

# Using moFF to Extract Peptide Ion Intensities from LC-MS experiments

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## Method Article

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# Abstract

Label free quantification approaches based on MS1 intensities extract directly from the raw file have become really popular due to low cost and the reliability of the result. Quantification softwares like MaxQuant provide accurate MS1 intensities but they need demanding computational steps that also limit their integration in automated pipeline for large number of LC-MS experiments. This protocols shows how to use moFF (modest Feature Finder), a scriptable and operating system independent software to for extracting peak intensities from Thermo raw files using an apex approach and match-between-runs functionality. This protocol shows also the use of the command line and the graphic-user interface version of moFF (<https://github.com/compomics/moff-gui>)

## Introduction

Quantitative mass spectrometry (MS) based proteomics aims to quantify all proteins in a sample<sup>1</sup>. Quantitative approaches fall in two main groups: labelled and label free. In labelled approaches the quantification is based on the labelling of the peptides using an isotopic or isobaric mass tag. Label-free approaches, does not require these additional costs for sample preparation and can be performed on unlimited number of samples. The most accurate label-free quantification methods are based on MS1 signals, extracting peptide intensities by finding the best peak in the three relevant dimensions (m/z, retention time, intensity). The associated workflow consist in the feature detection and the feature alignment<sup>2</sup>. A feature is a triplet composed by the mass-over-charge (m/z), RT and intensity founded in the raw data. In the feature combination step, features that belongs to the same peptides are grouped in cluster where the m/z values correspond to the isotopic masses of a peptides and the RT time interval correspond to the elution profile of the peptides. The intensity of possible peptide (a cluster of features) is the sum of all the peaks in the retention time interval identified. The feature alignment (called "match-between-runs") is intended to match features across runs that lack identified fragment spectra in some of the runs. MaxQuant<sup>3</sup> is the most popular software for protein quantification, it detects features by fitting a Gaussian peak shape to the three relevant dimensions (intensity, RT, and m/z) and then estimates peptide intensity as the volume of this complex 3D feature. Despite the precise intensities computed, MaxQuant suffers of speed penalties when the size of the dataset is increased and of a lack of integration in own pipeline. The increasing size also the complexity of the proteomics data in public repository (ProteomeXchange<sup>4</sup>) and their re-analysis has been shown to be promising for novel discovery<sup>5</sup>. To face this new challenge there is a need of quantification tool fast reliable and cluster friendly that can scale with the increasing size of complex quantitative data sets present in public proteomics repositories. **moFF Overview** moFF (modest Feature Finder) is a simple, fast and operating system independent MS1-based relative quantification algorithm. moFF is based on python and works directly on Thermo raw file and mzML as well. The access to Thermo raw file is based on the unthermo raw file library<sup>6</sup> that allow moFF to work both on Linux and Windows system. The access to mzML files is based on the python library pymzML<sup>7</sup>. moFF consists in two modules : the match-between-run and the apex extraction module. The complete workflow is showed in Figure 1 [See figure in Figures](#)

**section.** As input, moFF needs a list of identified features (e.g. the result of Mascot or X!Tandem) where each feature should be characterized by a minimum set of information. The match-between-runs module (mbr) performs a RT alignment across the runs, in order to match undefined features that are identified in other run. This process increases the number of quantified features across the replicates and reduces the missing values in the MS1 intensity matrix used in further analysis. Both matched and identified features are then processed by the apex module where the apex peaks are extracted directly from their XiC retrieved from the raw files (see Figure 2). **See figure in Figures section.** moFF provides two quality measures of the peak extracted: - Shape of the peak (\*\*log<sub>L</sub>R\*\*): if the peak has a symmetrical shape the value will be around 0, otherwise for left or right skewed shape the value is respectively greater or less than 0 - Signal-to-noise (\*\*SNR\*\*): this measure how the apex intensity is higher with respect to the level of the noise presence in the XiC extracted. The parameters of moFF are the following: - The size of XiC windows retrieved for each feature. - The retention time (RT) window used to search the apex. - The precursor mass tolerance The match-between-run has also other parameters: - The retention time (RT) windows used to search the apex intensity for the matched peak - Outlier filter and its width value. This filter works on the training set used to train the RT predicted models - Weighted or an unweighted combination of the predicted retention time model when a feature is matched in several runs.

