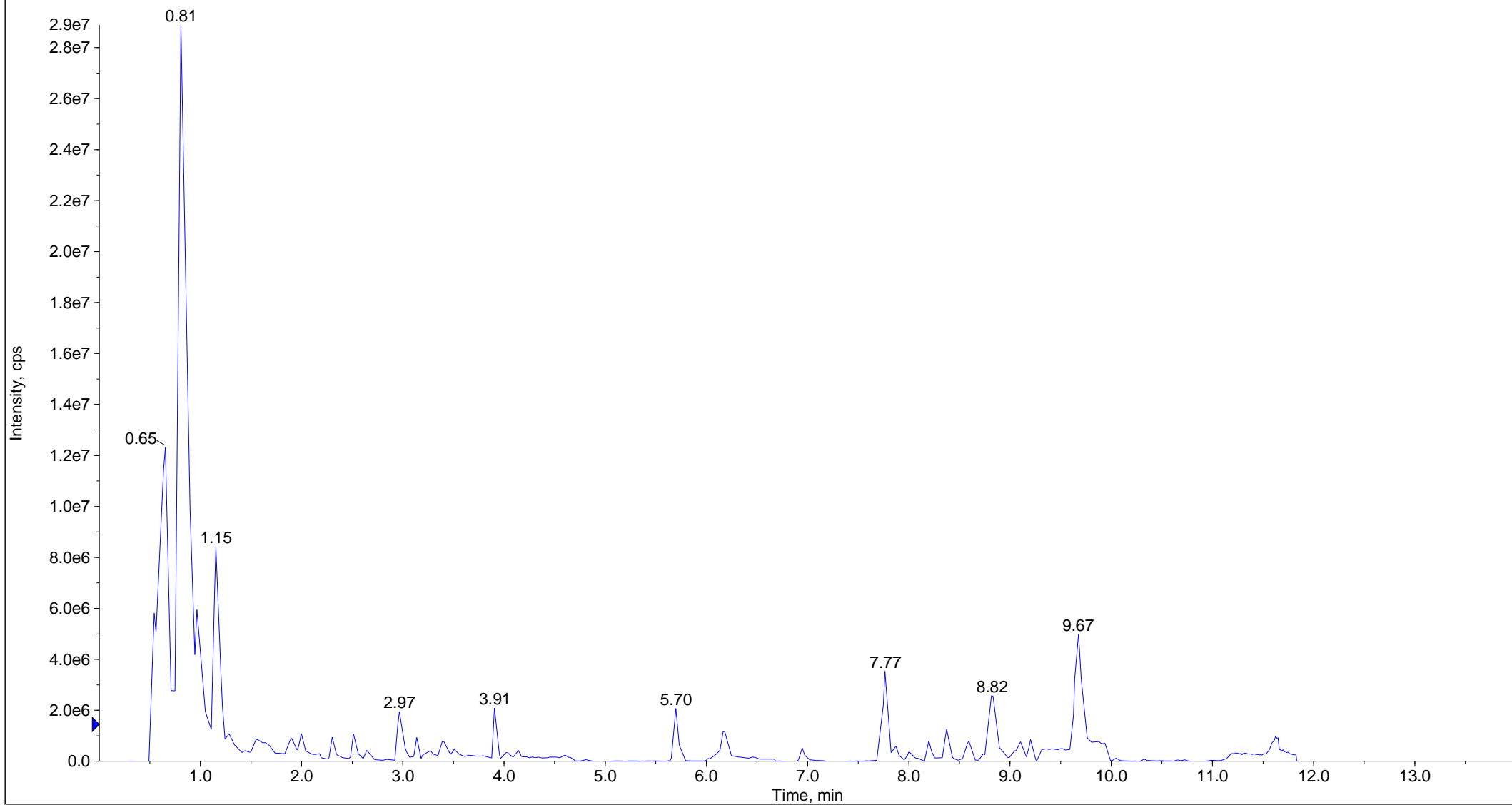
TIC of -MRM (791 pairs): from Sample 47 (A20106286a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.4e7 cps.



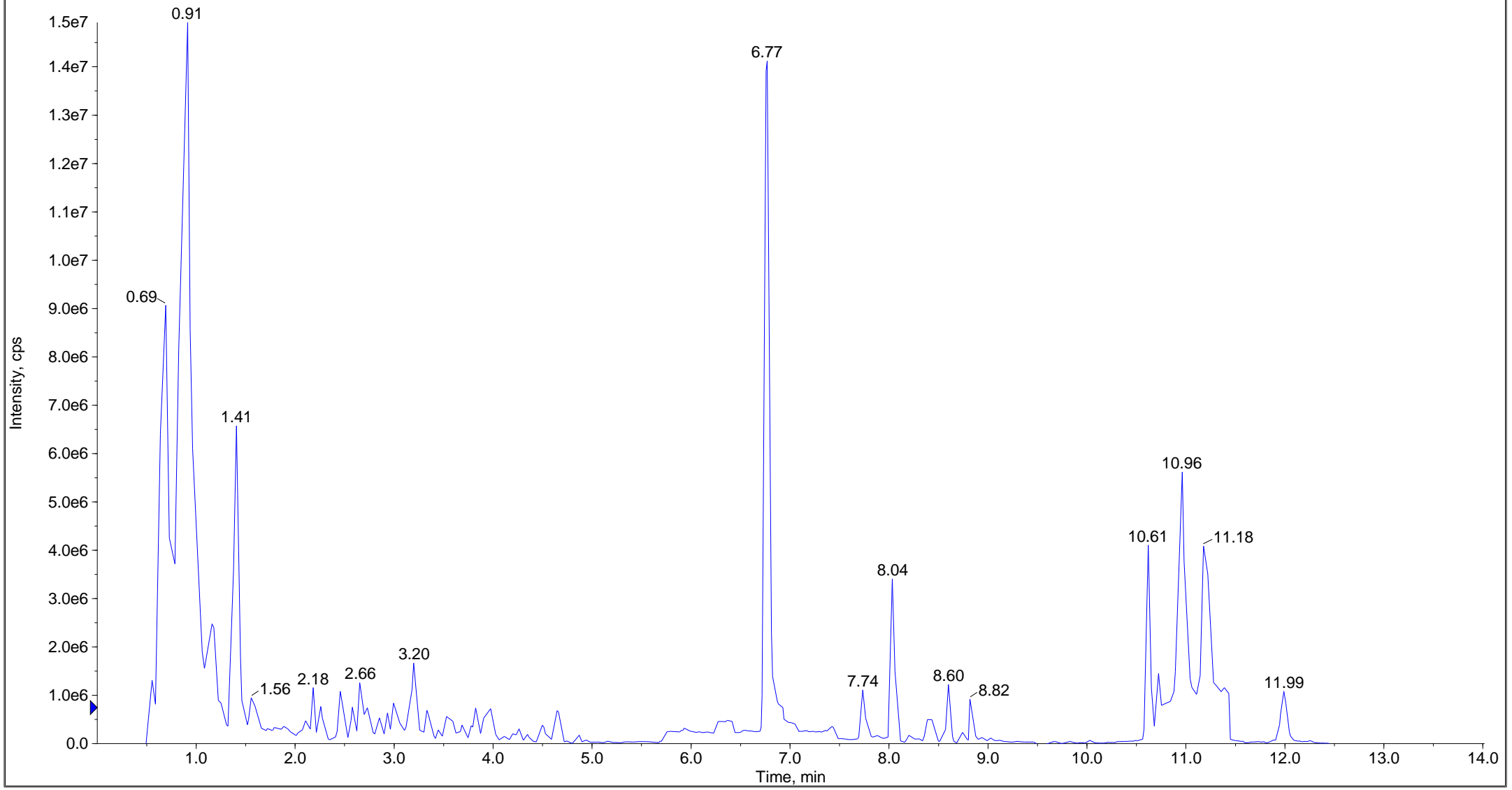
TIC of +MRM (625 pairs): from Sample 17 (A20106286a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.9e7 cps.



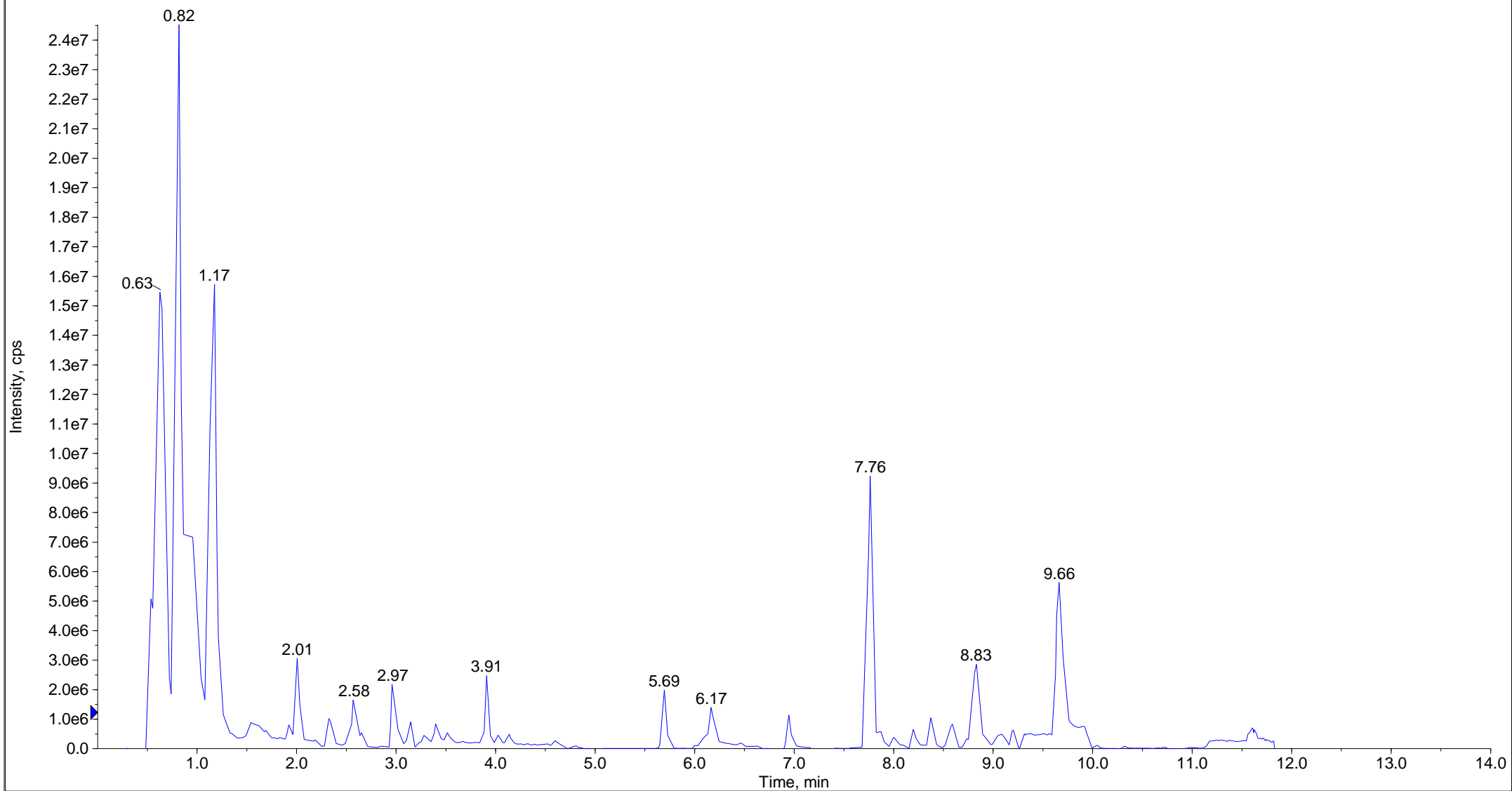
TIC of -MRM (791 pairs): from Sample 48 (A20106287a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.5e7 cps.



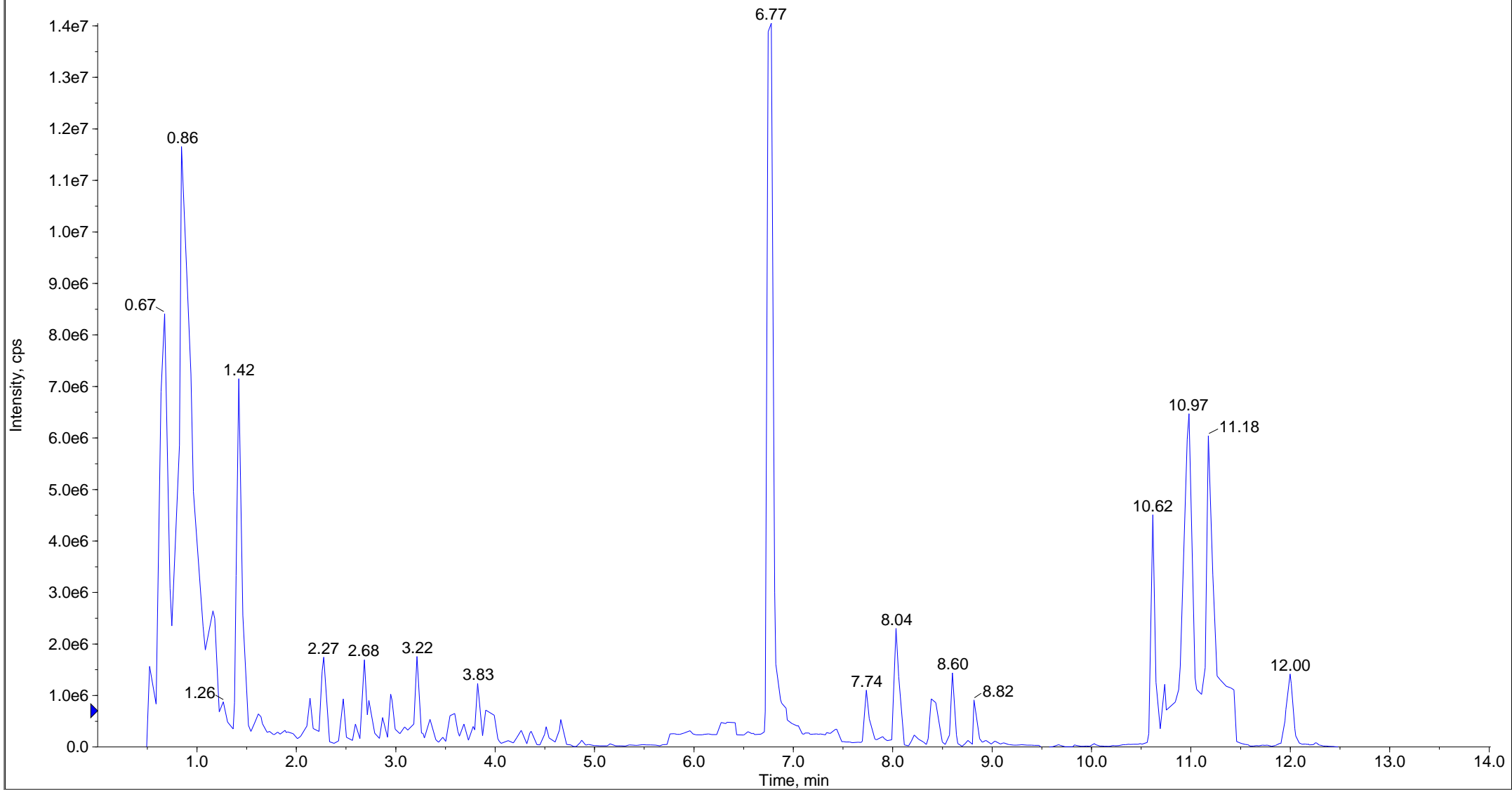
TIC of +MRM (625 pairs): from Sample 18 (A20106287a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.5e7 cps.



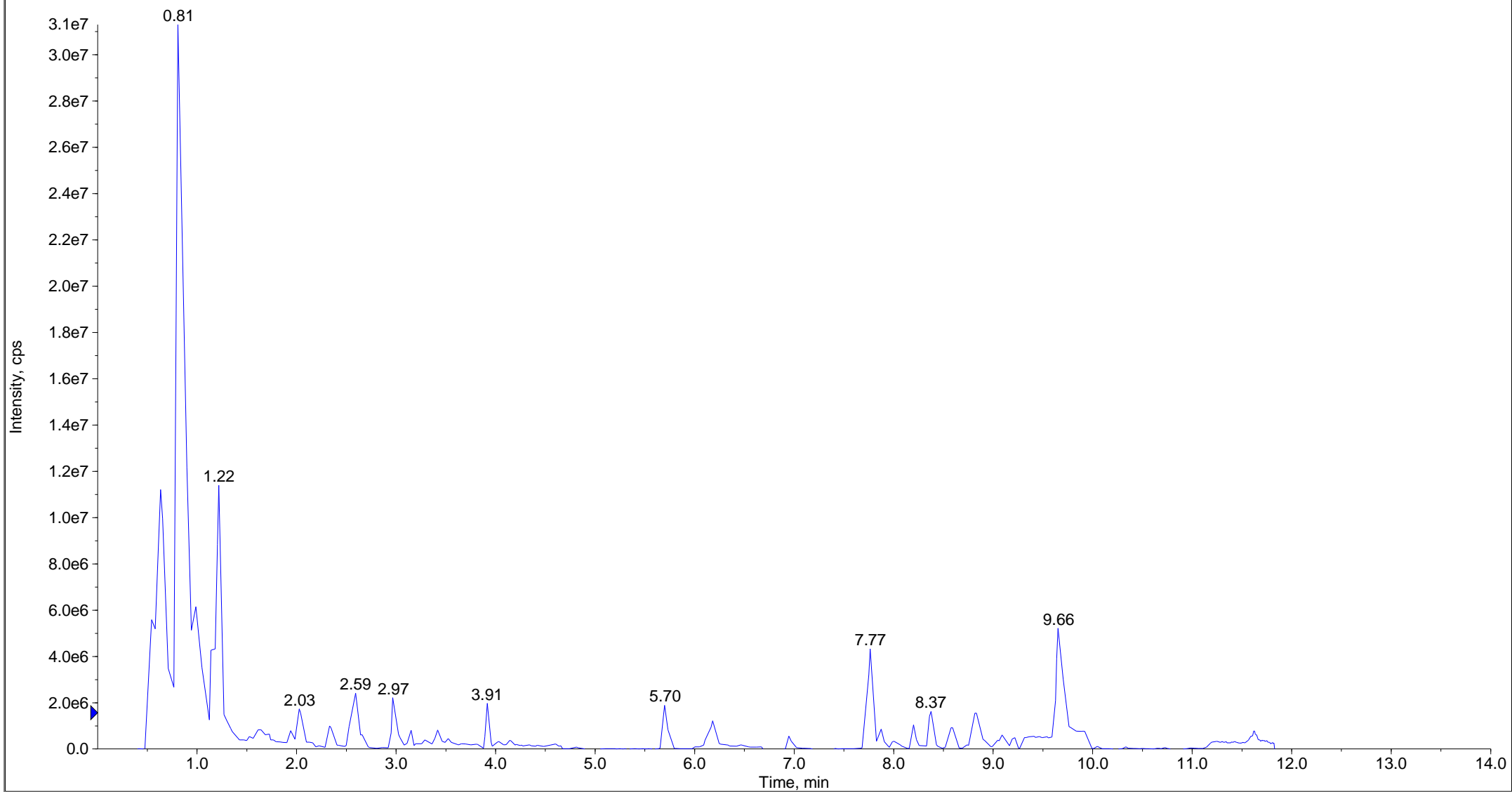
TIC of -MRM (791 pairs): from Sample 49 (A20106288a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.4e7 cps.



