

Supplementary material

Optimizing MS -based multi-omics: comparative analysis of protein, metabolite, and lipid extraction techniques

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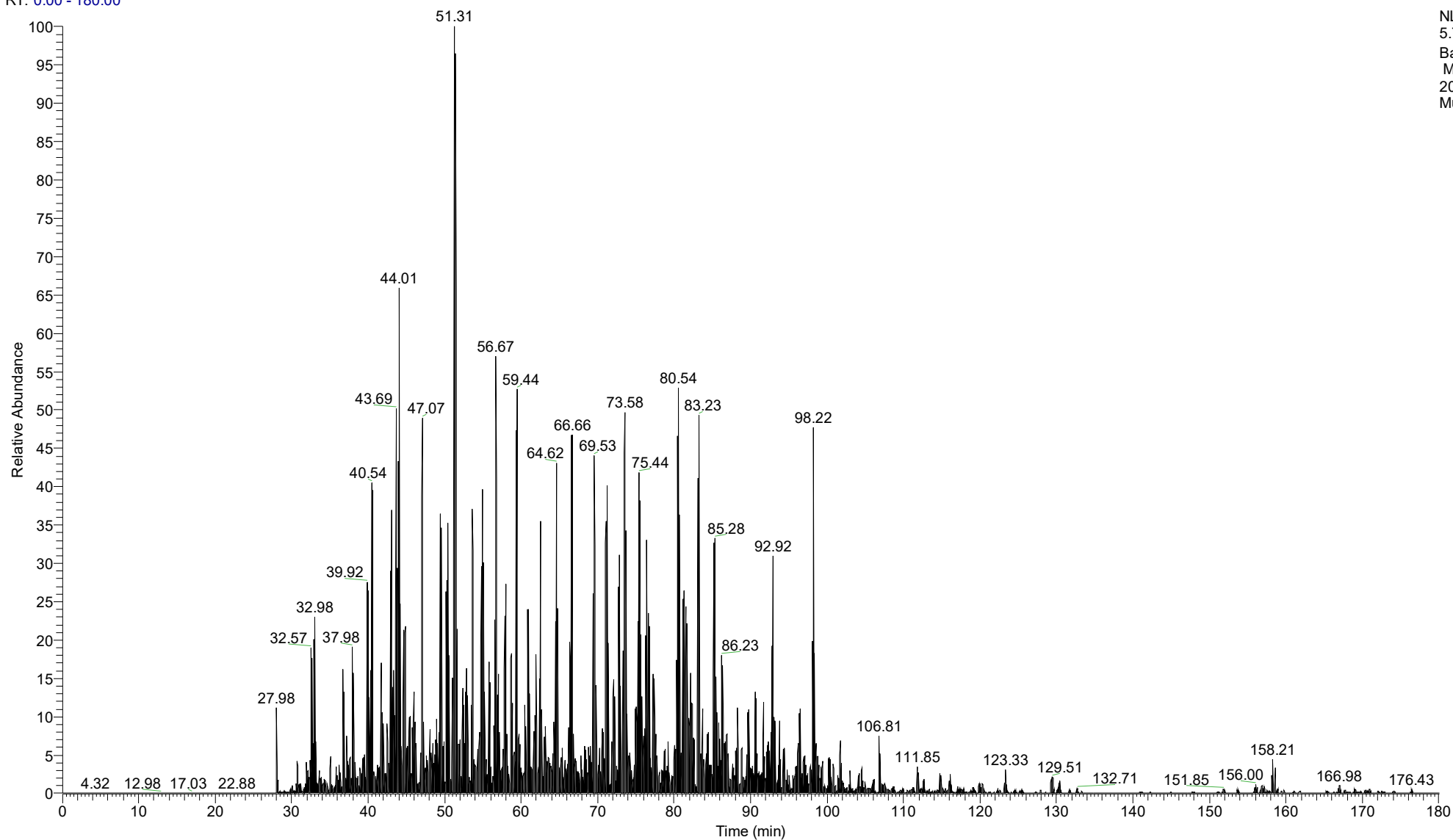
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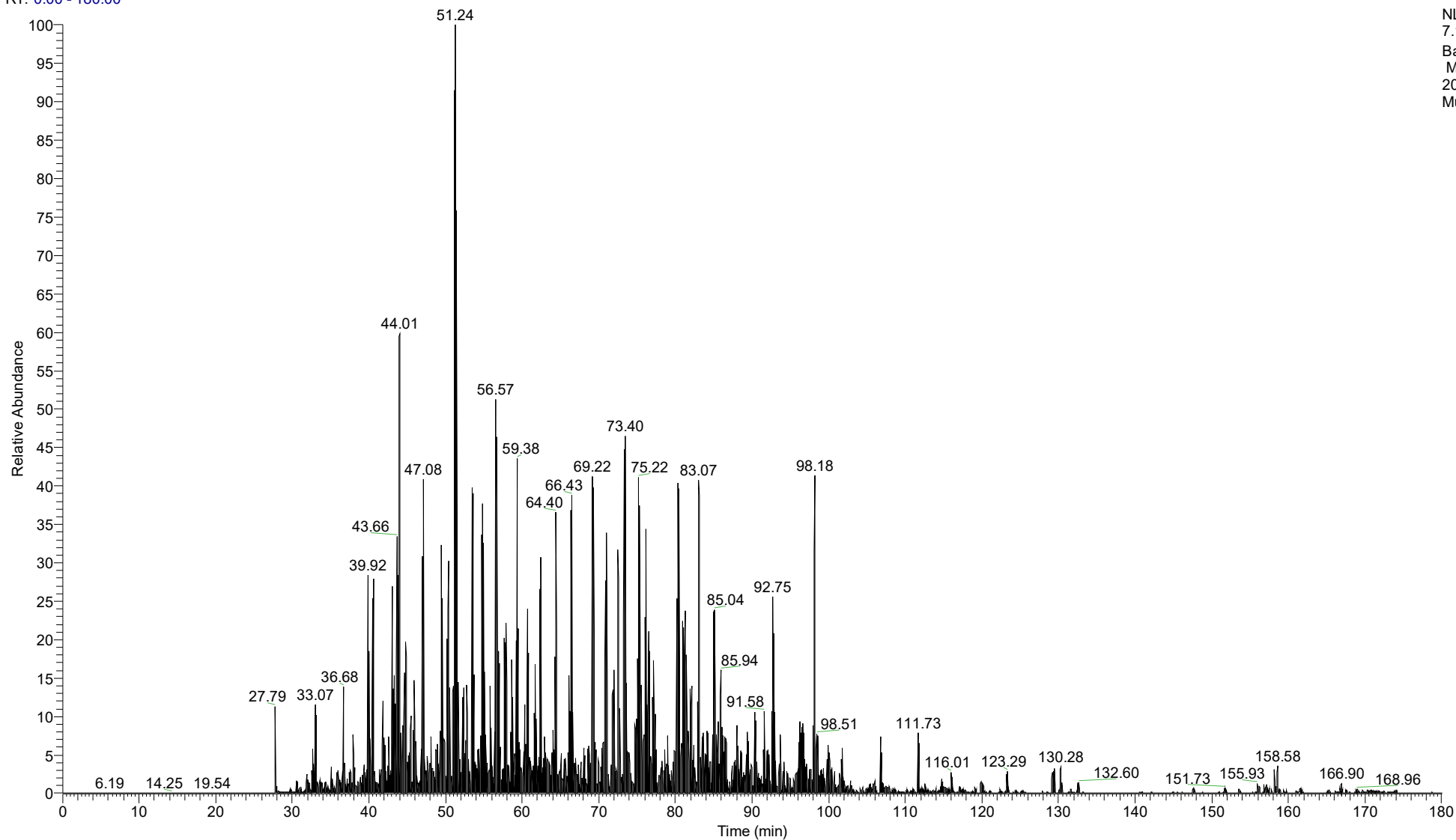
RT: 0.00 - 180.00