## Equipment

**Computer** - Operating system: Windows or Linux - Python 2.7 installed and also Java 1.7 for moFF-GUI - Download "moFF-GUI": <https://github.com/compomics/moff-gui> or "moFF": <https://github.com/compomics/moFF> **Input data** - Raw file: Thermo raw file of mzML file - Identified features listed in a tab delimited file. The minimum information required for each feature are: **\_peptide\_:** sequence of the peptide **\_prot\_:** protein ID **\_rt\_:** feature retention time (The retention time must be specified in second) **\_mz\_:** mass over charge **\_mass\_:** mass of the feature **\_charge\_:** charge of the ionized feature - PeptideShaker cps files along with the sequence database (FASTA) and spectra (MGF) used in SearchGui (only for moFF-GUI)

## Procedure

**moFF from the command line with identified features in tab-delimited file as input** 1. Put your input identified features files in **\_input\_**. Put your raw file in another folder a called **\_rawFolder\_**. 2. Run moFF (match-between-runs and apex) using the following command: **python moff\_all.py -inputF input/ -raw\_repo rawFolder/ -output\_folder my\_output** To set all the parameters and options of moFF, please read the full list in the **"documentation"**: <https://github.com/compomics/moFF/blob/master/README.md#entire-workflow> 3. Collect all the results in the output folder **moFF-GUI with PeptideShaker result as input** 1. Run moFF-GUI and set the folder where PeptideShaker is installed and the output folder where all the results are collected. Click **\_proceed\_** to continue 2. Choose which module to run. 'Apex' is just the apex MS1 extraction, and 'matching-between-run' for the match-between-runs module plus the apex module. Click

\_proceed\_ to continue \(\Figure 3). [See figure in Figures section](#). 3. Insert the Thermo RawFile or mzML files. For each raw file you have to associate also the relative cpsx file. Moreover, you can also insert the fasta and the mgf files used in PeptideShaker/SearchGui. Click \_proceed\_ to continue \(\Figure 4). [See figure in Figures section](#). 4. Setting of the moFF parameters \(\Figure 5): - XiC retention window - Peak retention time windows - Precursor mass tolerance - Match-between-run parameters\_: -Peak retention time windows for matched peak - Weighting/unweighting and the activation of outlier filtering and its width value - Selection of a set of specific peptides \(\loaded as tab-delimited file) and use them as training set of the mbr procedure instead of the shared features of the runs. [See figure in Figures section](#). 5 Start the procedure clicking on \_start\_. Collect your result in the output folder

## Timing

The time taken largely depend by the number of input feature and by the length of the XiC extracted \(\XiC retention window).