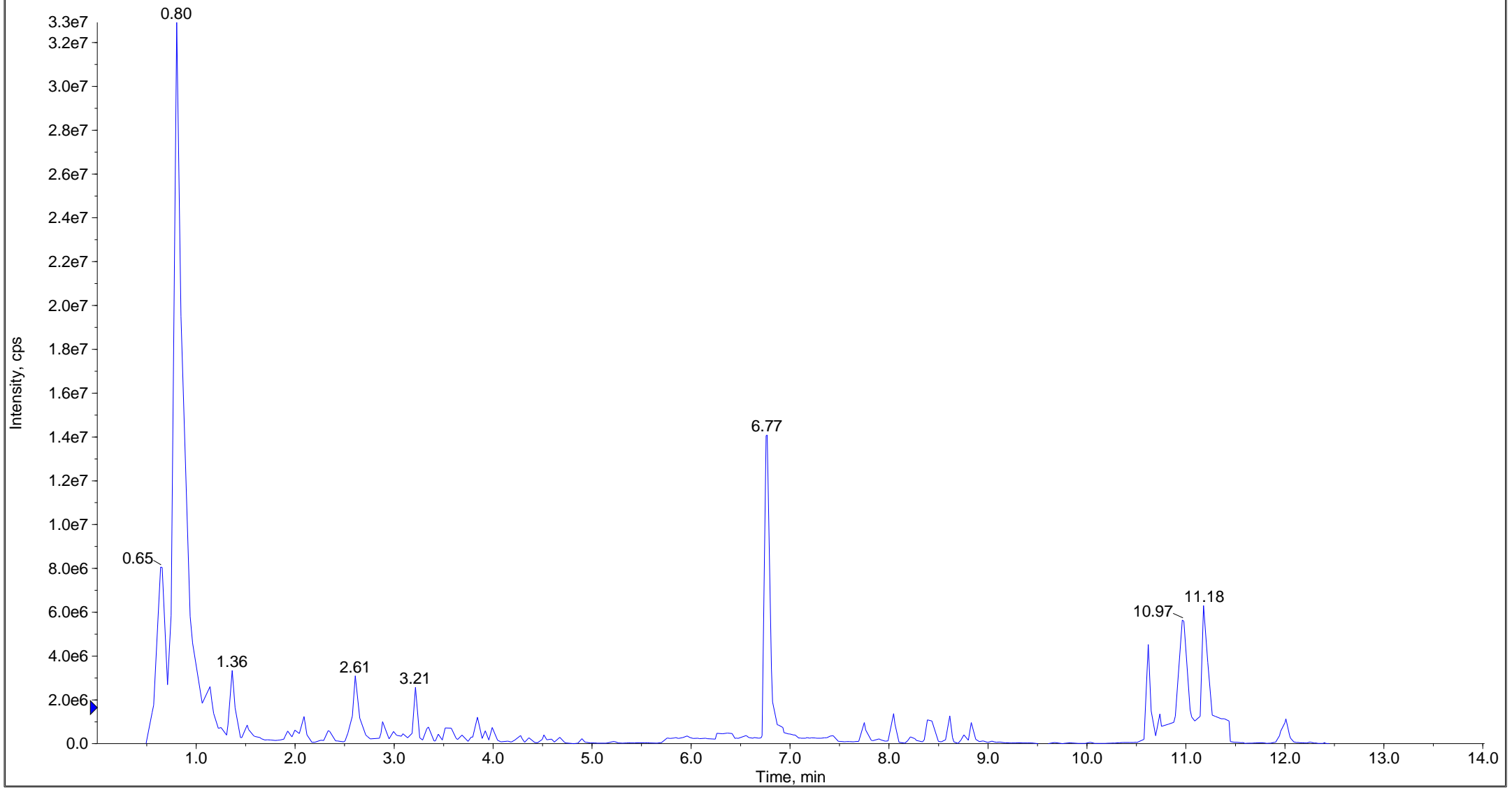
TIC of +MRM (625 pairs): from Sample 19 (A20106288a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.1e7 cps.



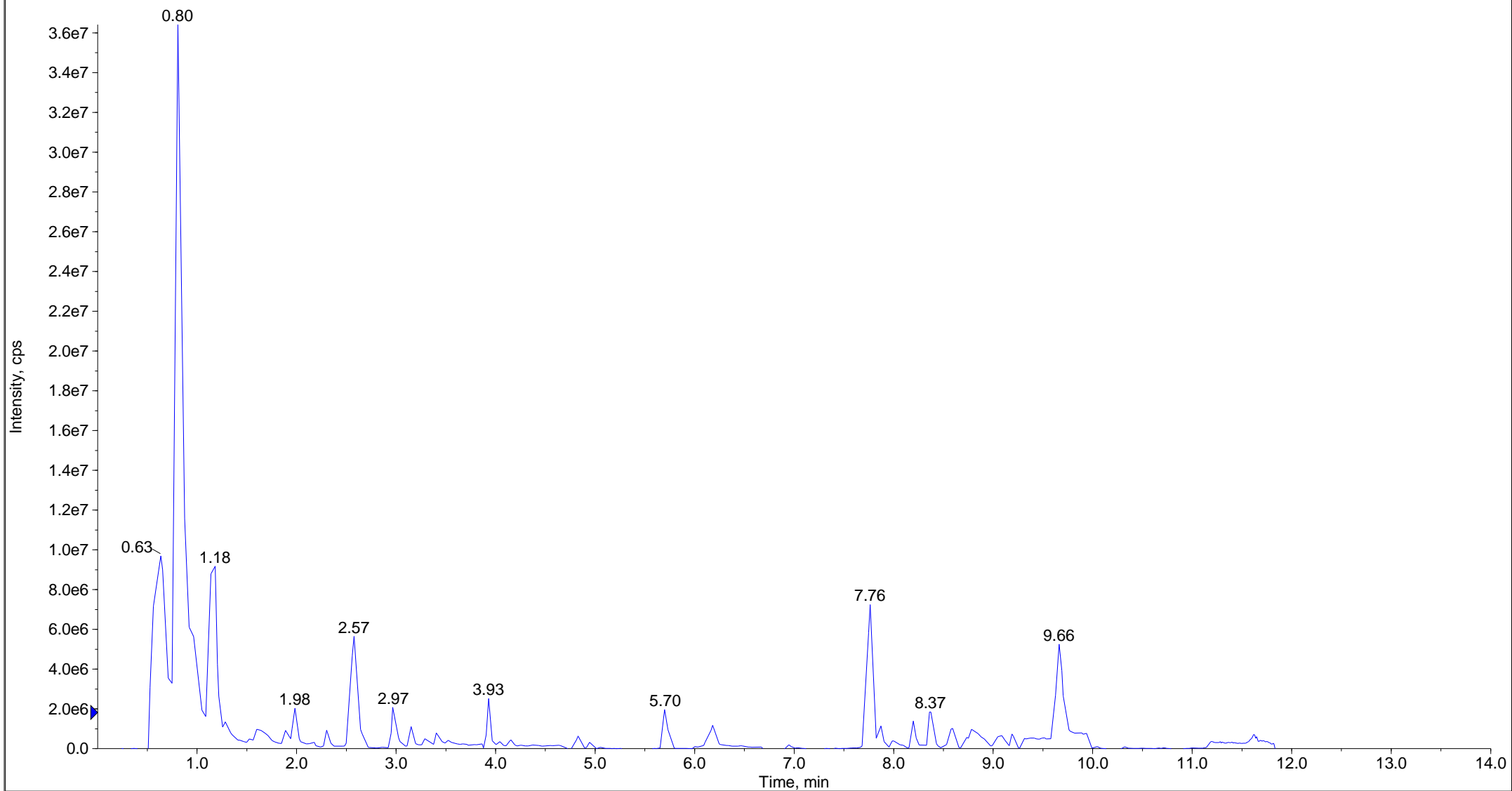
TIC of -MRM (791 pairs): from Sample 50 (A20106289a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.3e7 cps.



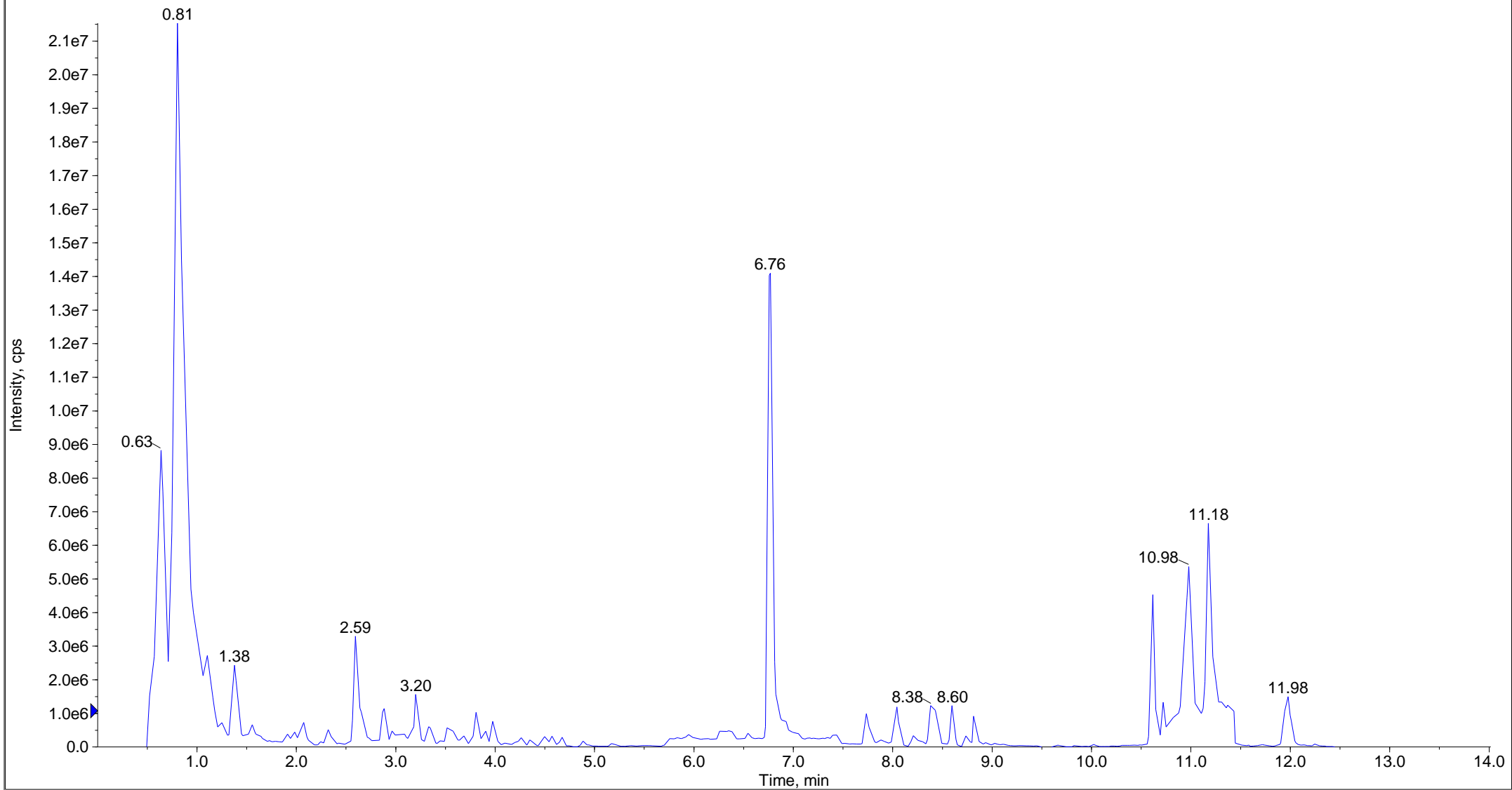
TIC of +MRM (625 pairs): from Sample 20 (A20106289a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.6e7 cps.



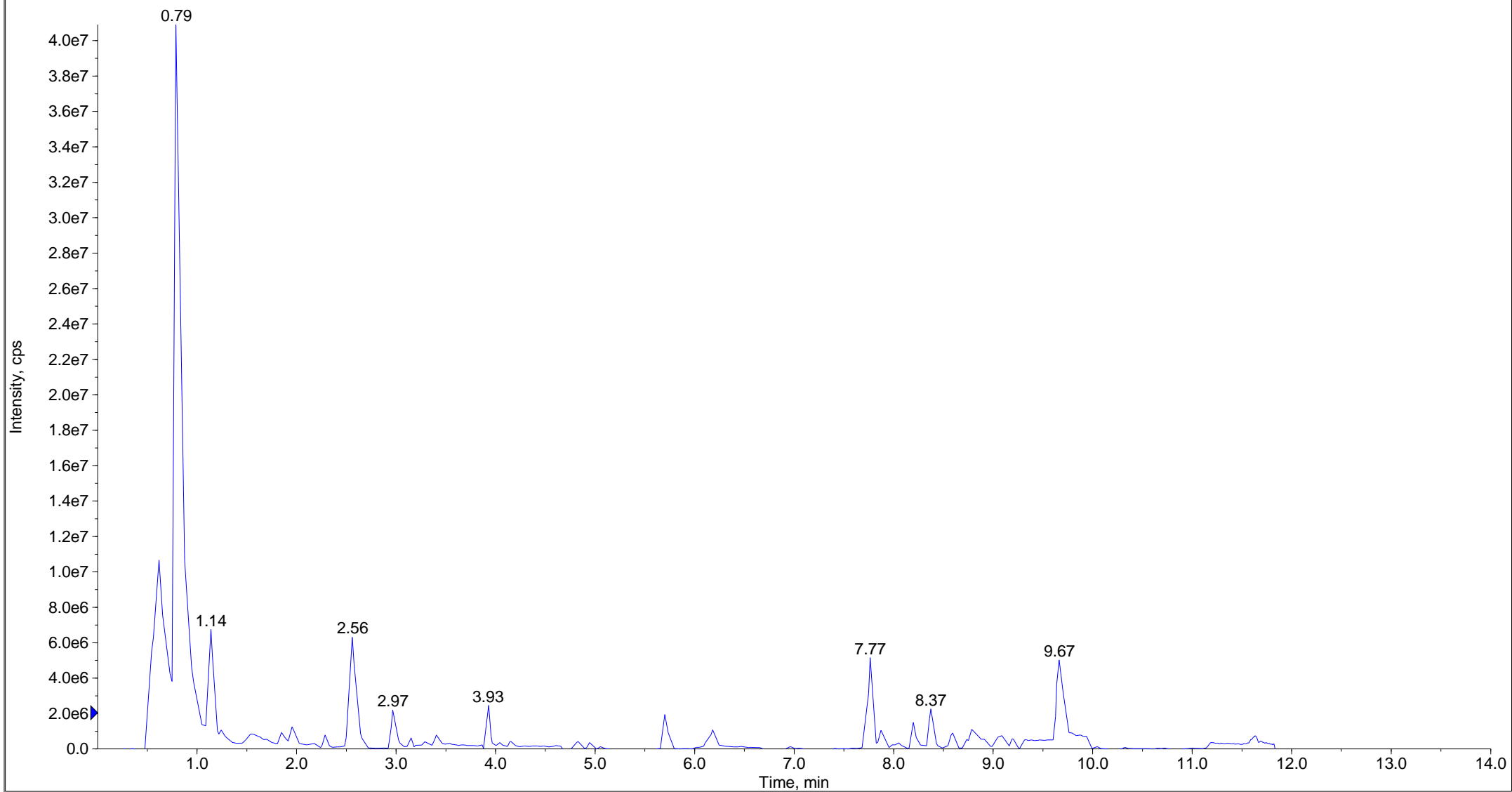
TIC of -MRM (791 pairs): from Sample 51 (A20106290a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.2e7 cps.



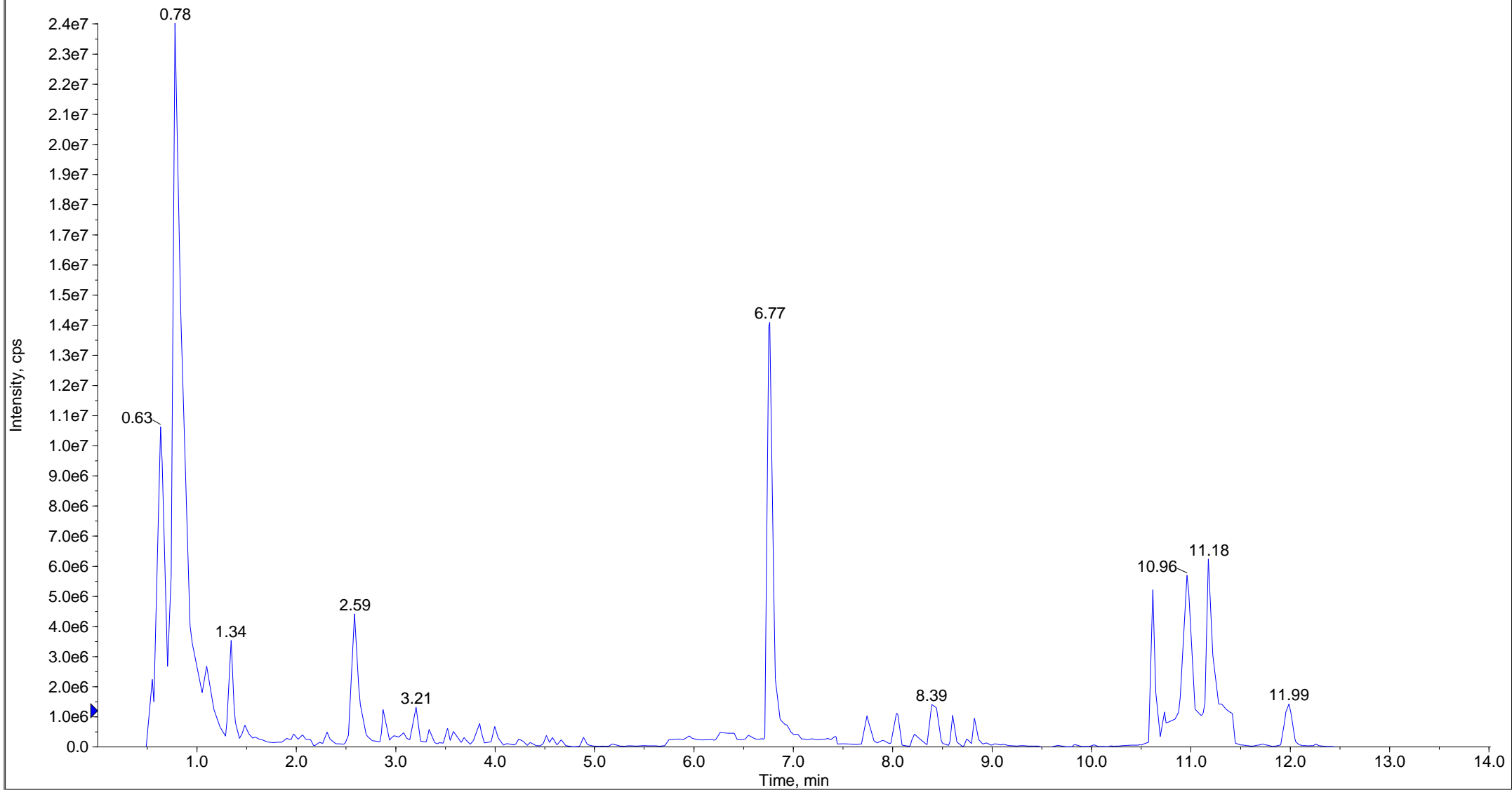
TIC of +MRM (625 pairs): from Sample 21 (A20106290a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.1e7 cps.



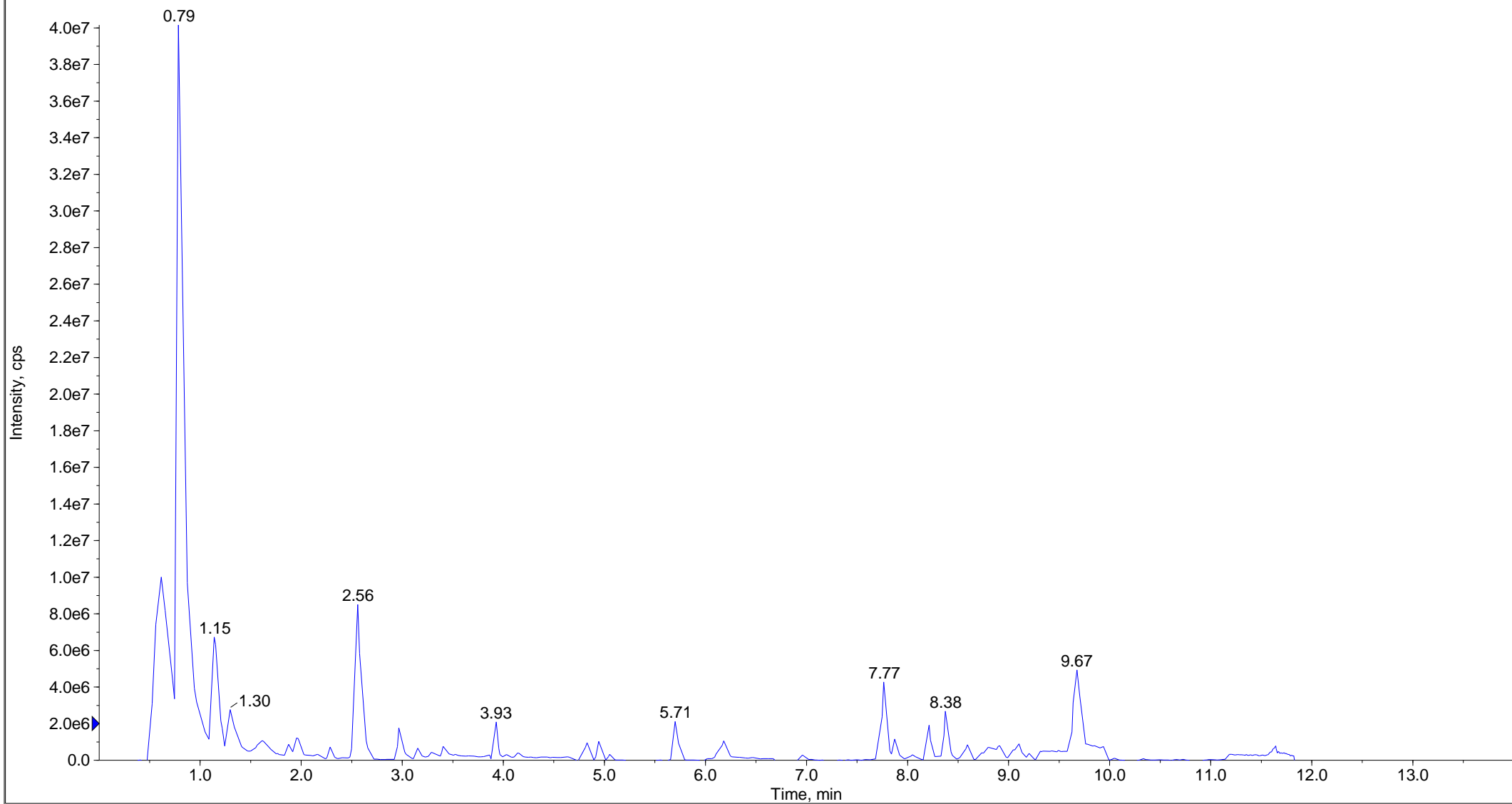
TIC of -MRM (791 pairs): from Sample 52 (A20106291a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.4e7 cps.



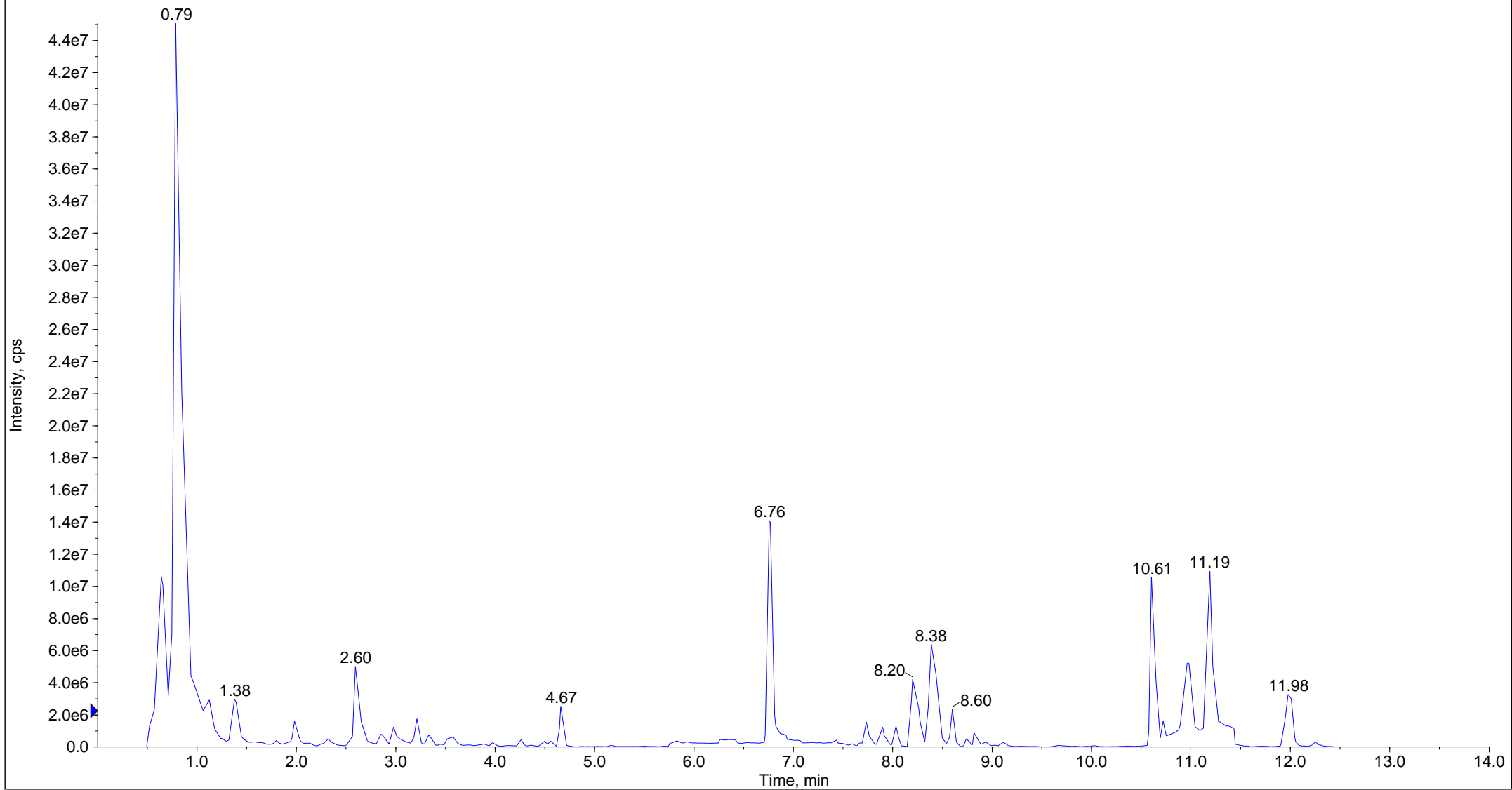
TIC of +MRM (625 pairs): from Sample 22 (A20106291a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.0e7 cps.



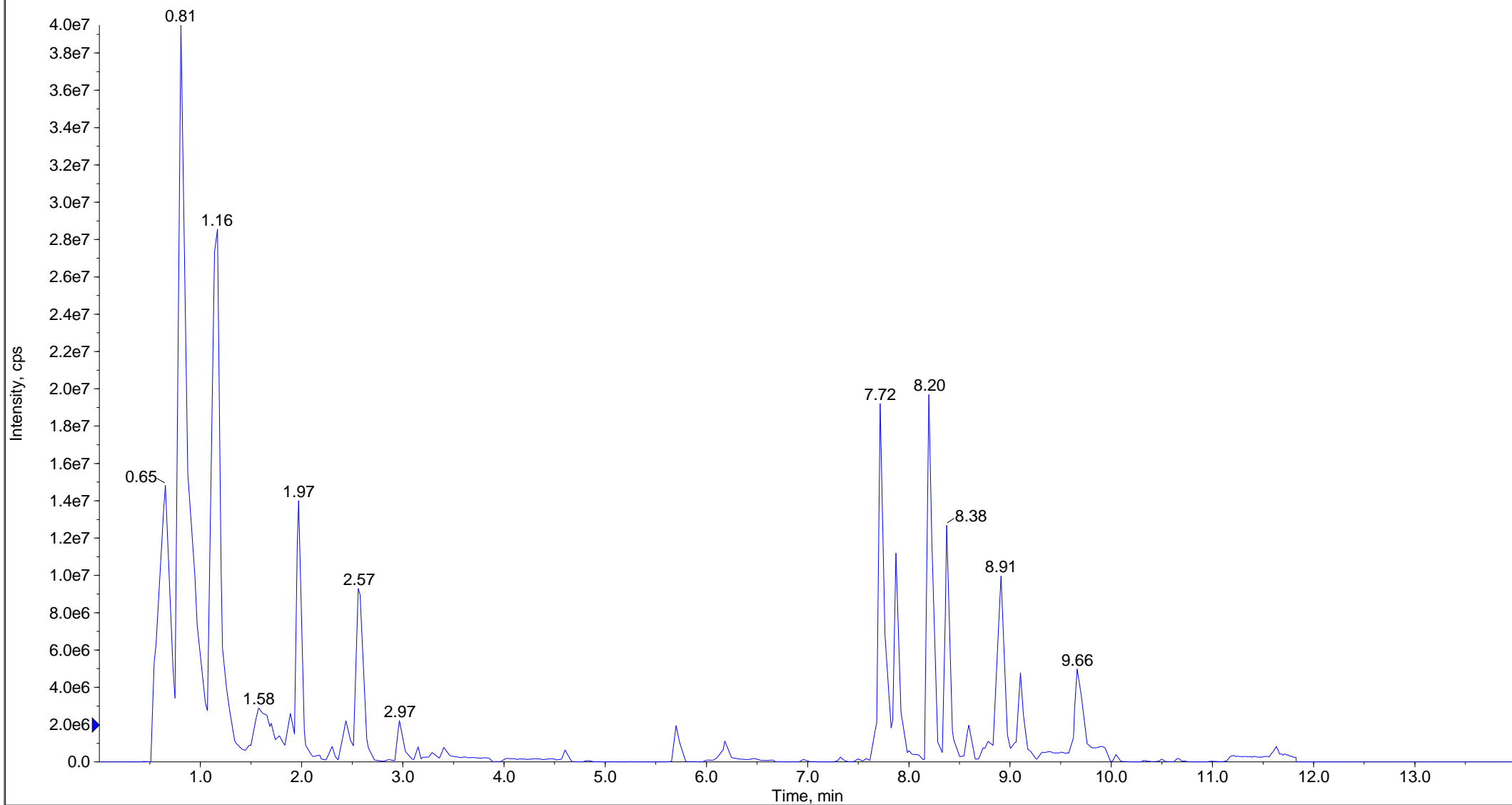
TIC of -MRM (791 pairs): from Sample 53 (A20106292a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.5e7 cps.



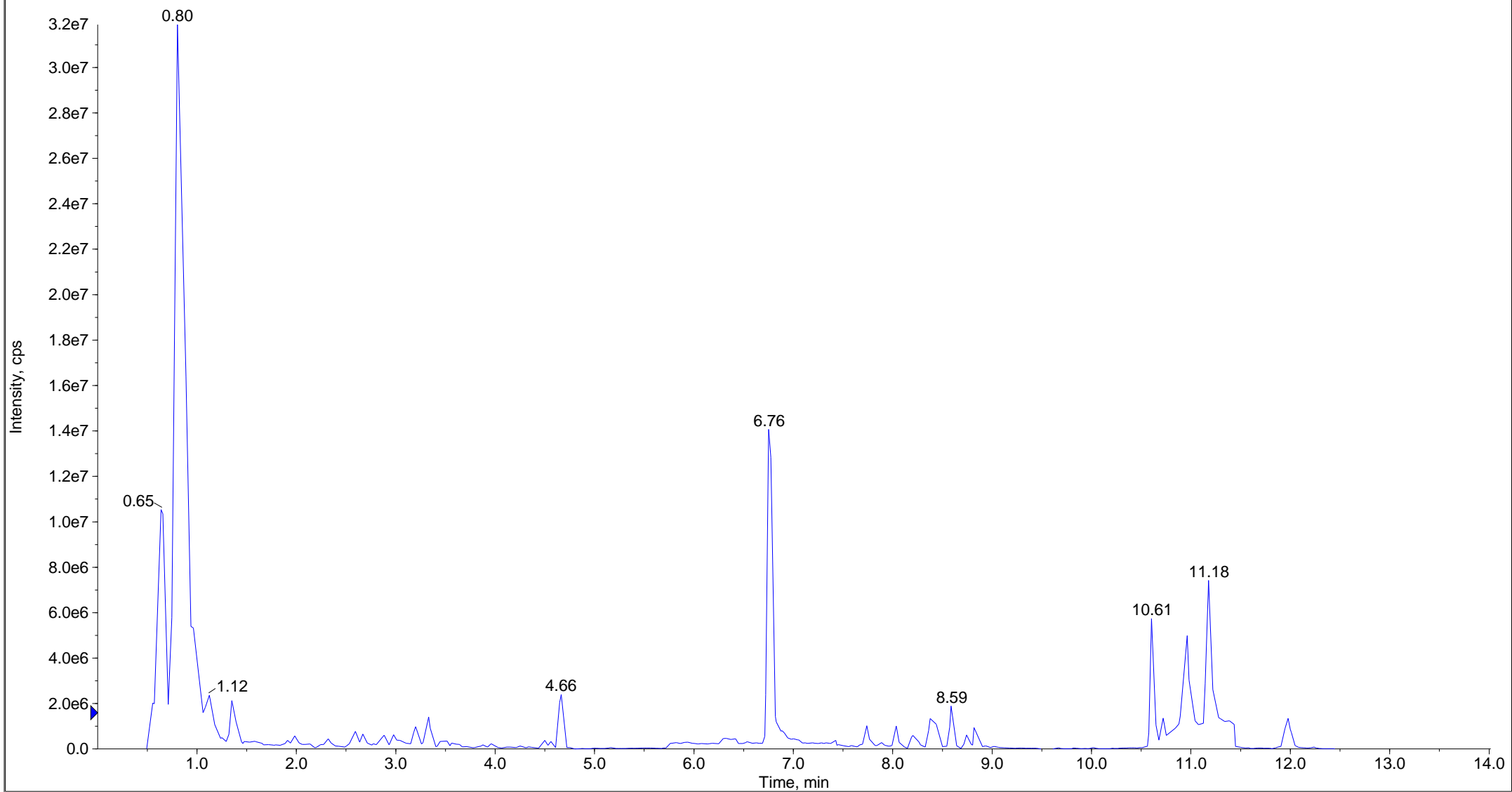
TIC of +MRM (625 pairs): from Sample 23 (A20106292a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.0e7 cps.