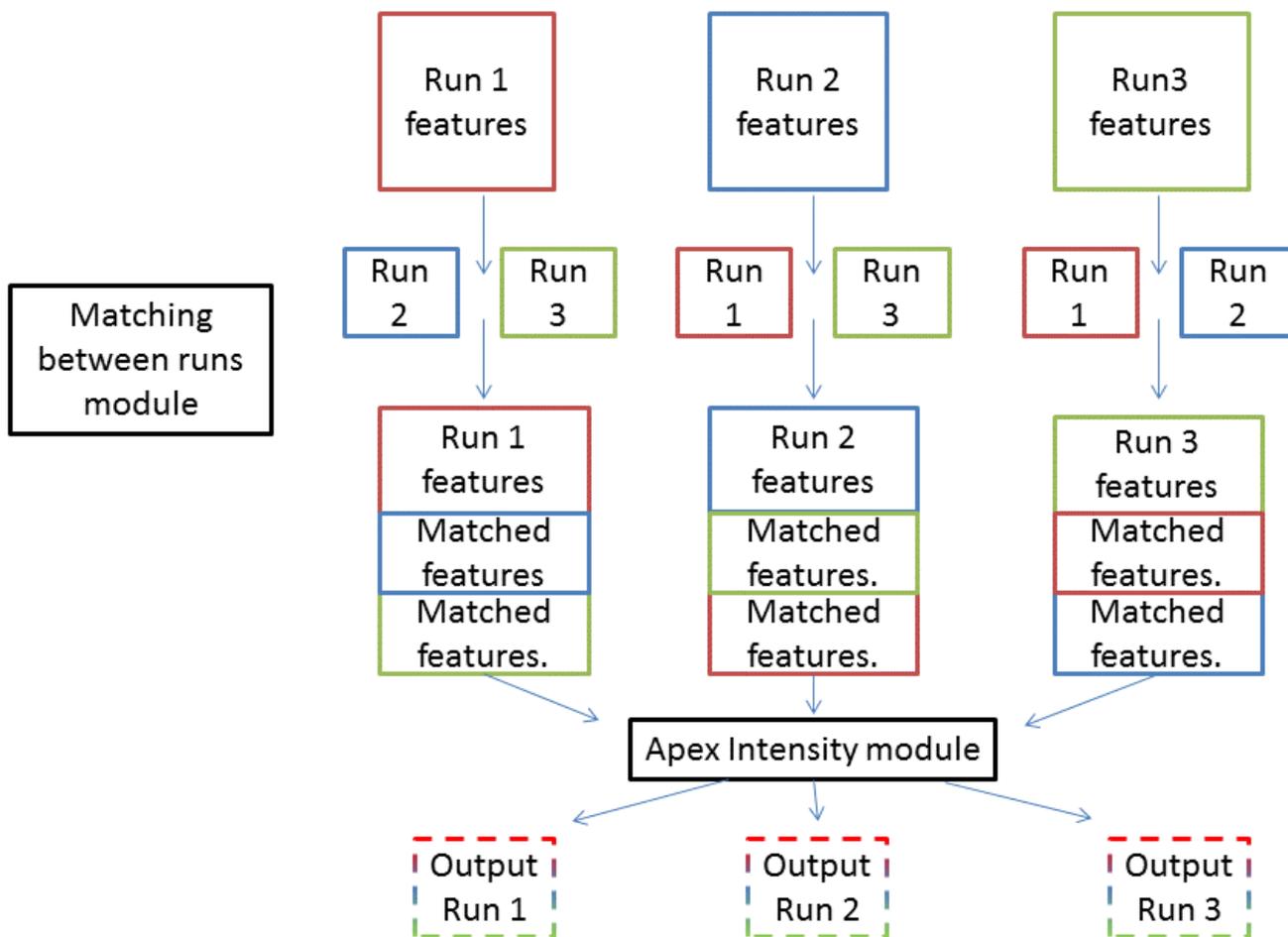
## Anticipated Results

moFF produces for each run/raw file a file with the results and a log file with detailed information about the apex intensity extraction \(\see Figure 6). [See figure in Figures section](#). The output of match-between-run module is the set of the input files enriched with the matched features founded and a separated log file that contains all the detail of procedure.

## References

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## Figures



**Figure 1**

Figure 1 moFF workflow overview. The optional match-between-runs module takes as input a list of features of interest for a given run, and then matches the corresponding features in other runs. Upon matching, all peptides (either identified directly, or indirectly by matching between runs) are processed by the Apex intensity module to extract feature intensity and associated quality measures. The results are then written to tab-delimited output files.