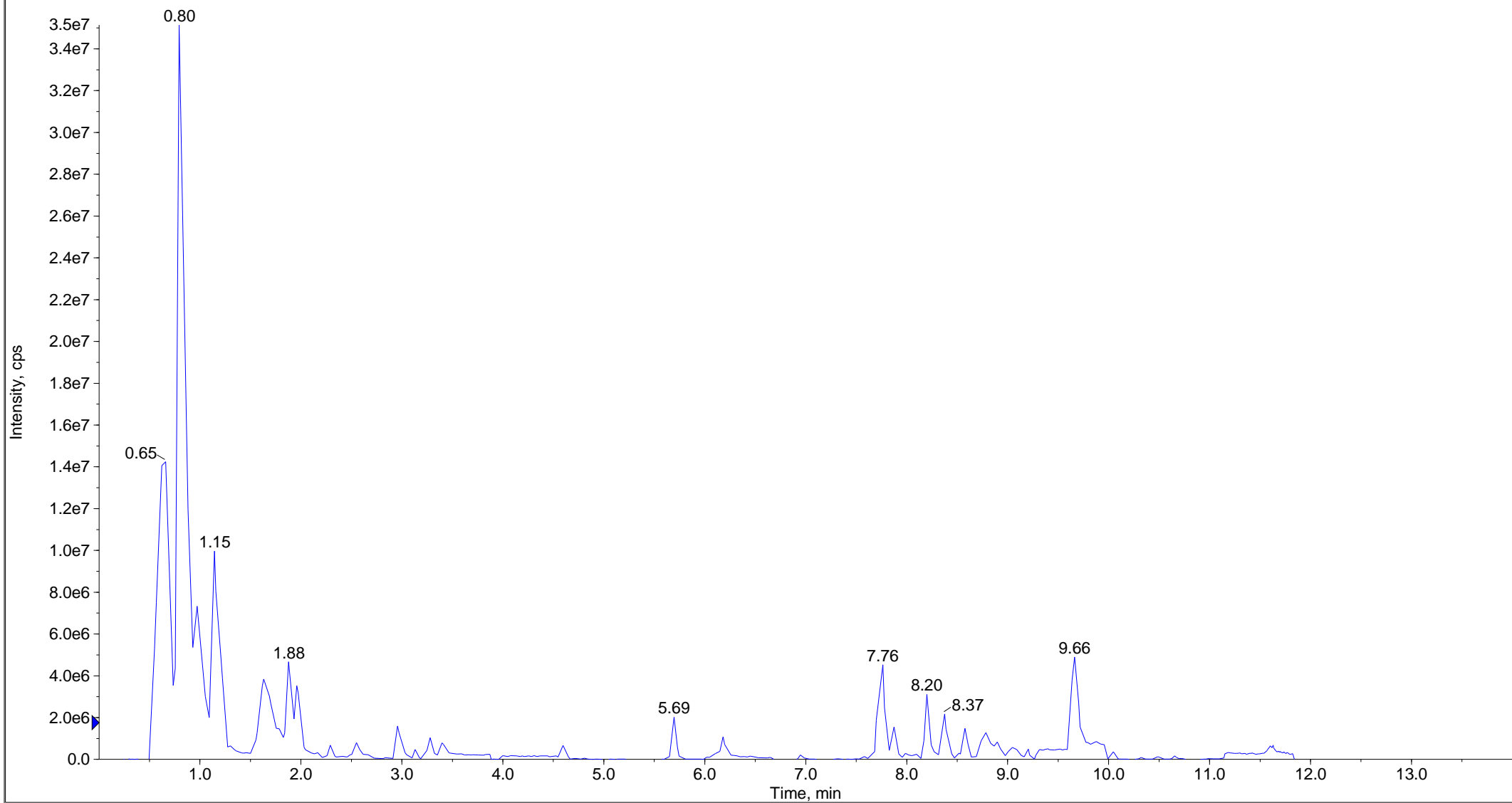
TIC of -MRM (791 pairs): from Sample 54 (A20106293a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.2e7 cps.



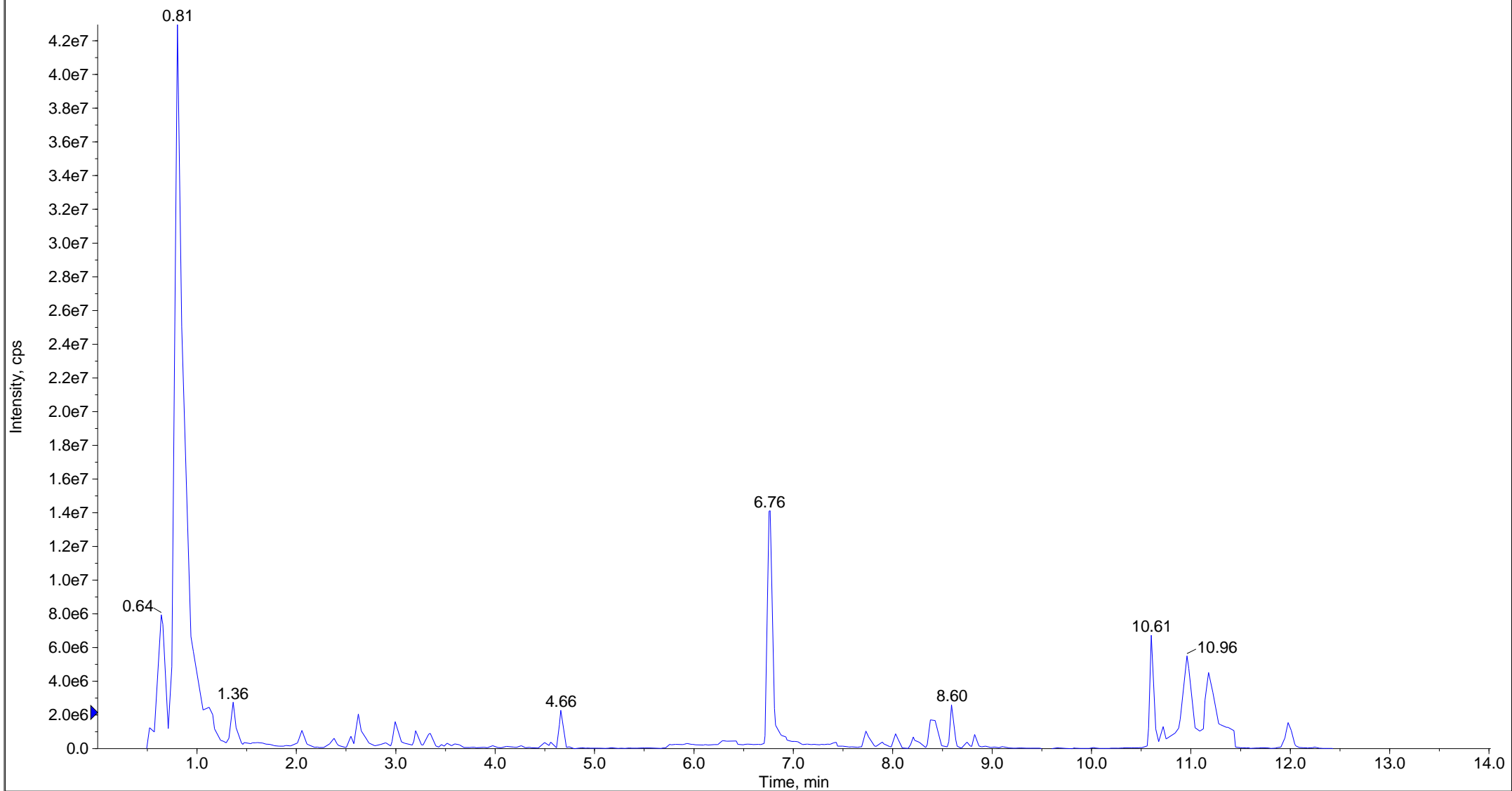
TIC of +MRM (625 pairs): from Sample 24 (A20106293a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.5e7 cps.



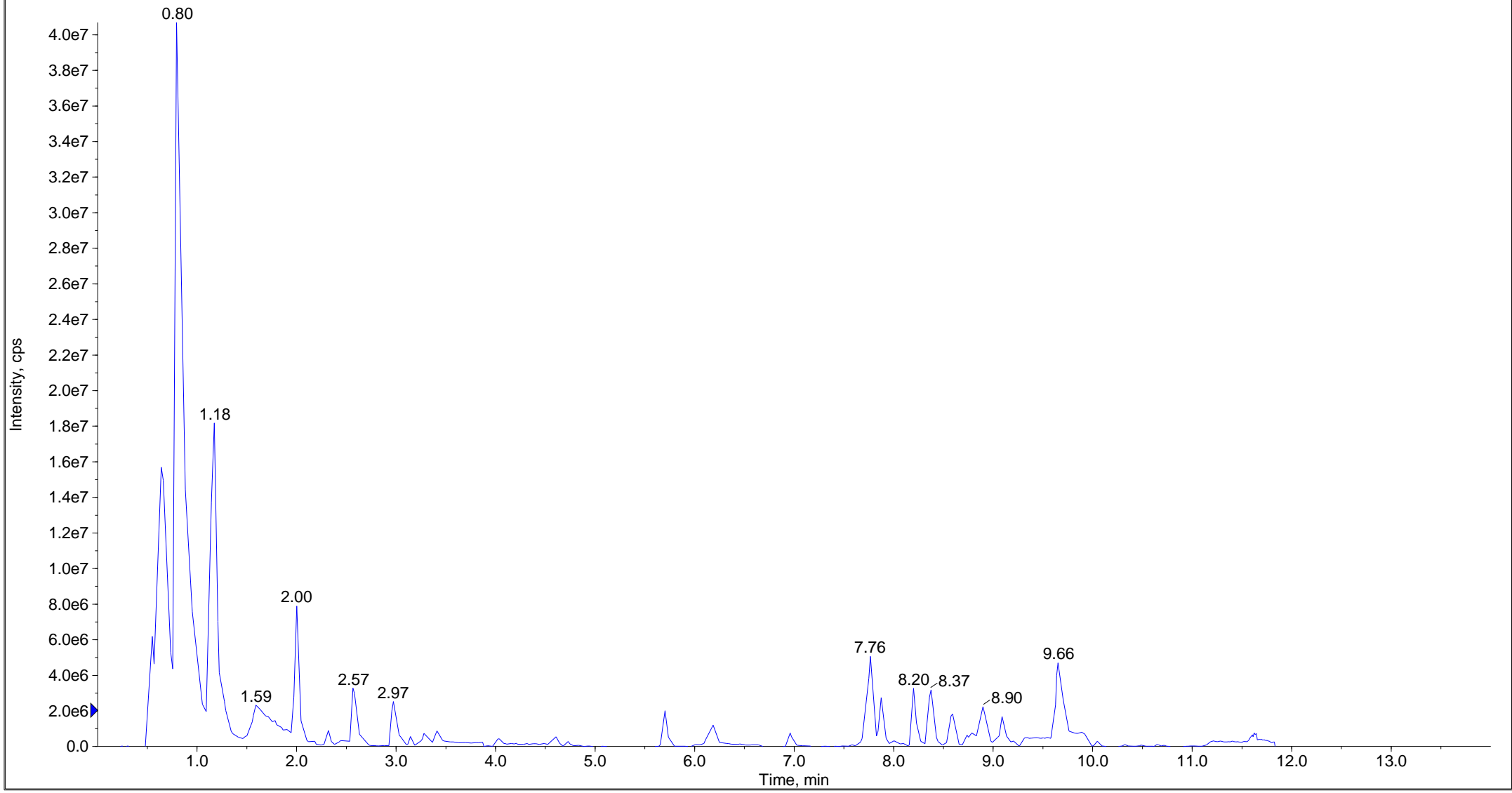
TIC of -MRM (791 pairs): from Sample 55 (A20106294a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.3e7 cps.



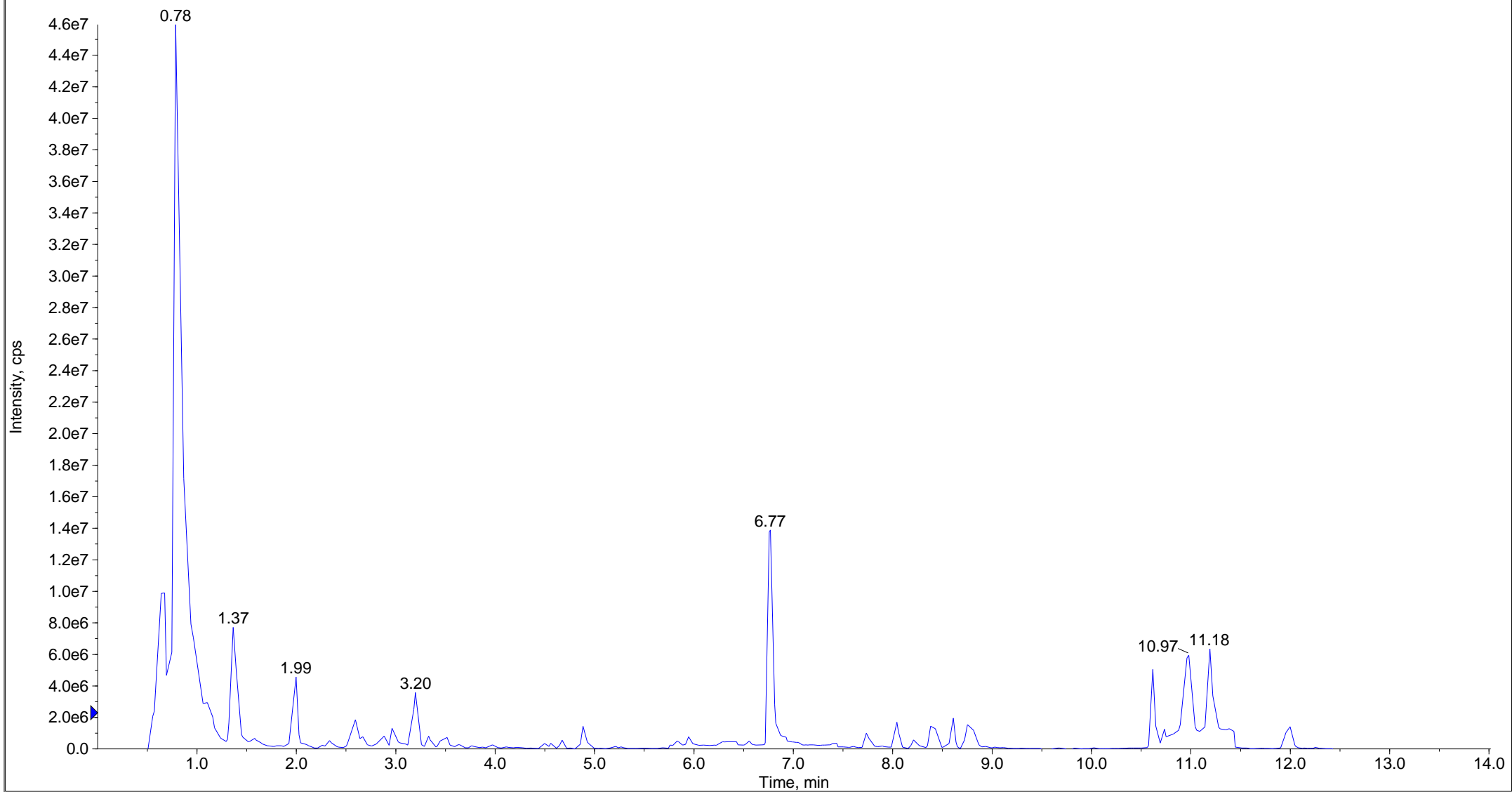
TIC of +MRM (625 pairs): from Sample 25 (A20106294a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.1e7 cps.



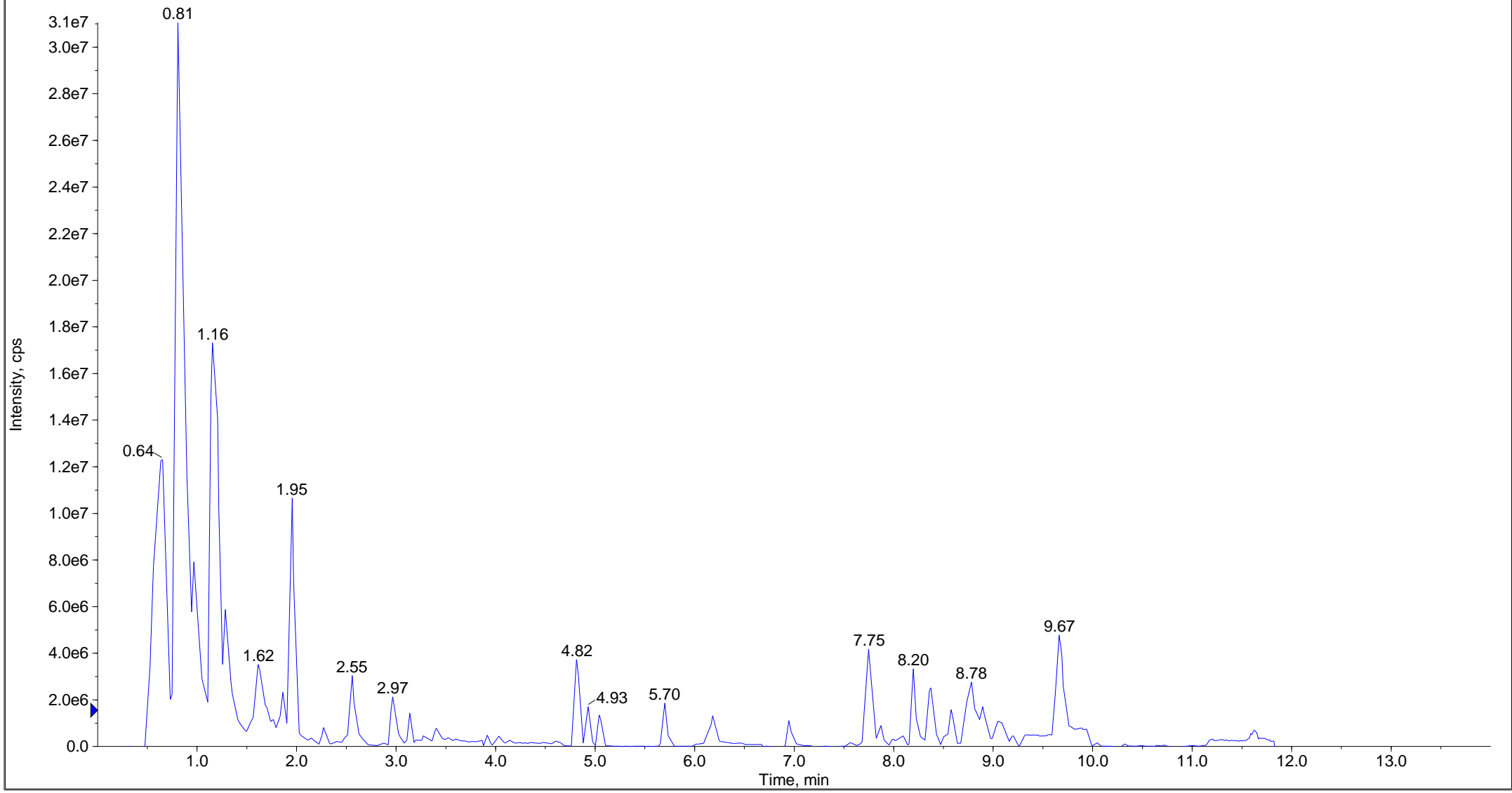
TIC of -MRM (791 pairs): from Sample 56 (A20106295a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.6e7 cps.



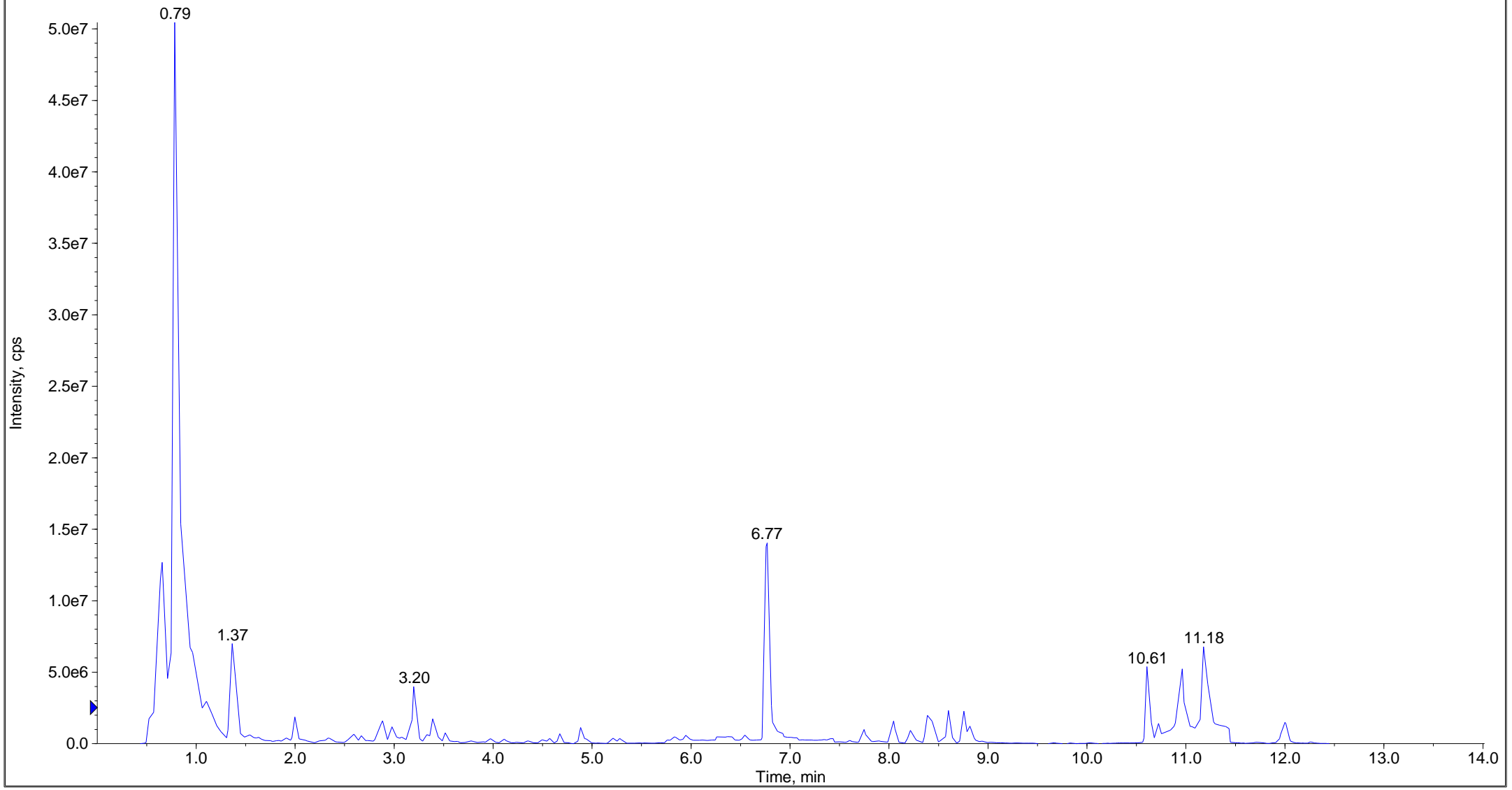
TIC of +MRM (625 pairs): from Sample 26 (A20106295a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.1e7 cps.



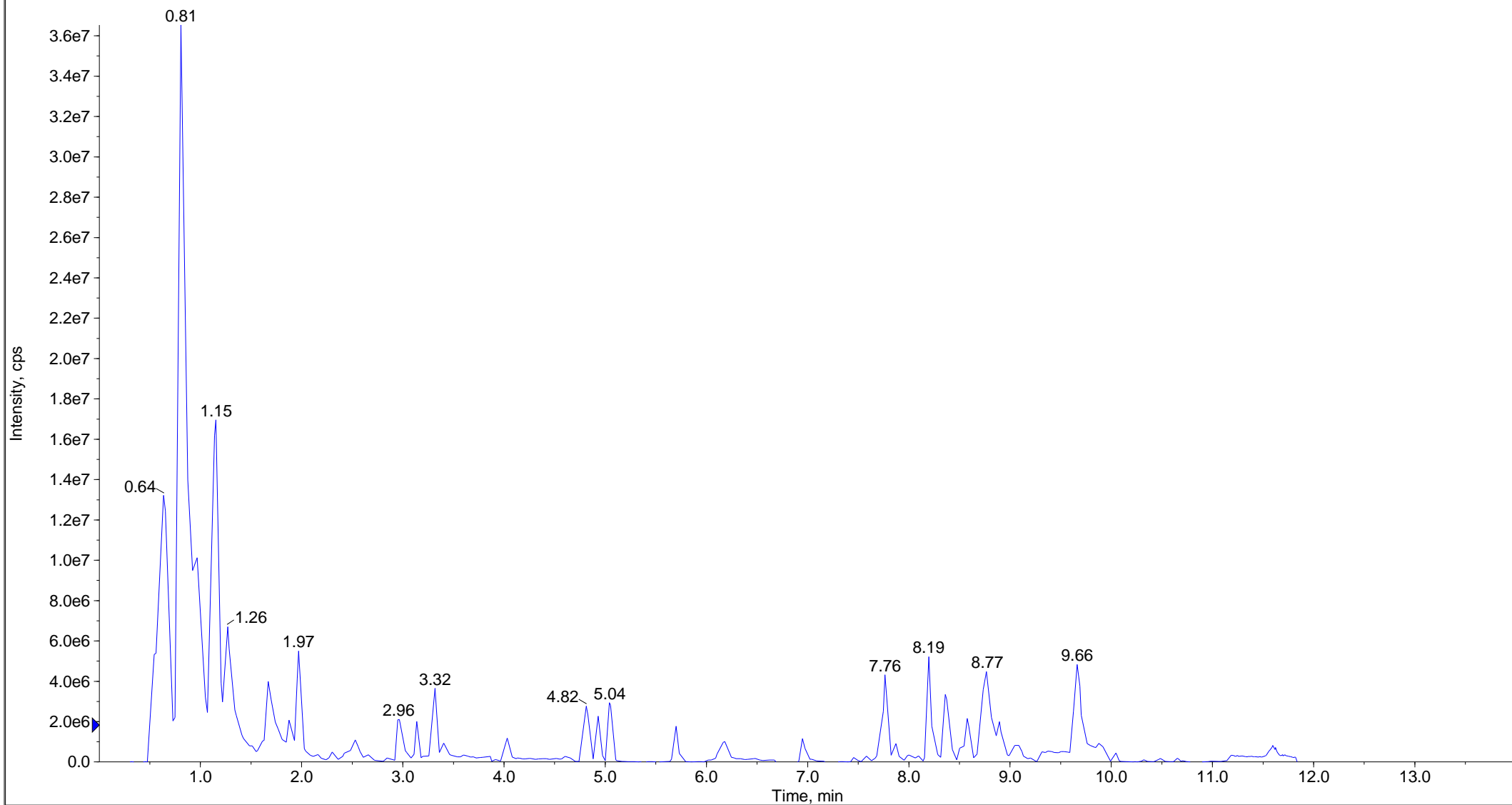
■ TIC of -MRM (791 pairs): from Sample 57 (A20106296a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 5.0e7 cps.



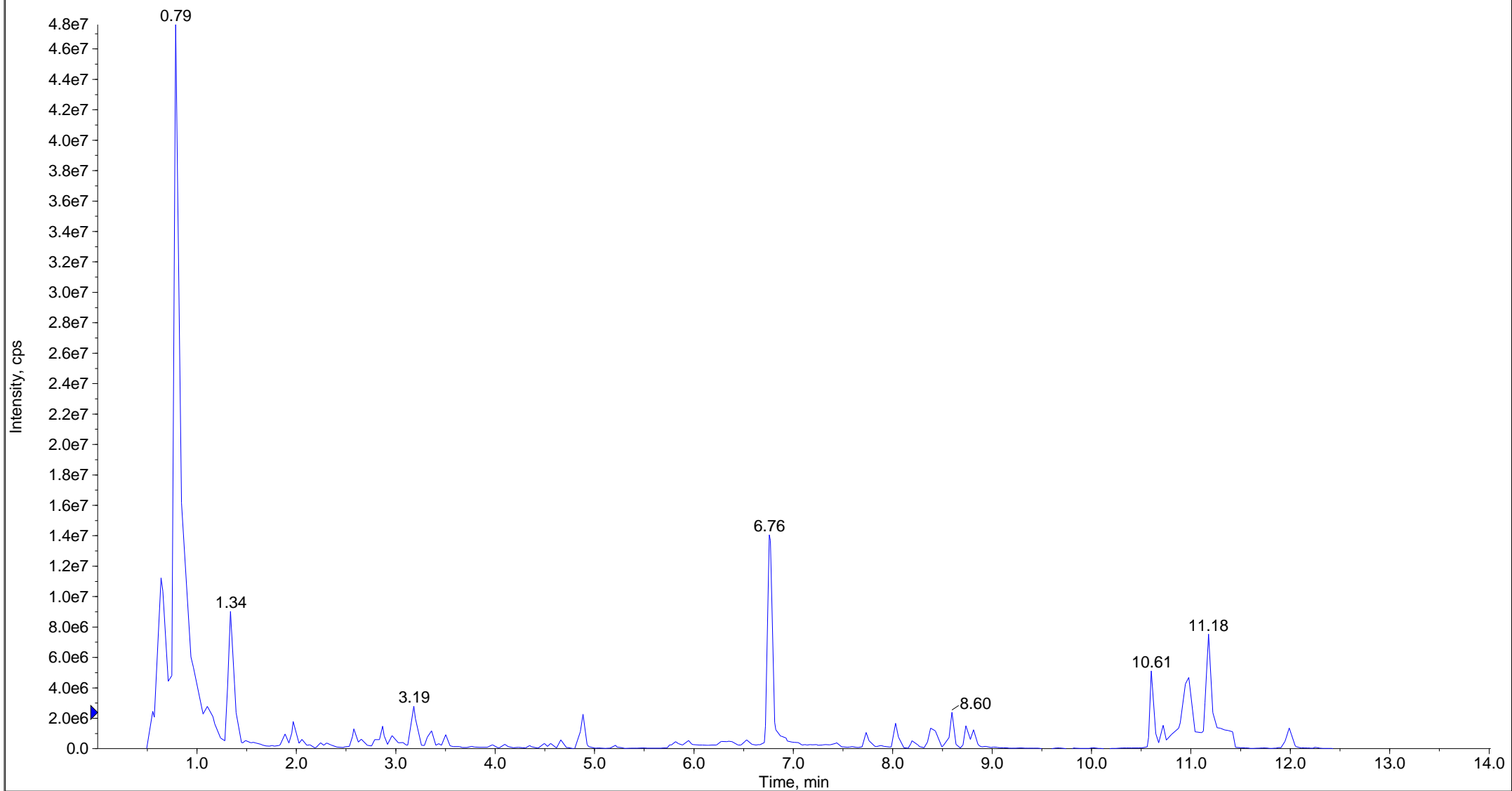
TIC of +MRM (625 pairs): from Sample 27 (A20106296a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.7e7 cps.



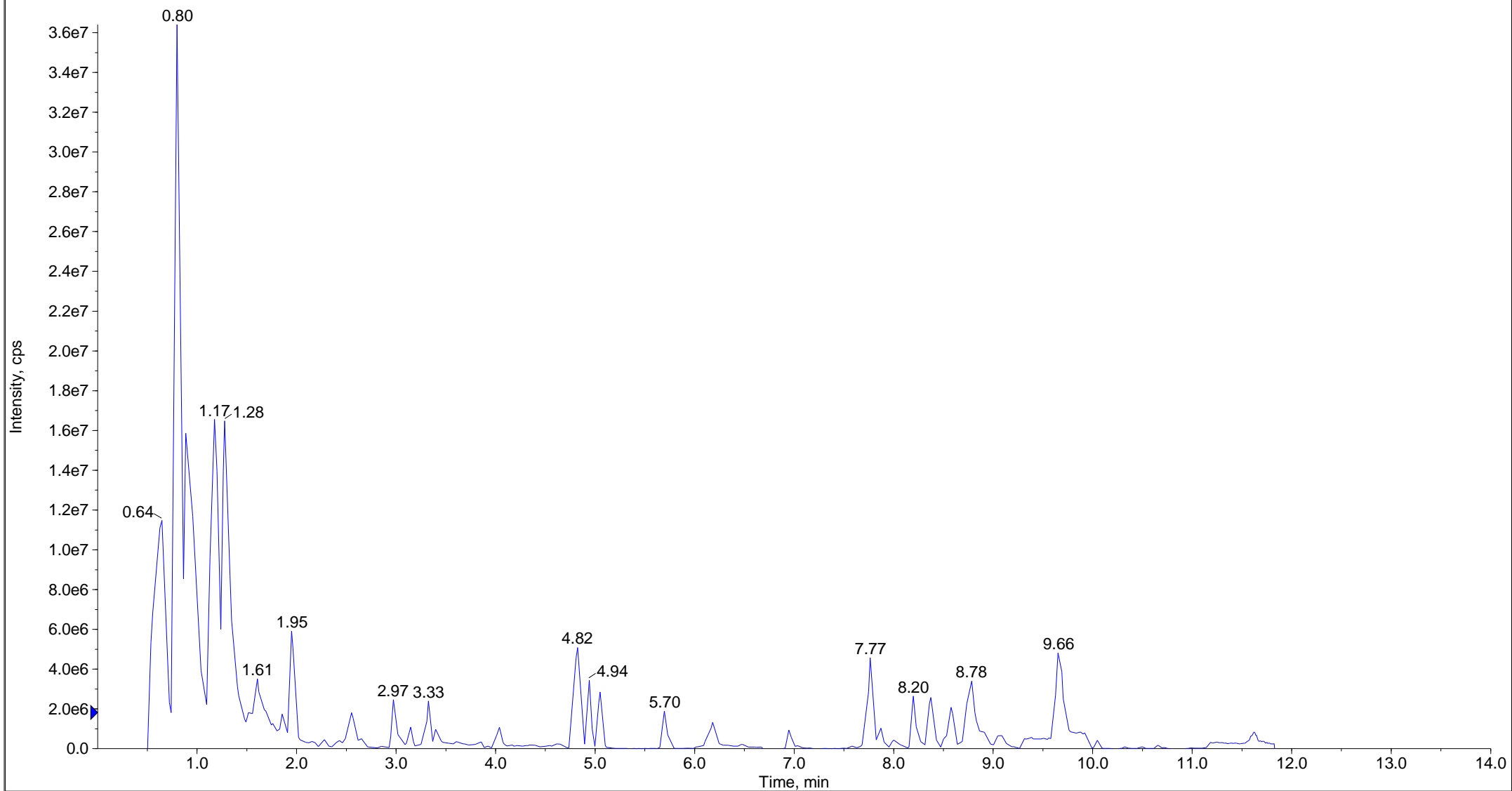
TIC of -MRM (791 pairs): from Sample 58 (A20106297a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 4.8e7 cps.