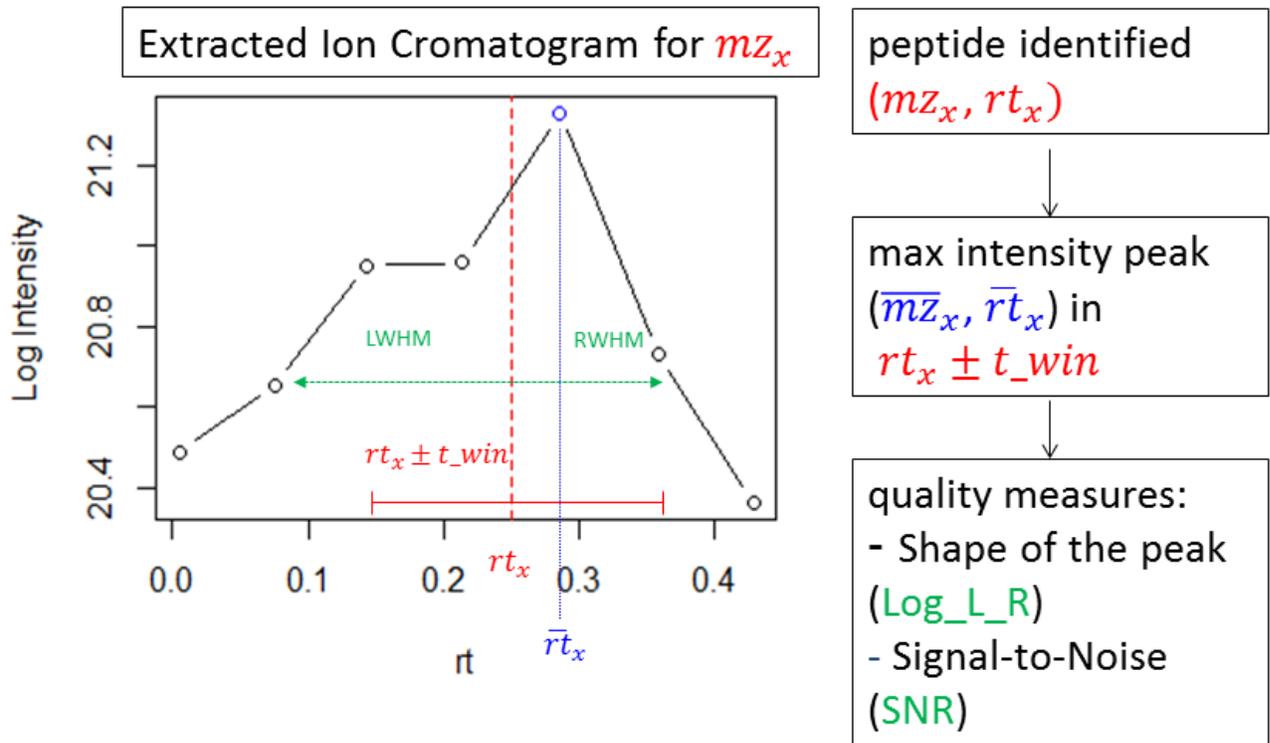


Figure 2

Overview of the apex intensity module Around the RT of the input feature, a time window is constructed which results in a local XIC. The peak apex is then located in this local XIC. The  $log\_L\_R$  metric measures the skewness of the peak around the RT of the obtained apex point. The SNR metric provides the ratio of peak height to noise, where the noise value is set as the lowest intensity value in the local XIC