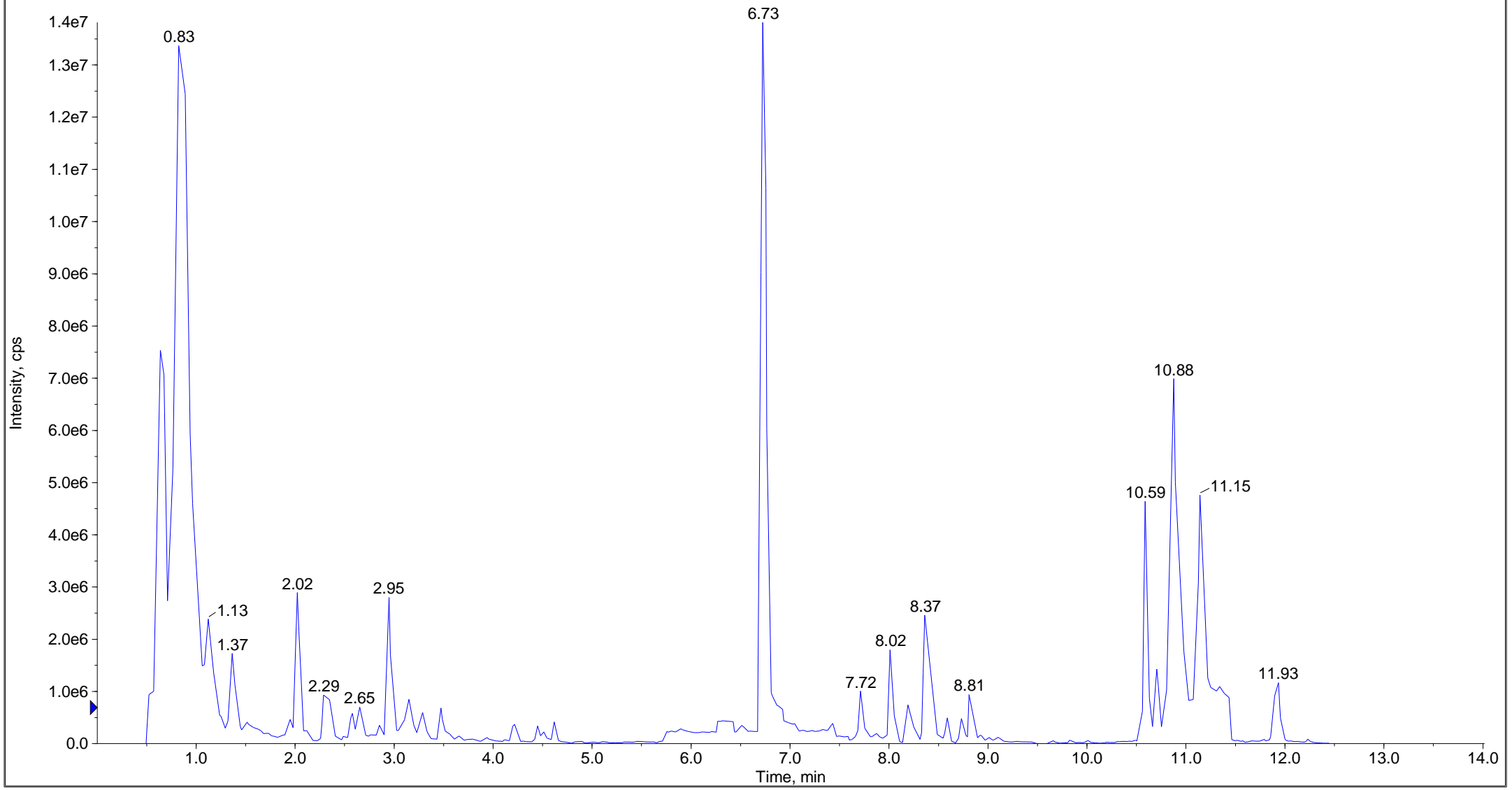
TIC of +MRM (625 pairs): from Sample 28 (A20106297a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 3.6e7 cps.



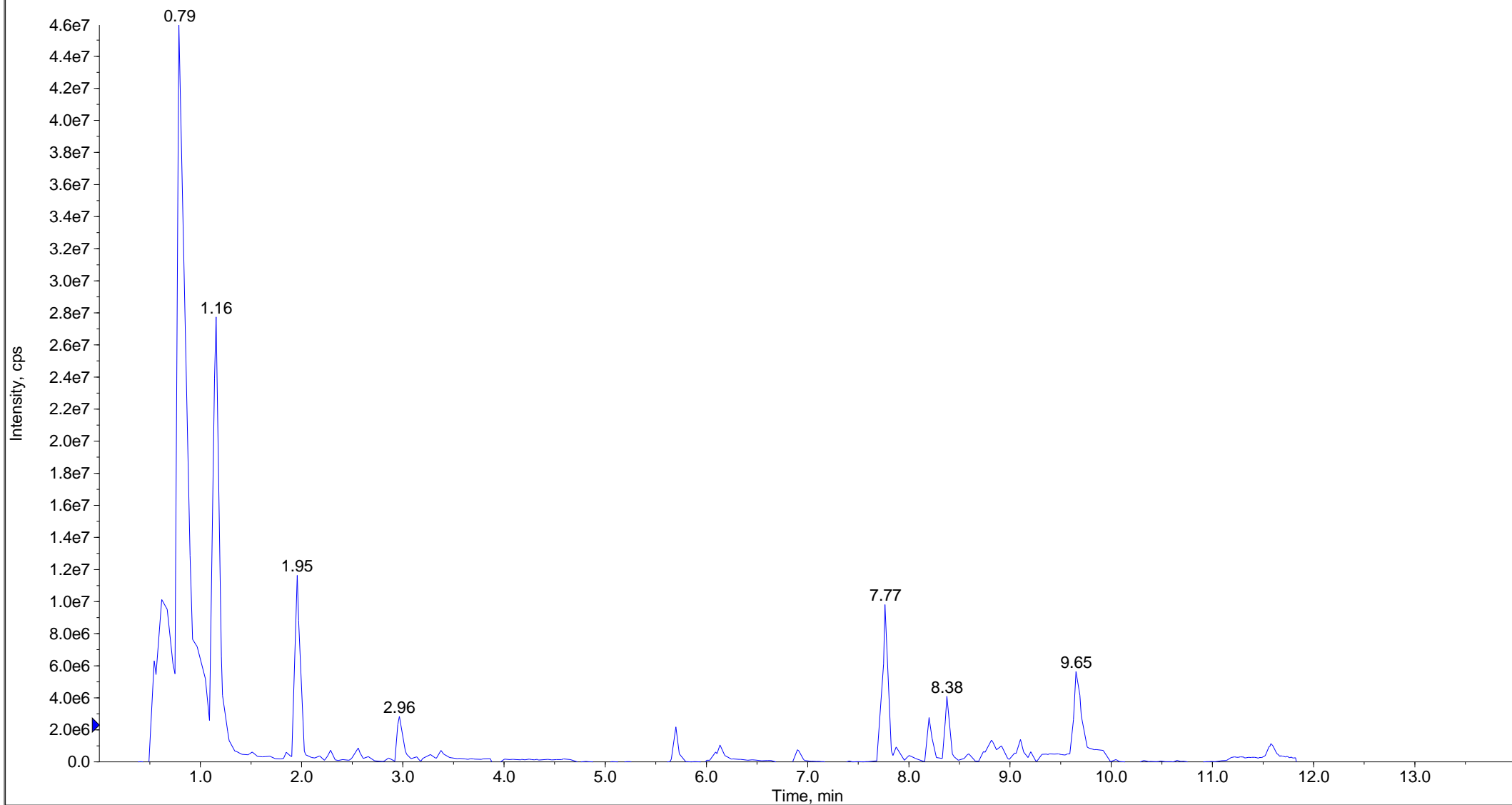
TIC of -MRM (791 pairs): from Sample 33 (A20106274a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.4e7 cps.



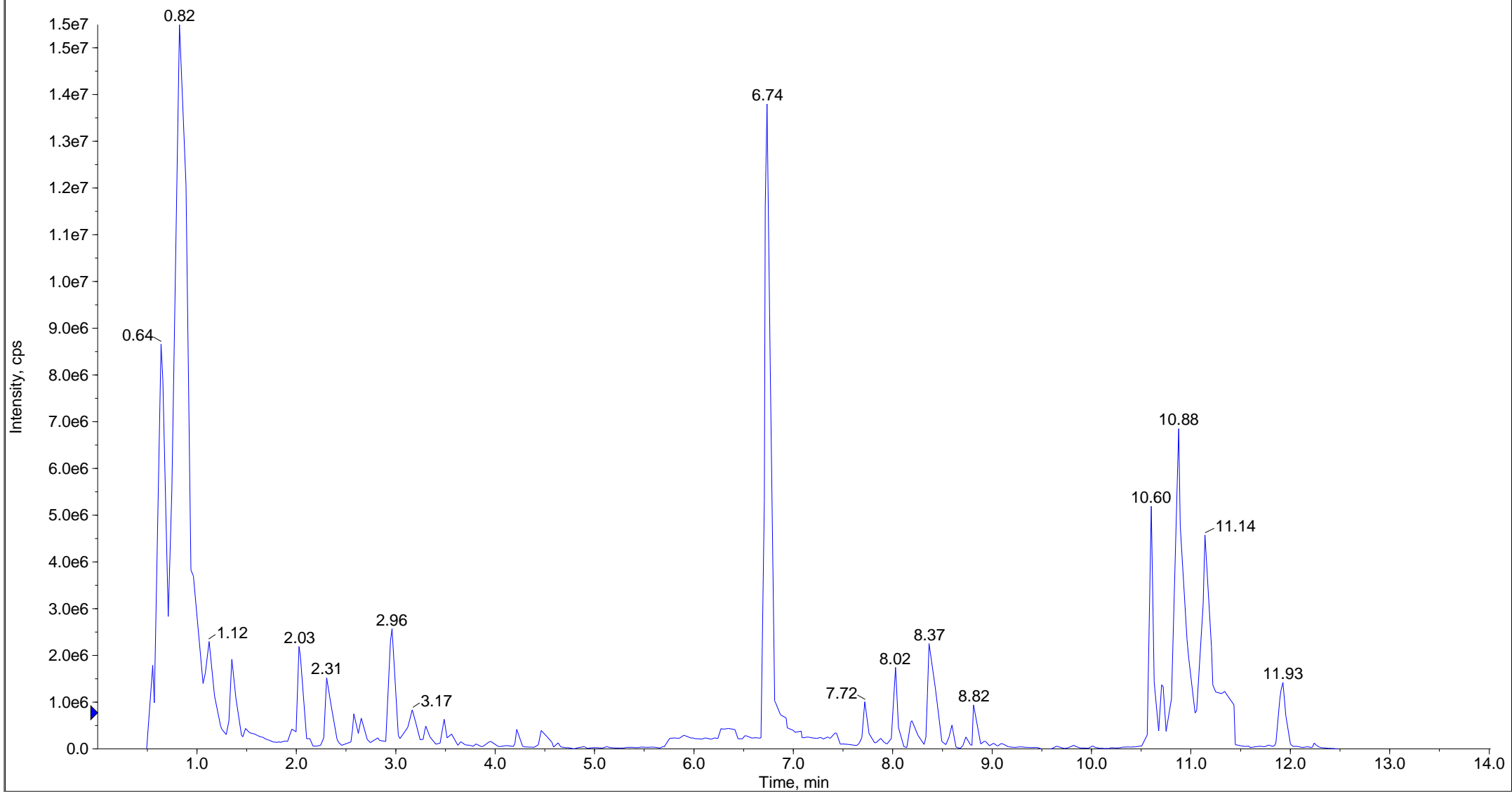
TIC of +MRM (625 pairs): from Sample 3 (A20106274a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 4.6e7 cps.



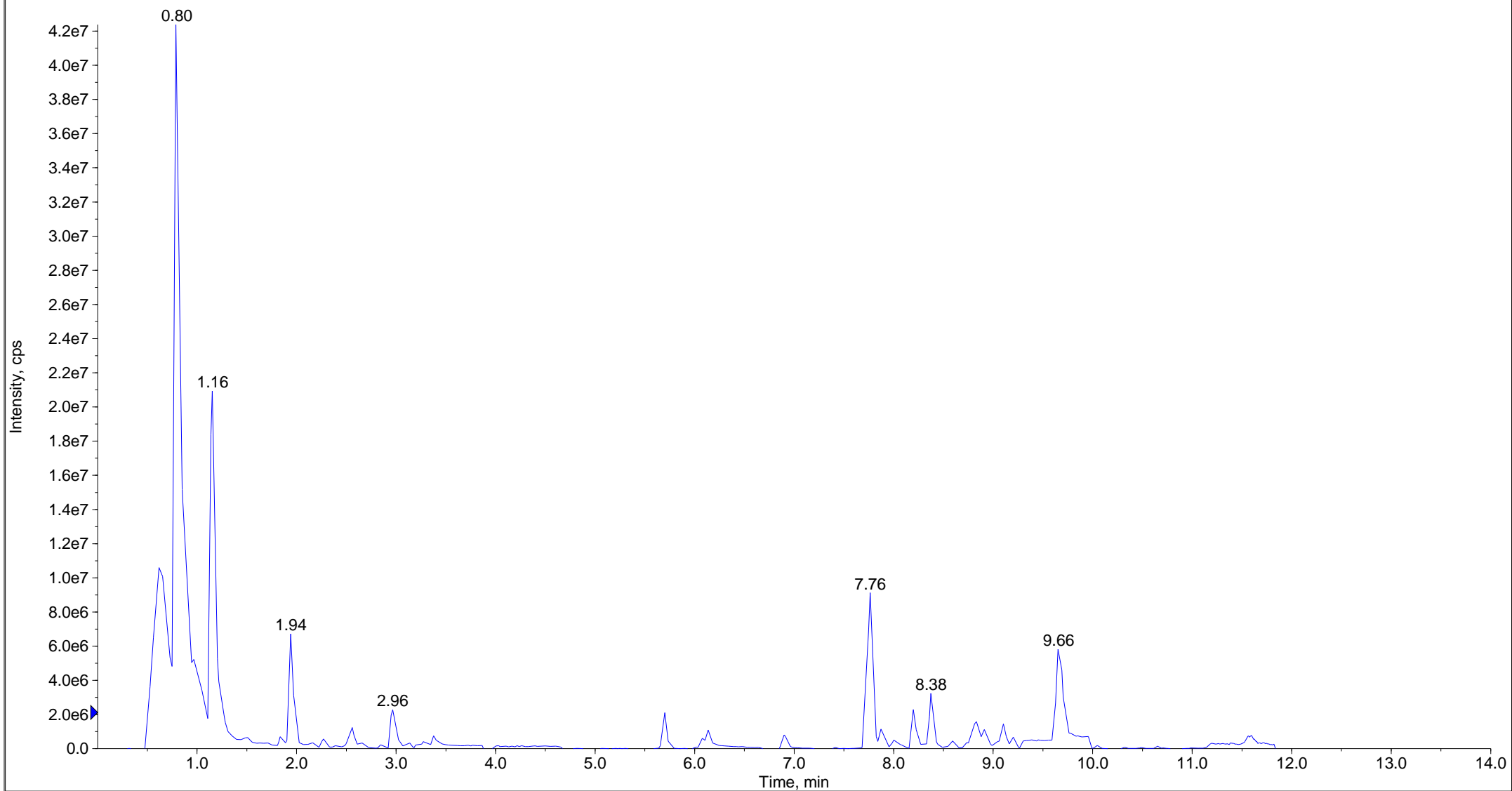
TIC of -MRM (791 pairs): from Sample 34 (A20106275a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.5e7 cps.



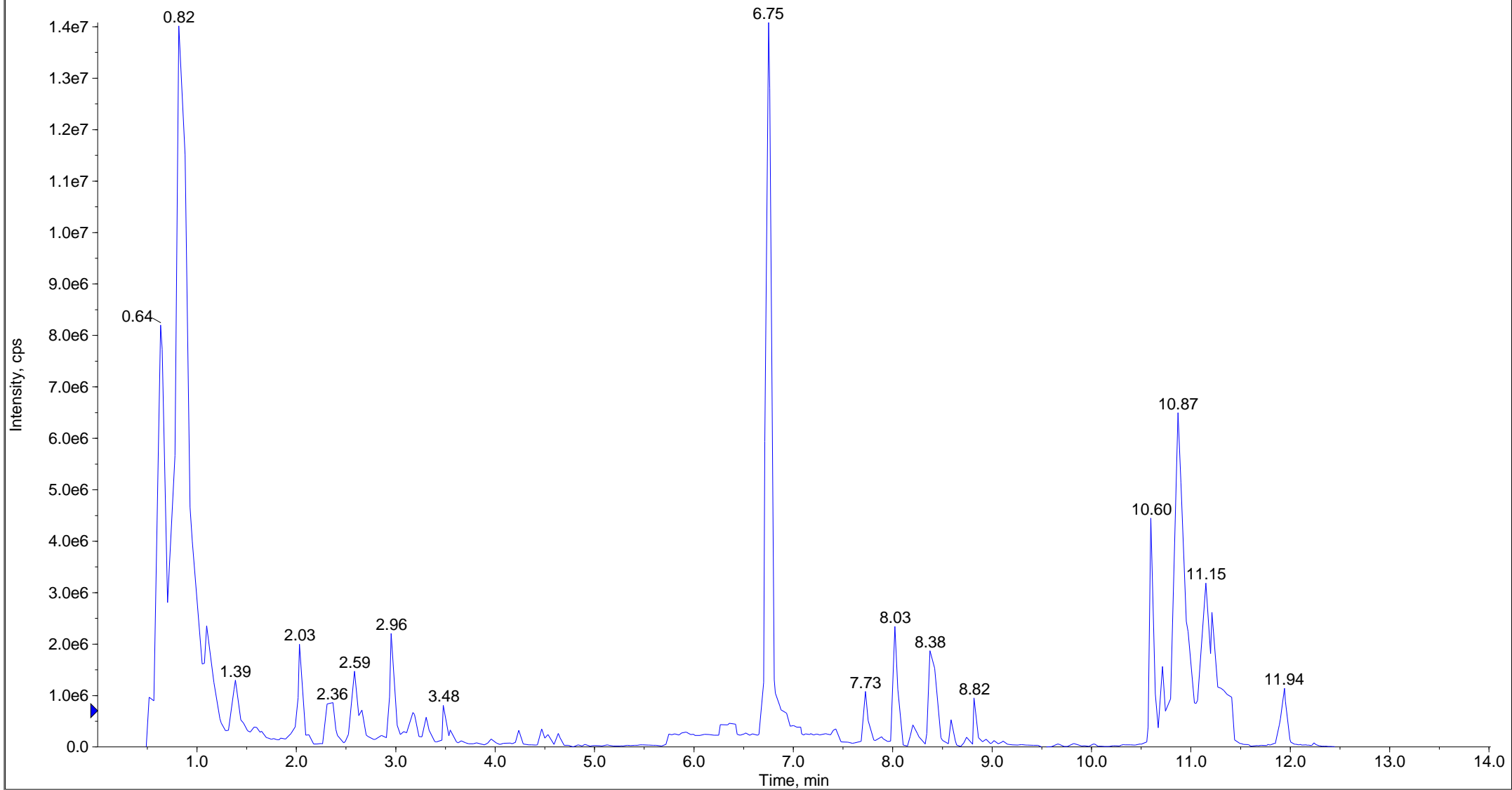
TIC of +MRM (625 pairs): from Sample 4 (A20106275a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 4.2e7 cps.