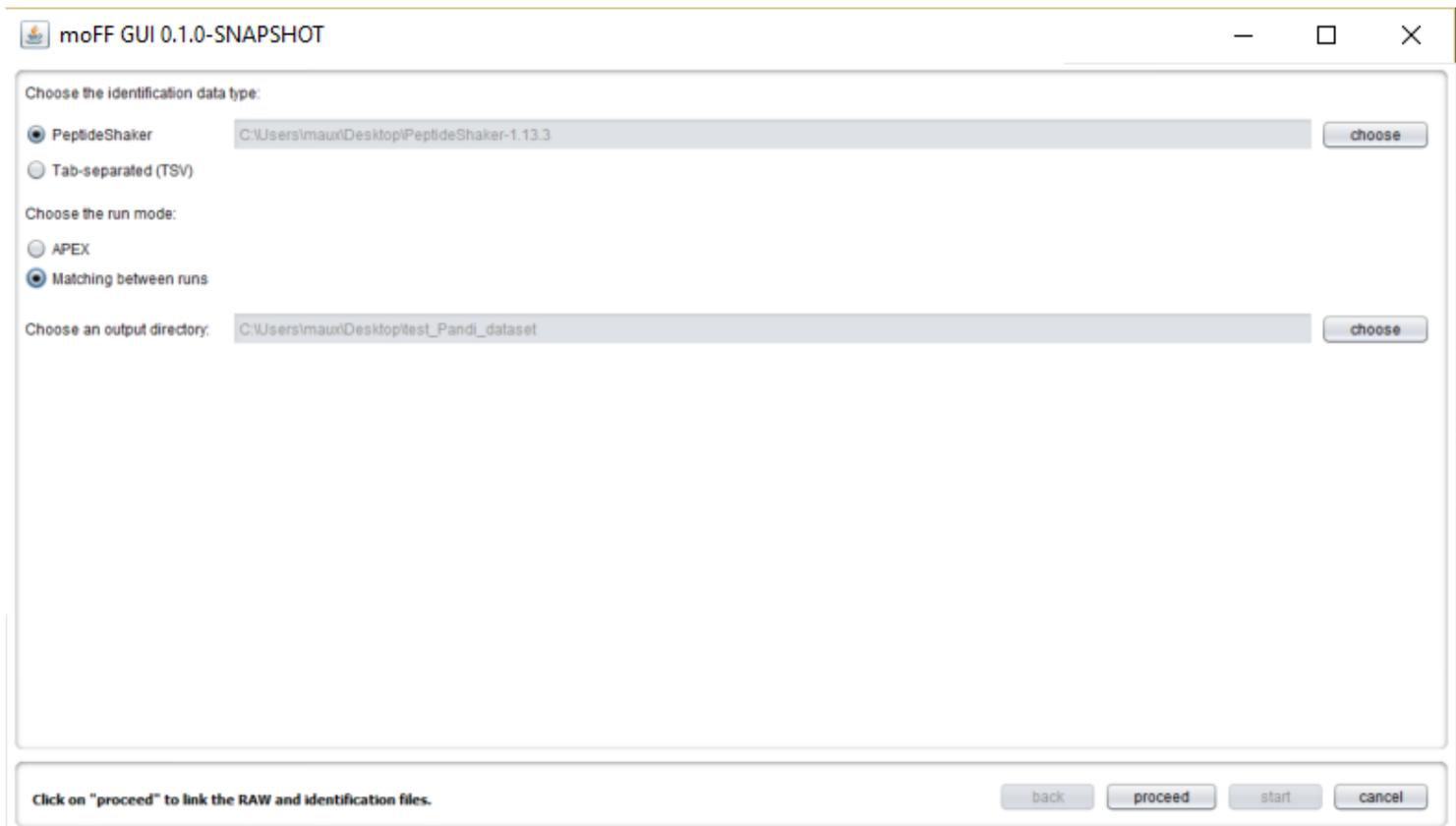


Figure 3

moFF GUI Overview Setting the PeptideShaker folder and the moFF output folder where to collect your results.

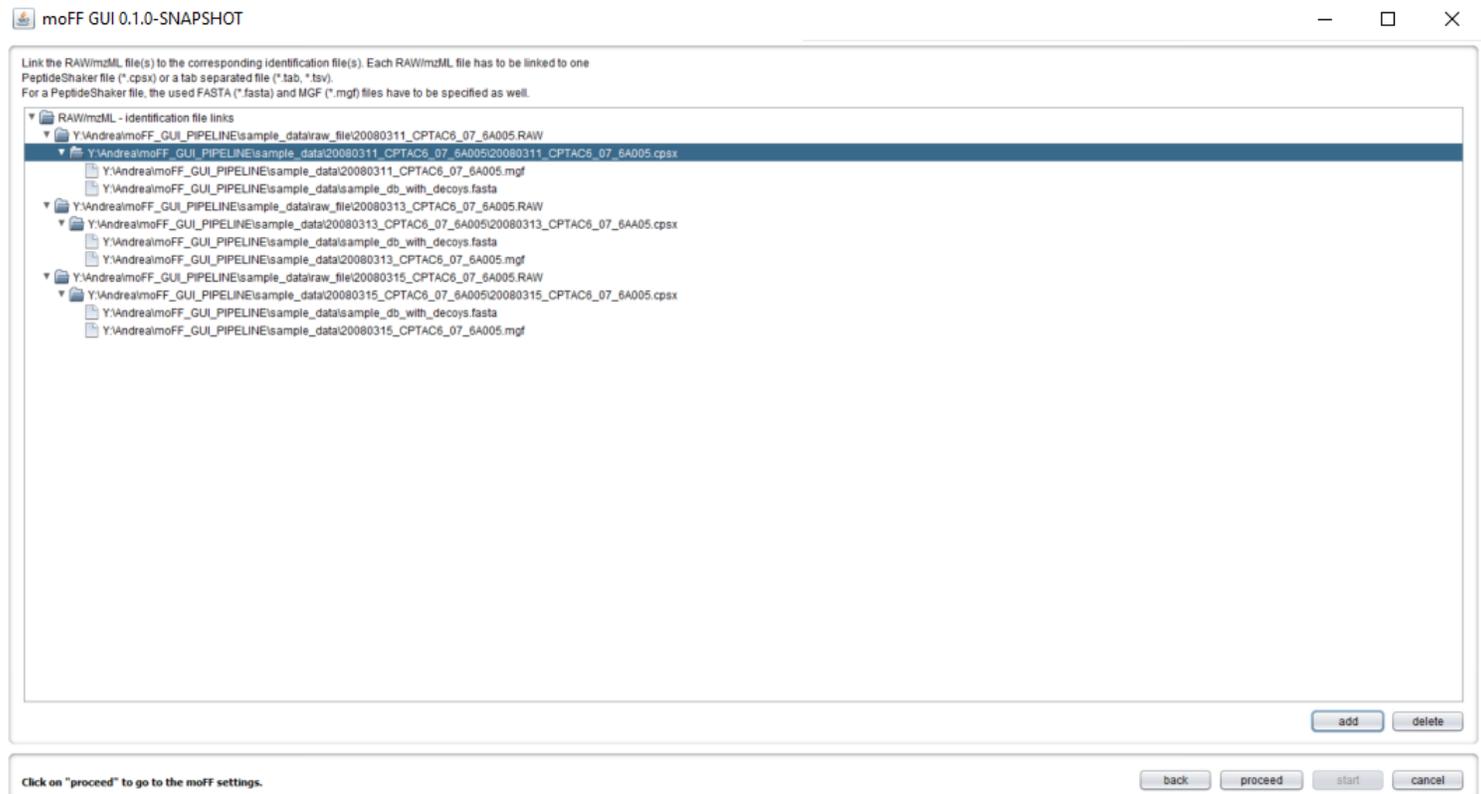


Figure 4

moFF GUI Overview (2) Load the raw and cps files into moFF-GUI

moFF GUI 0.1.0-SNAPSHOT

**APEX settings**

XIC retention time window (minutes): 5.0

Peak retention time window (minutes): 0.3

Precursor mass tolerance (ppm): 10

**Matching between runs settings**

Matched peaks retention time window (minutes): 0.6

Use combination weighing

Filter outliers      Width: 1.5

use custom peptides      choose

Click on "start" to run moFF.