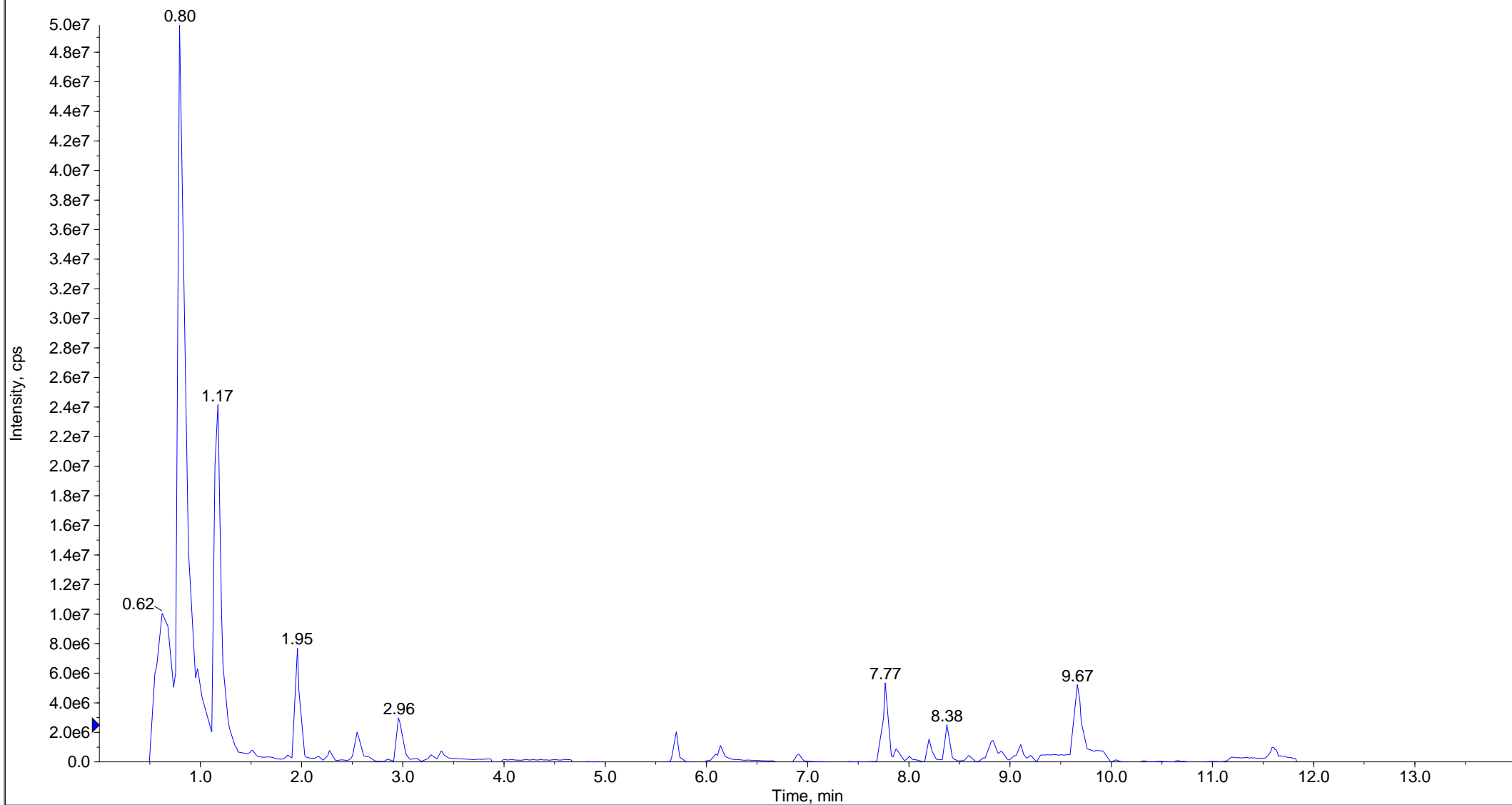
TIC of -MRM (791 pairs): from Sample 35 (A20106276a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.4e7 cps.



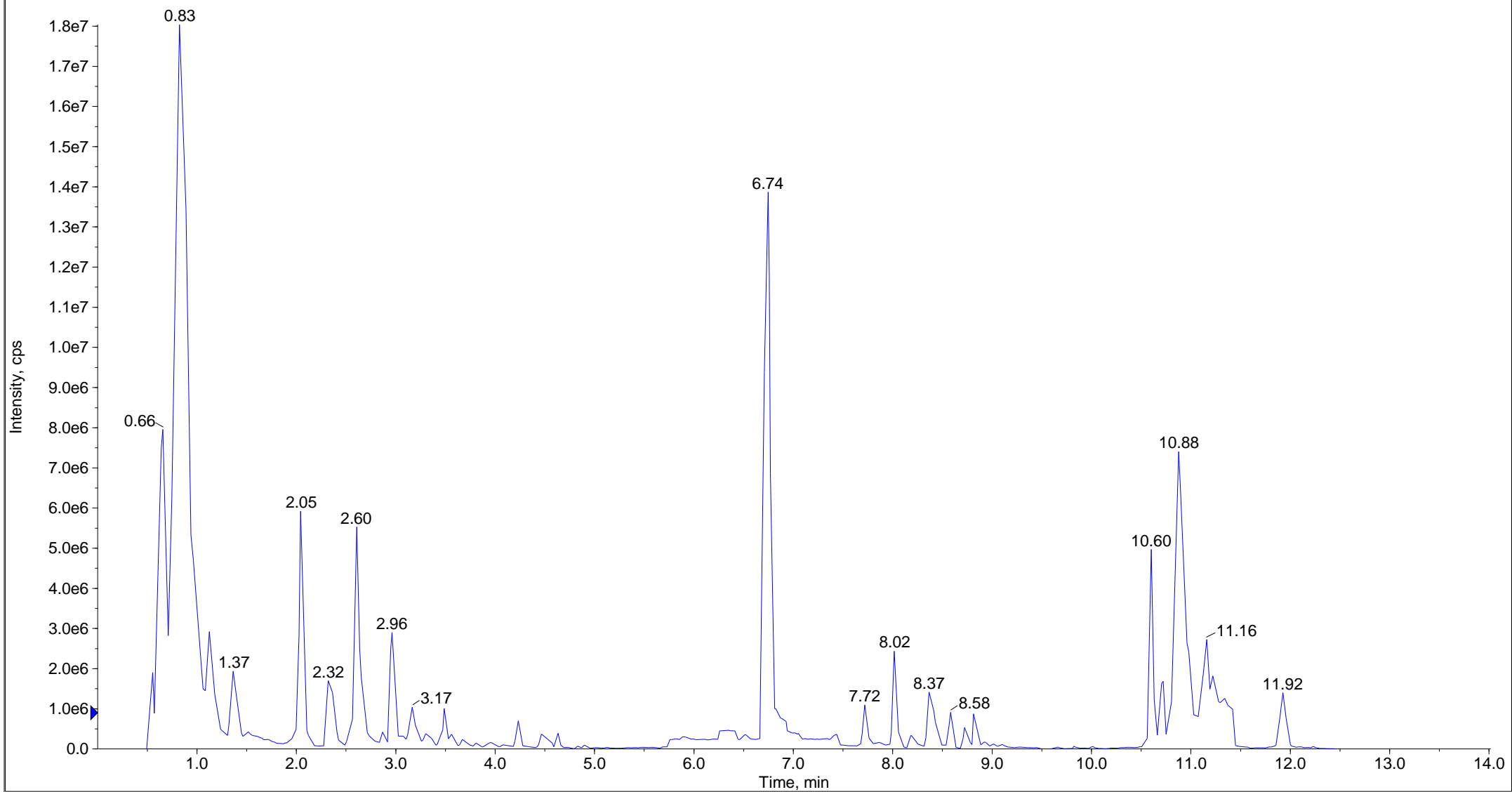
TIC of +MRM (625 pairs): from Sample 5 (A20106276a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 5.0e7 cps.



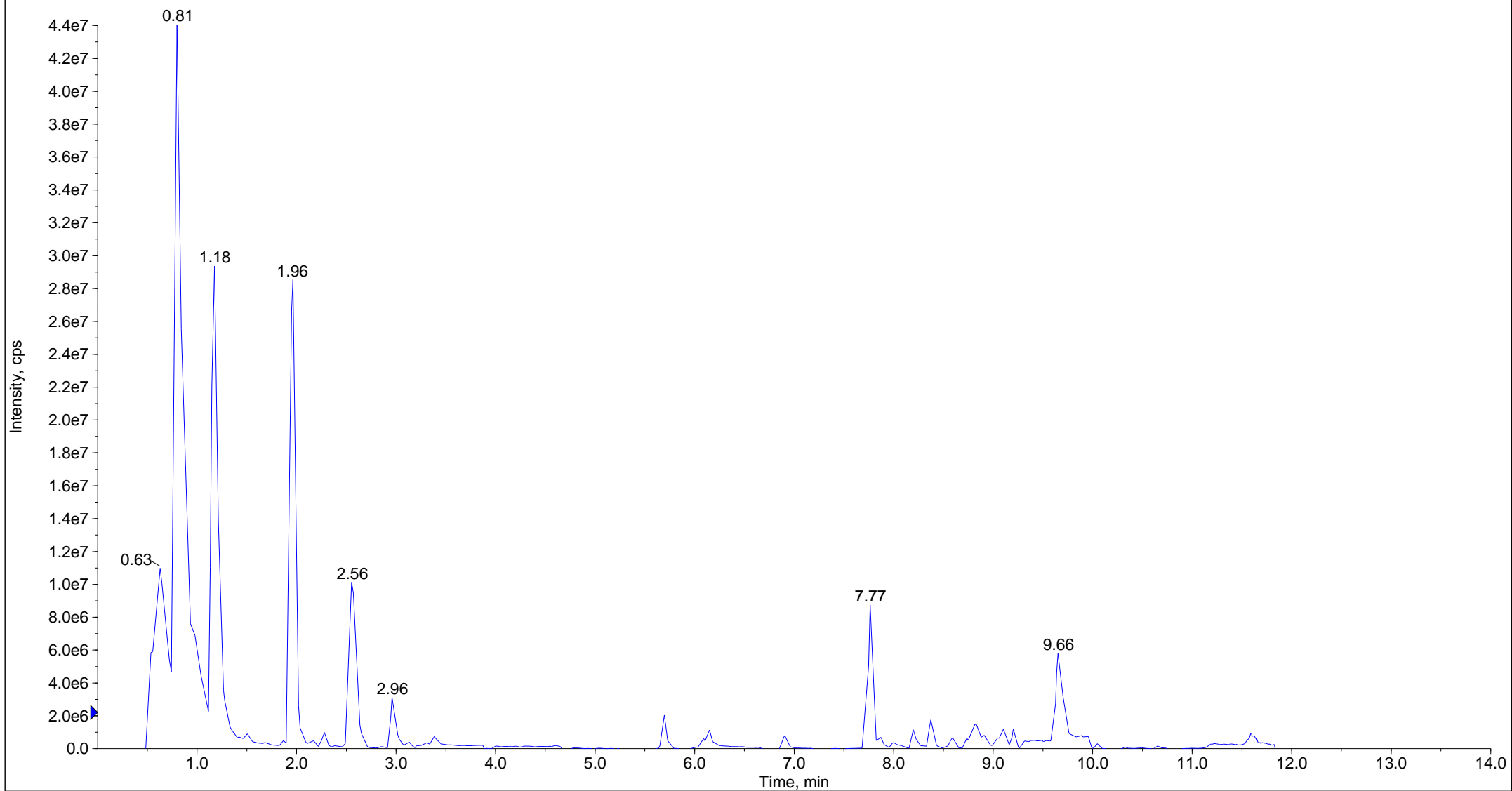
TIC of -MRM (791 pairs): from Sample 36 (A20106277a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.8e7 cps.



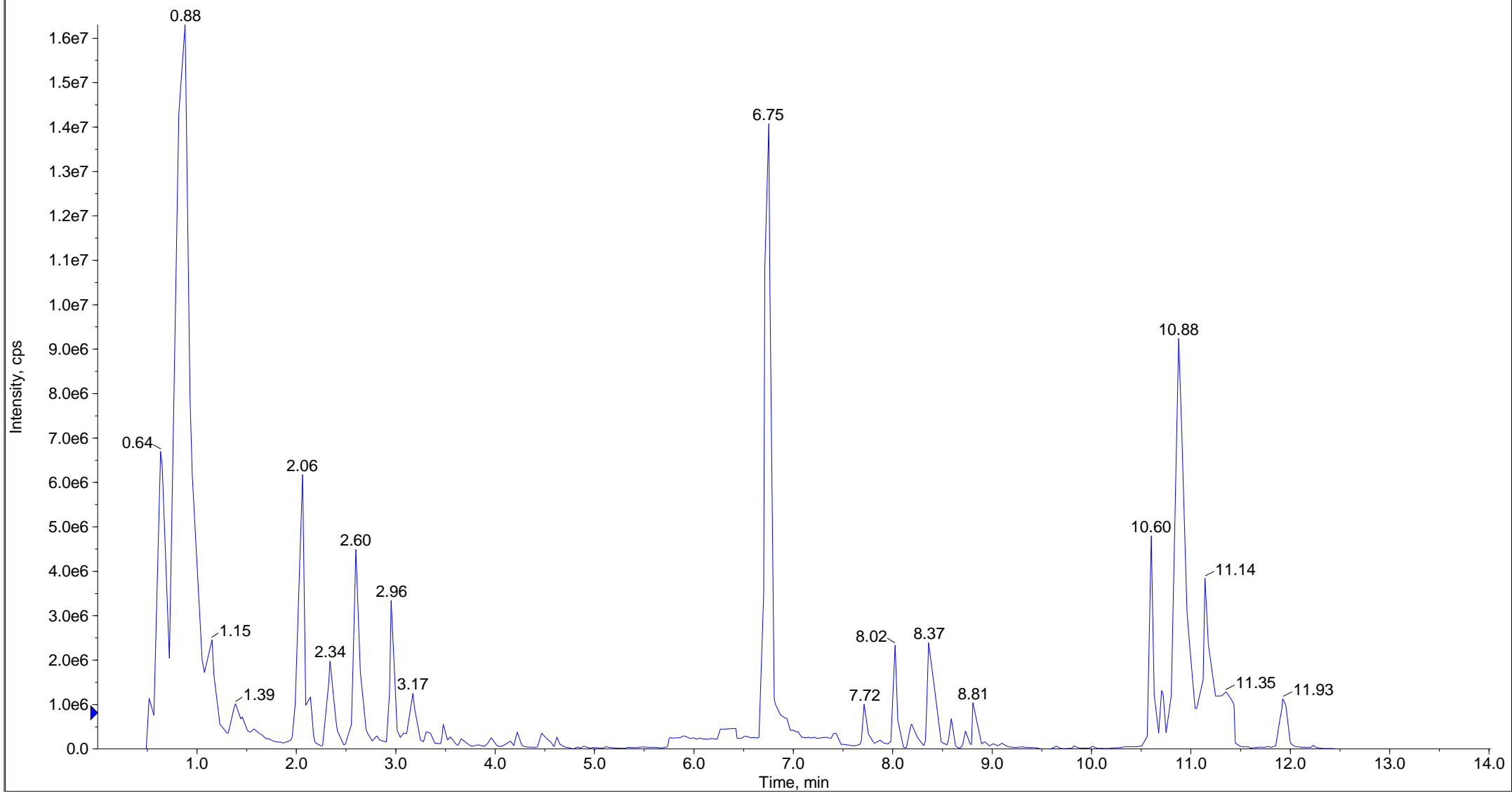
TIC of +MRM (625 pairs): from Sample 6 (A20106277a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 4.4e7 cps.