back    proceed    start    cancel

Figure 5

moFF GUI Overview (3) Setting the moFF parameters

peptide	length	peak	type	raw_file	charge	calib_mz	mass	ppm_correction	rt	ms_intensity	ms_intensity	rt_peak	label	xcvm	sp_noise	log_noise	snr	log_L_R	log_int
AAAEIETKELAFEGSDQK	20	015042	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1066.4964	2130.9746	0.16208	32.555	2447600.0	1066.49477284	173072.92	1929.7116	1924.9515	1939.4216	2842.46725	3247.7581		
AAAEIETKELAFEGSDQK	20	015042	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	711.33214	2130.9746	0.80289	32.285	1323300.0	711.33211121	94461.464	1929.7116	1924.9515	1939.4216	1890.562815	2474.09745		
AAALGAGGAGGADGQDFQFQFQK	27	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	870.05639	2607.1474	0.35518	24.905	7540000.0	870.056499027	504040.44	1489.3915	1482.8115	1502.9315	14608.4996	17897.28		
AAAEYEVAVDTGK	16	000273	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	818.89429	1635.774	0.48734	23.93	2610300.0	818.89469808	898664.44	1431.5016	1422.7915	1434.6116	13997.9261	16244.2874		
AAQDLEIPIQDQIQRARFQK	30	045924	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	975.50155	2923.4828	0.38225	28.812	2446000.0	975.50122889	123463.12	1724.1214	1714.5115	1740.4016	4853.08254	7054		
AAIYGVYGGDGT	13	030770	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	425.31221	1248.6099	0.19331	23.649	21711000.0	425.31232928	2784509.8	1416.7415	1410.8915	1422.7915	28319.0464	31479.2468	39.85942	
AAEAALIVYEVK	12	002111	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	638.8445	1275.674	-0.48957	22.472	4540300.0	638.844187241	864072.7	1344.9515	1339.3415	1353.6416	25699.5236	35793.1838	30.1	
AAEYDQKQKELQDFQK	20	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1129.5415	2207.0485	-1.3704	22.422	2870200.0	1129.53995208	248916.1	1344.9515	-1.0	1353.6416	23744.489	24468.66	20.4	
AAEAALIVYEVK	12	002111	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	735.37079	1460.727	0.42454	23.855	1522000.0	735.37102194	2252400.2	1434.6116	1428.5516	1443.8217	20382.473	22047.5542	40.1	
AAAVATLTVYGVYEVK	18	022314	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	947.02511	1932.0357	0.42584	29.058	1973100.0	947.025521508	137534.17	1740.6016	1736.3416	1744.9716	2914.11609	4064.1242	33.4	
AAVYDQKQKELQDFQK	16	000273	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	606.95247	1817.8362	-0.69982	21.209	14930000.0	606.95224767	1323156.2	1269.7615	1264.3716	1279.0615	13979.308	35482.0164		
AAVYDQKQKELQDFQK	16	000273	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	902.97562	1803.9367	0.74789	26.915	104900.0	902.97429326	94013.984	1421.1015	1404.0115	1425.0115	8774.4002			
AAQDFQKQKELQDFQK	14	043313	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	791.3587	1580.7028	-0.49524	21.159	15701000.0	791.358308088	15749708.0	1292.015	1283.7816	1297.6415	41601.8546	58123.1146	51.1	
AAQDFQKQKELQDFQK	14	015075	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	632.3133	1893.9181	-1.019	20.832	4594100.0	632.31255673	658991.06	1245.3316	1242.6016	1253.4215	24306.11225	30620.8945	28.4	
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1080.0274	2159.0403	-1.1499	22.287	4704600.0	1080.02594207	424726.38	1339.3415	1328.1615	1344.9515	21761.1904	26935.43		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	958.40468	2072.1981	0.84821	25.45	19720000.0	958.407184601	10202935.0	1516.5115	1506.0016	1523.0015	28364.9338	38305.07		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1437.1063	2872.1981	0.13711	25.252	2048600.0	1437.1063197	120139.72	1516.5115	1509.4276	1523.0015	17061.3001	1753		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	4	719.05681	2872.1981	0.83377	25.301	4140600.0	719.057409528	212138.72	1516.5115	1509.4276	1523.0015	14295.5034	1523		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	892.72543	2478.1846	0.17467	27.219	4502100.0	892.73558076	40789.66	1405.0715	1399.3616	1407.9218	21849.5425	2414		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	942.456	2884.3462	0.24292	27.386	8947300.0	942.4562338	493451.9	1438.6515	1432.2215	1449.3015	13455.370425	14139.94		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1443.1804	2884.3462	-0.24036	27.357	3311100.0	1443.18005312	173931.36	1438.6515	1432.2215	1449.3015	13455.370425	14139.94		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	954.94471	1907.8749	0.70145	25.591	8185500.0	954.94378946	765848.94	1530.3116	1523.0015	1541.8516	10340.99405	11050.7814	37.1	