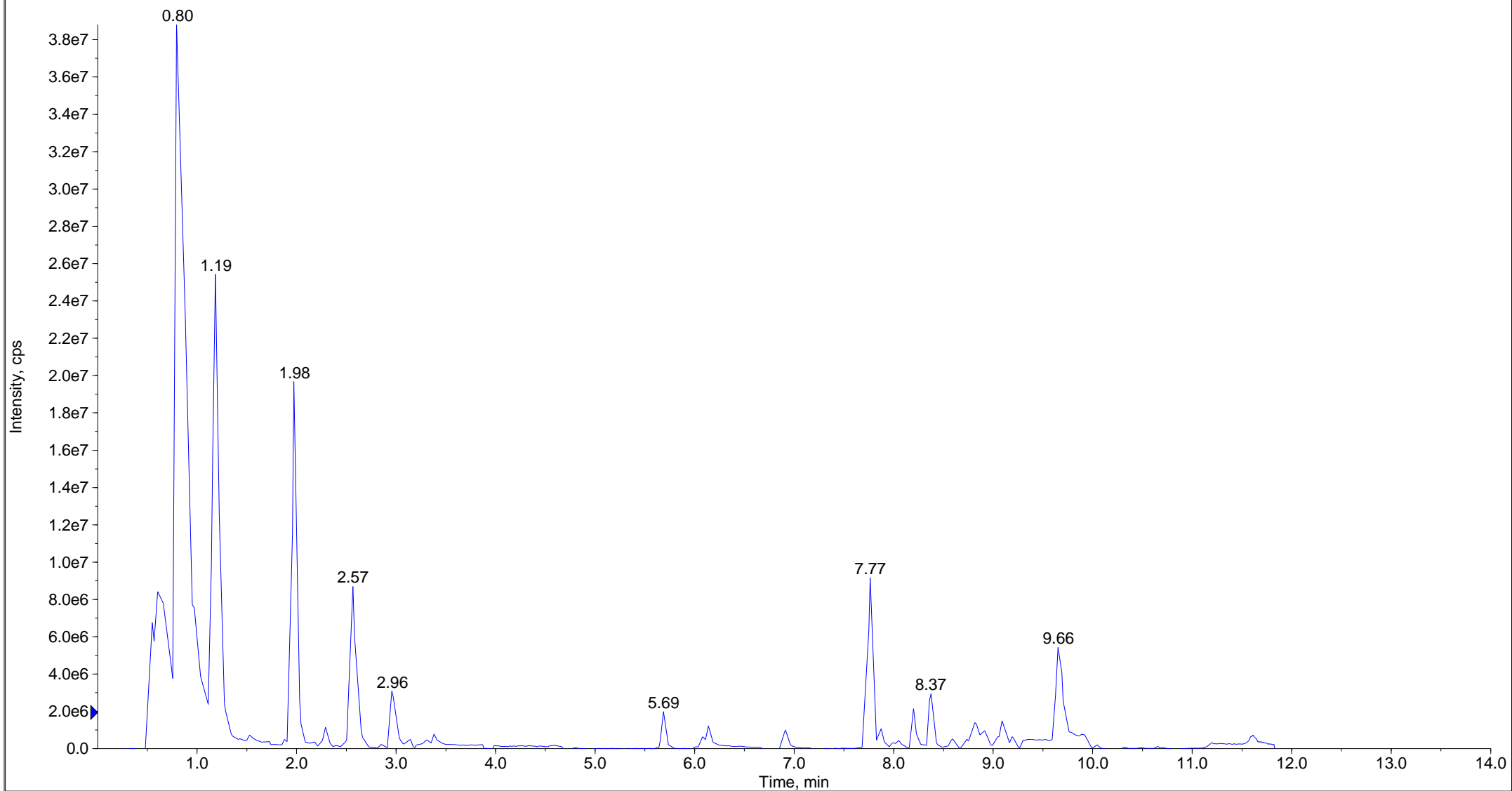
TIC of -MRM (791 pairs): from Sample 37 (A20106278a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.6e7 cps.



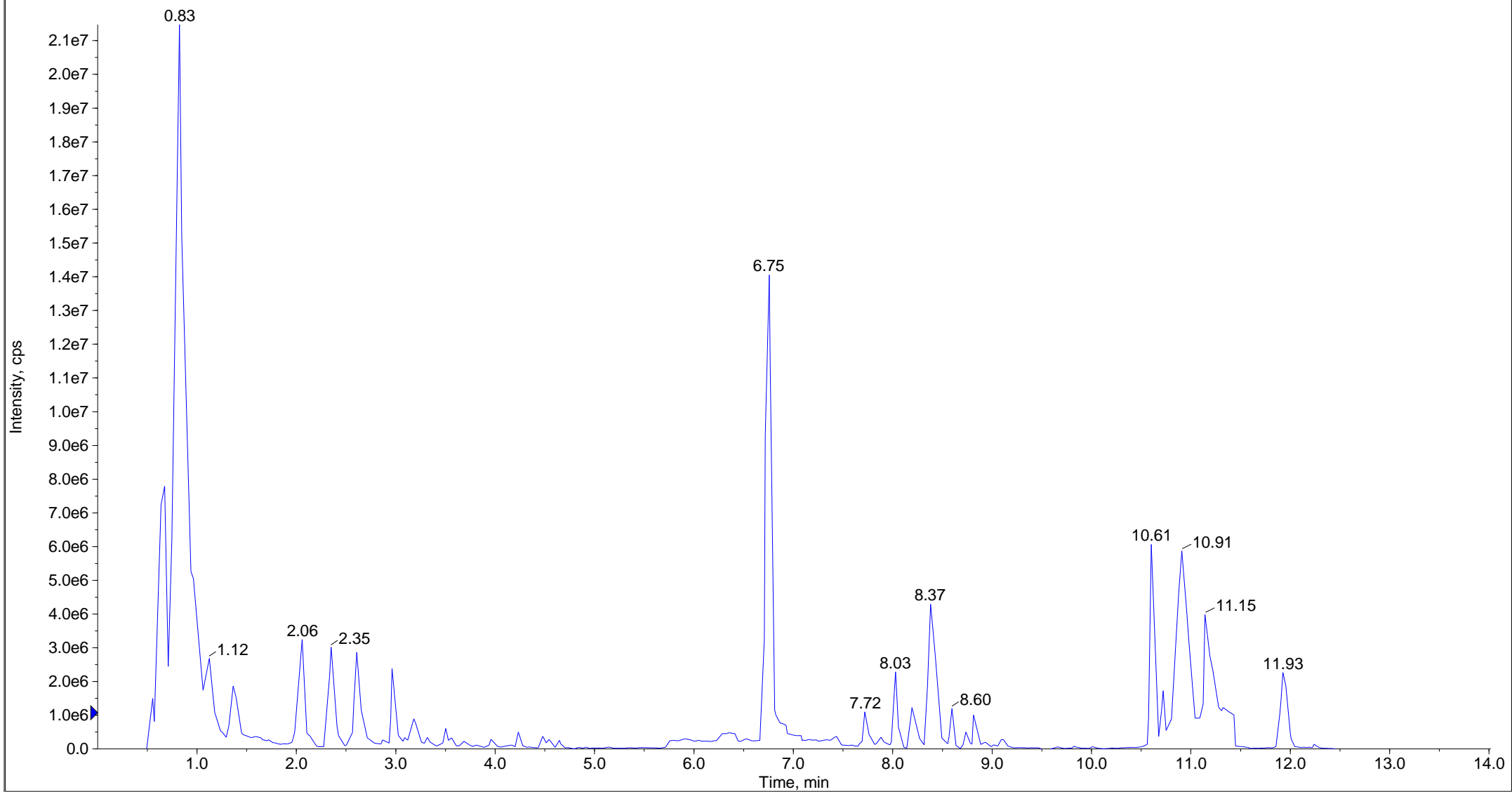
TIC of +MRM (625 pairs): from Sample 7 (A20106278a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 3.9e7 cps.



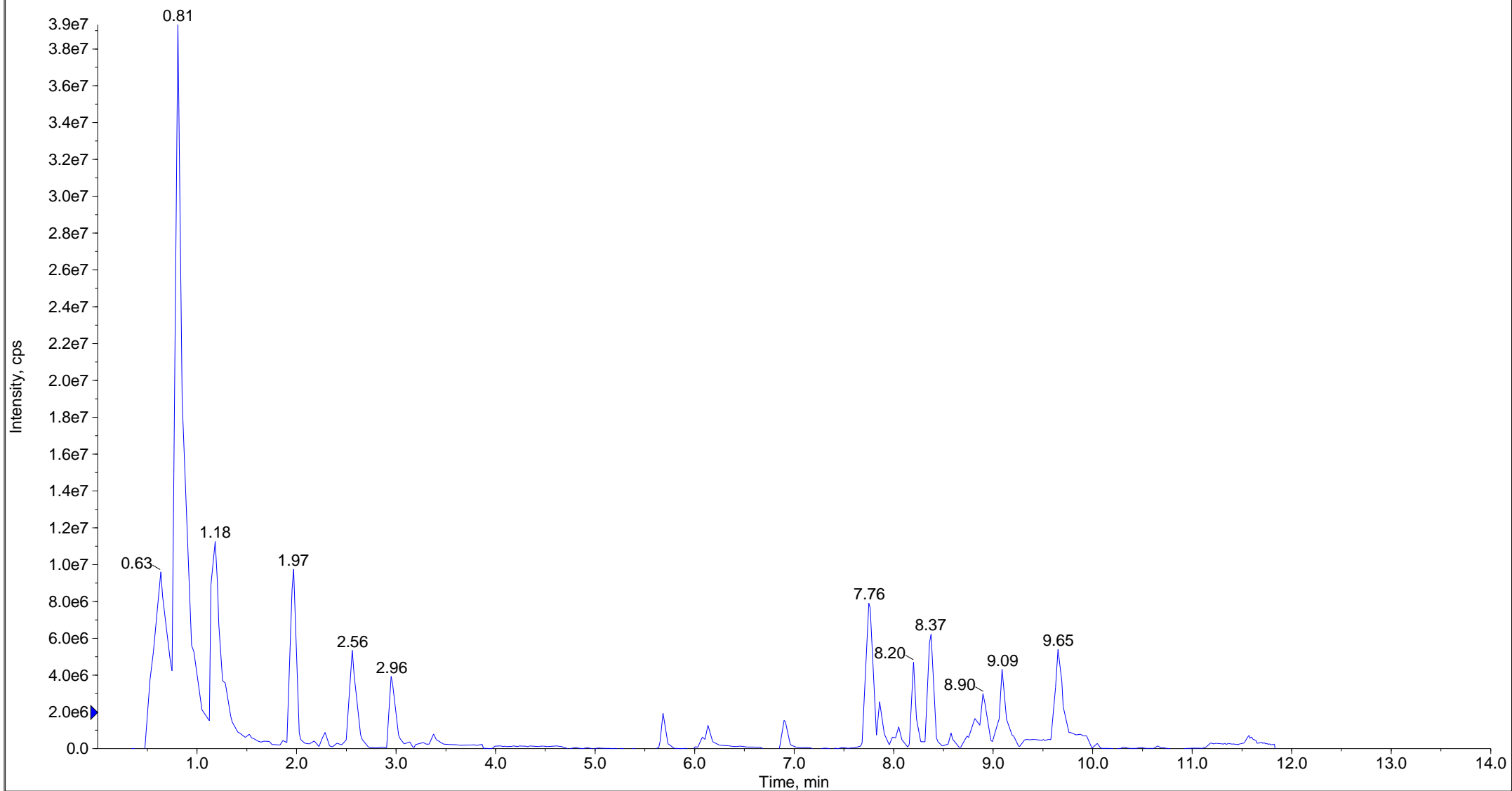
TIC of -MRM (791 pairs): from Sample 38 (A20106279a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 2.1e7 cps.



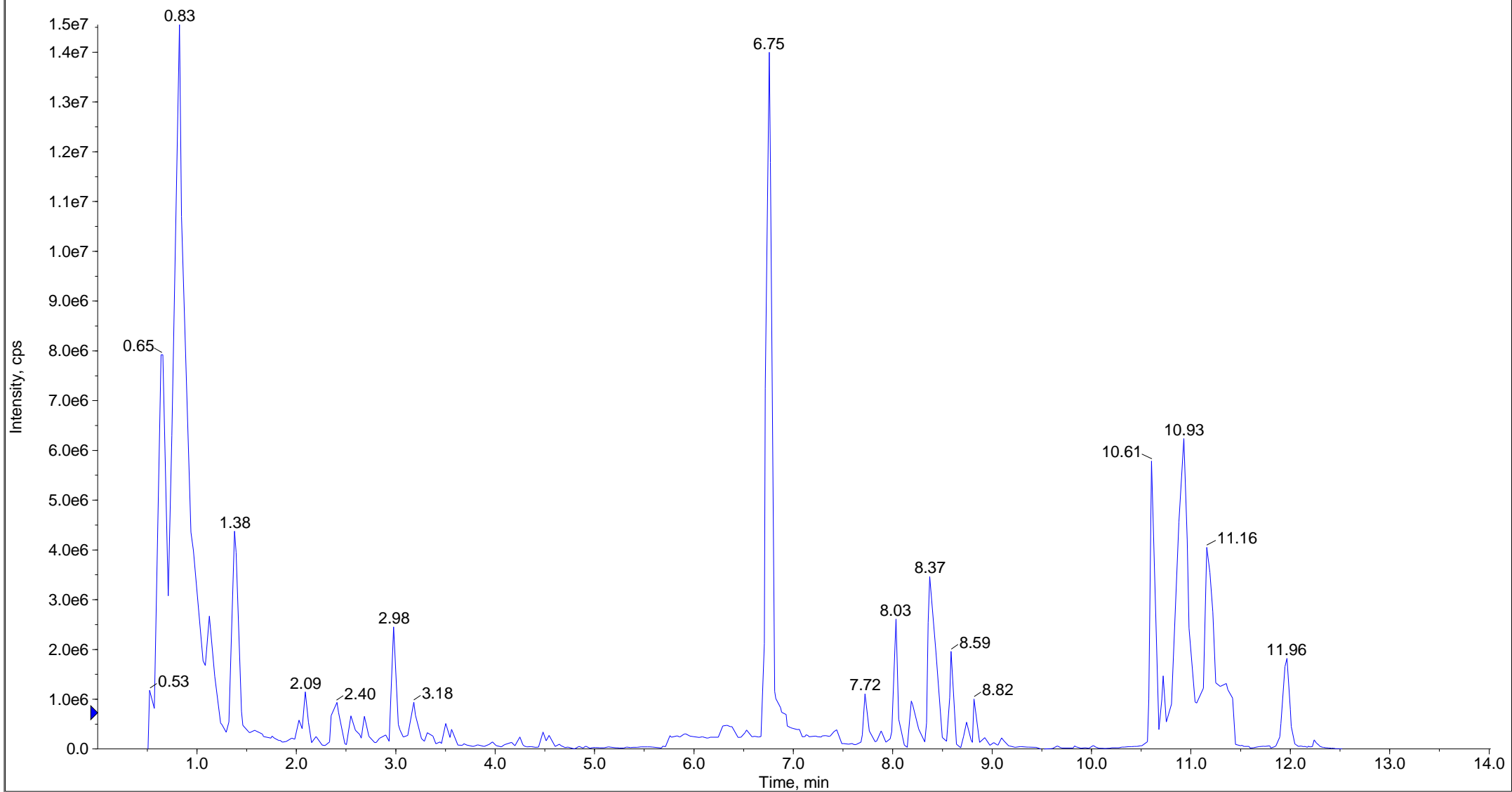
■ TIC of +MRM (625 pairs): from Sample 8 (A20106279a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 3.9e7 cps.



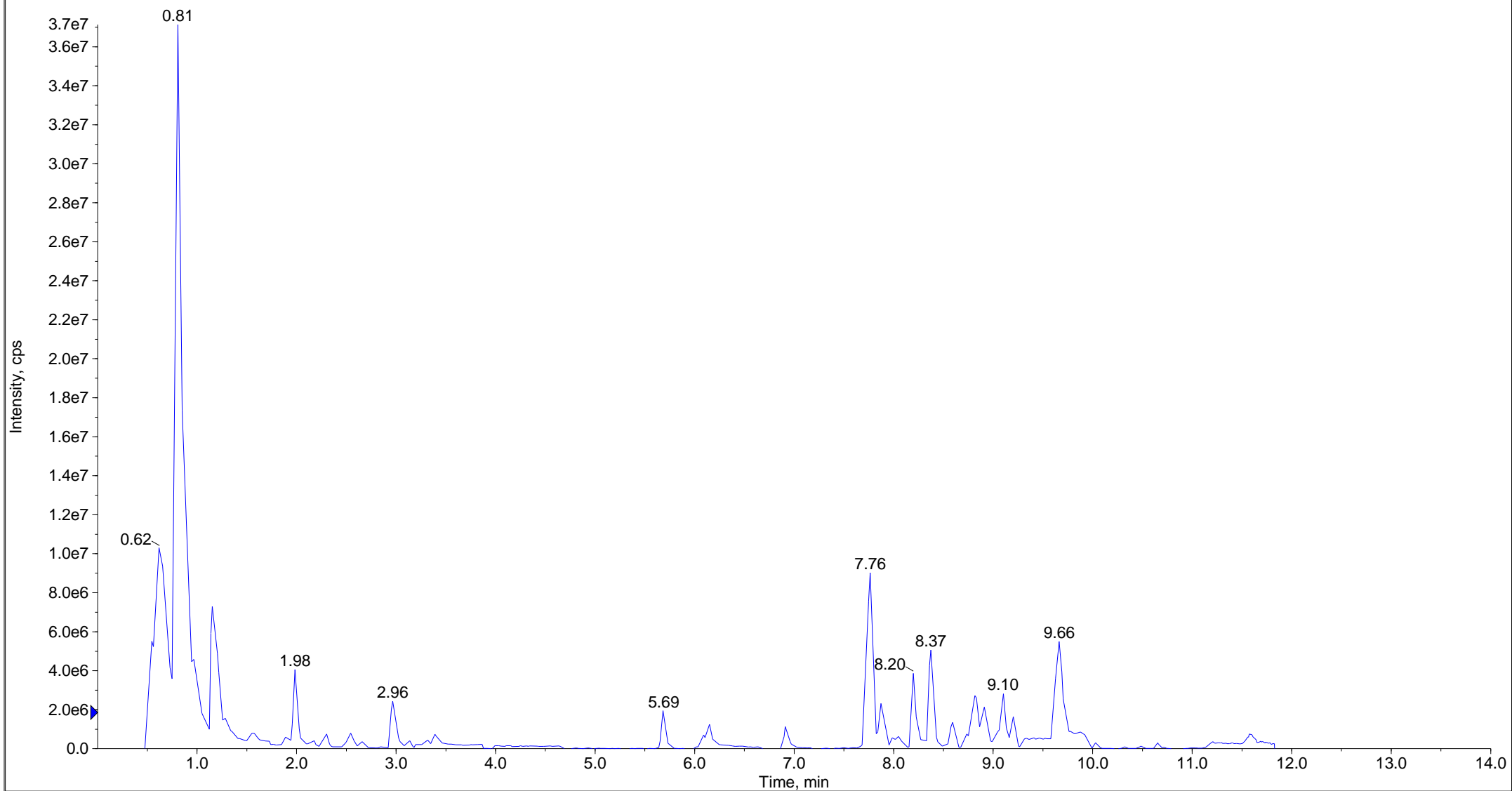
TIC of -MRM (791 pairs): from Sample 39 (A20106280a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.5e7 cps.



TIC of +MRM (625 pairs): from Sample 9 (A20106280a_P) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spray...

Max. 3.7e7 cps.



TIC of -MRM (791 pairs): from Sample 40 (A20106281a_N) of MWXS-20-1657D_24_JS4500-2_C02_MWDB4.0_LH_20210121.wiff (Turbo Spra...

Max. 1.5e7 cps.