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	721.9621	1440.7096	0.42307	24.564	9039500.0	721.96241524	1093945.2	1473.1415	1462.8515	1479.1215	3747.24655	21584.324	35.12192	
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1049.4478	2086.811	0.098718	24.99	4240700.0	1049.4479036	305309.8	1496.4015	1493.2515	1509.6276	17422.869	19467.383		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	4	661.11316	2046.4235	1.0002	27.492	1255200.0	661.113821245	104330.74	1441.2116	1439.1515	1444.9616	6955.3731	8234.66928		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	891.99602	1781.9775	0.74849	35.039	524830.0	891.99648474	44461.273	2100.2815	2090.4216	2107.1016	944.24812	1204.2133	33.2	
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	4	660.86086	2439.4143	1.2094	26.188	422460.0	660.861459245	65420.76	1549.2316	1530.3116	1552.9116	9634.4998	1145		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	1061.8384	3182.4934	-0.032899	29.803	4172500.0	1061.83836507	146886.06	1781.5816	1769.7816	1797.4615	4673.127125			
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	3	1016.1849	3045.3329	0.48254	30.459	23452000.0	1016.1839303	912316.06	1823.2515	1815.2016	1831.6615	4313.44525	5411		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	1523.7337	3045.3329	0.022464	30.409	1321300.0	1523.73374339	70410.4	1823.2515	1815.2016	1831.6615	4200.33964	4792		
AAQDFQKQKELQDFQK	14	024927	MULTI-MHMS	V14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057	2	982.00827	1962.002	0.47888	33.046	425610.0	982.00874024	44460.004	1982.4915	1972.7915	1987.4115	1785.74166	2113.482		

```

raw file select
moFF input file: ../second_dir/PRD000446/input_m_2_run/v14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057.LAI XIC_out_10.0 XIC_win_5.0000 moFF_stwin_peak_4.0000
RAW file : ../second_dir/PRD000446/raw_rep/v14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057.raw
Output file in : ../second_dir/PRD000446/moFF_output/v14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057_moFF_result.LAI
RAW file location : ../second_dir/PRD000446/raw_rep/v14790_PolyAEM_tesst_445_Durkat_31-05-2013_LMAD_fer_130617185057.raw
Starting mrm .....
peptide at line 0 -> MZI 1066.4948 RT: 32.5550
peptide at line 1 -> MZI 711.3327 RT: 32.2850
peptide at line 2 -> MZI 870.0547 RT: 24.9050
peptide at line 3 -> MZI 818.8949 RT: 23.9300
peptide at line 4 -> MZI 975.5019 RT: 28.8120
peptide at line 5 -> MZI 425.3123 RT: 23.6490
peptide at line 6 -> MZI 638.8442 RT: 22.4720
peptide at line 7 -> MZI 1129.5415 RT: 22.4220
peptide at line 8 -> MZI 735.3711 RT: 23.9550
peptide at line 9 -> MZI 947.0255 RT: 29.0580
peptide at line 10 -> MZI 606.9522 RT: 21.2090
peptide at line 11 -> MZI 902.9743 RT: 26.9150
peptide at line 12 -> MZI 791.3583 RT: 21.5900
peptide at line 13 -> MZI 632.3127 RT: 20.8320
peptide at line 14 -> MZI 1080.0259 RT: 22.2870
peptide at line 15 -> MZI 958.4072 RT: 25.4500
peptide at line 16 -> MZI 1437.1063 RT: 25.2520
peptide at line 17 -> MZI 719.0574 RT: 25.3010
peptide at line 18 -> MZI 892.7354 RT: 23.5190
peptide at line 19 -> MZI 892.4562 RT: 27.3860
peptide at line 20 -> MZI 1443.1801 RT: 27.3570
peptide at line 21 -> MZI 954.9448 RT: 21.5910
peptide at line 22 -> MZI 721.9629 RT: 24.5640
peptide at line 23 -> MZI 1049.4479 RT: 24.9900
peptide at line 24 -> MZI 661.1139 RT: 27.4920
peptide at line 25 -> MZI 891.9967 RT: 35.0390
peptide at line 26 -> MZI 660.8617 RT: 26.1880
peptide at line 27 -> MZI 1061.8384 RT: 29.8030
peptide at line 28 -> MZI 1016.1854 RT: 30.4590
peptide at line 29 -> MZI 1523.7337 RT: 30.4090
peptide at line 30 -> MZI 982.0087 RT: 33.0460
peptide at line 31 -> MZI 735.3534 RT: 19.9940
peptide at line 32 -> MZI 839.3970 RT: 23.6440

```

↑  
moFF result

← moFF log

Figure 6

output files of the apex module The output of the apex module is composed by two files: the result file and log file. In the result file , you notice the intensity and log intensity extracted by moFF along with the quality measures log\_L\_R and SNR. The log file contains details information to each apex intensity extracted. Here you can easily spot spot eventually errors in the apex intensity extraction from the XIC data