NL:
5.72E9
Base Peak
MS
20201109_
Multi_S1-1

(A)80%methanol + S-trap-2

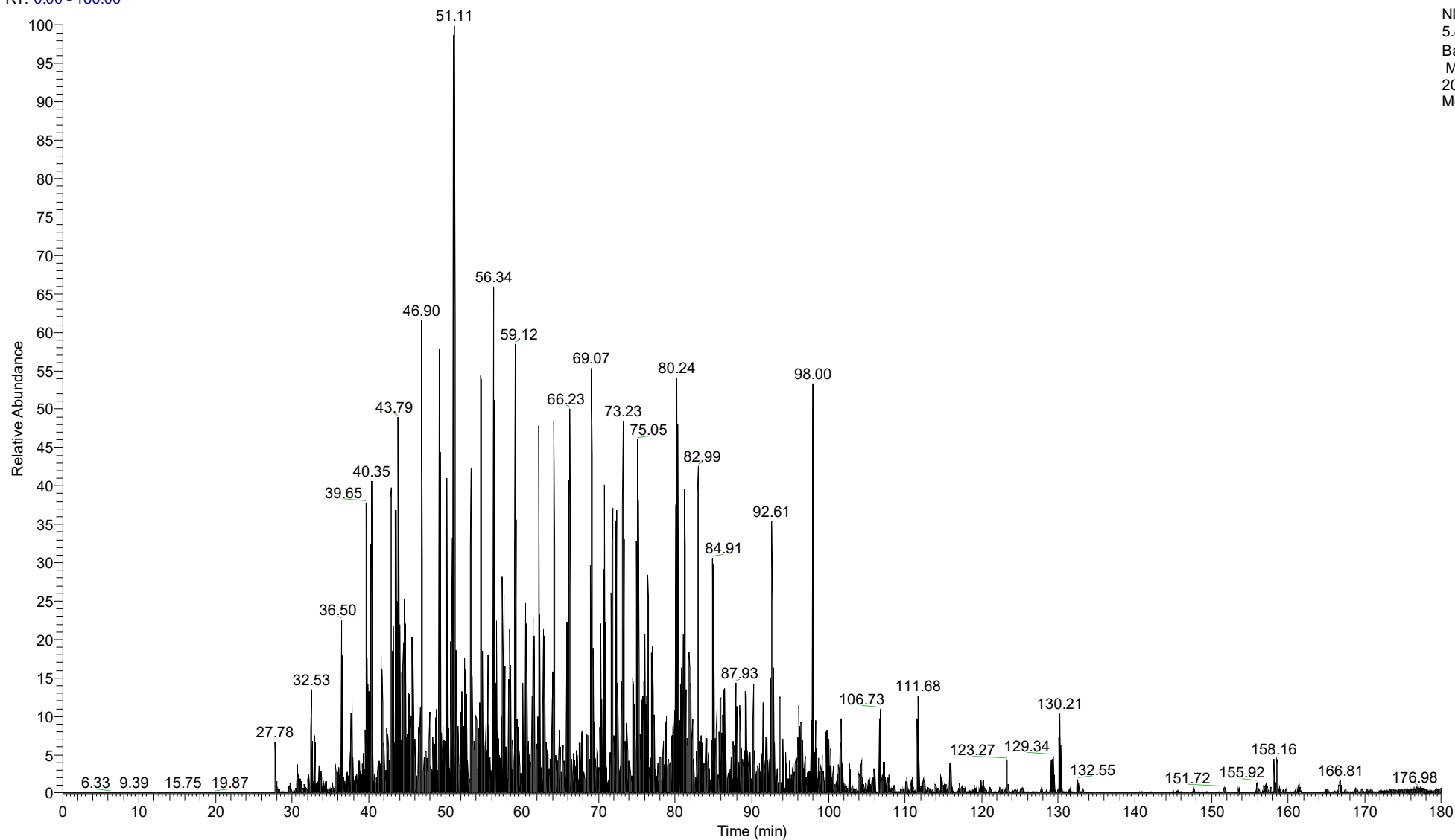
RT: 0.00 - 180.00



NL:
7.10E9
Base Peak
MS
20201109_
Multi_S1-2

(A)80%methanol + S-trap-3

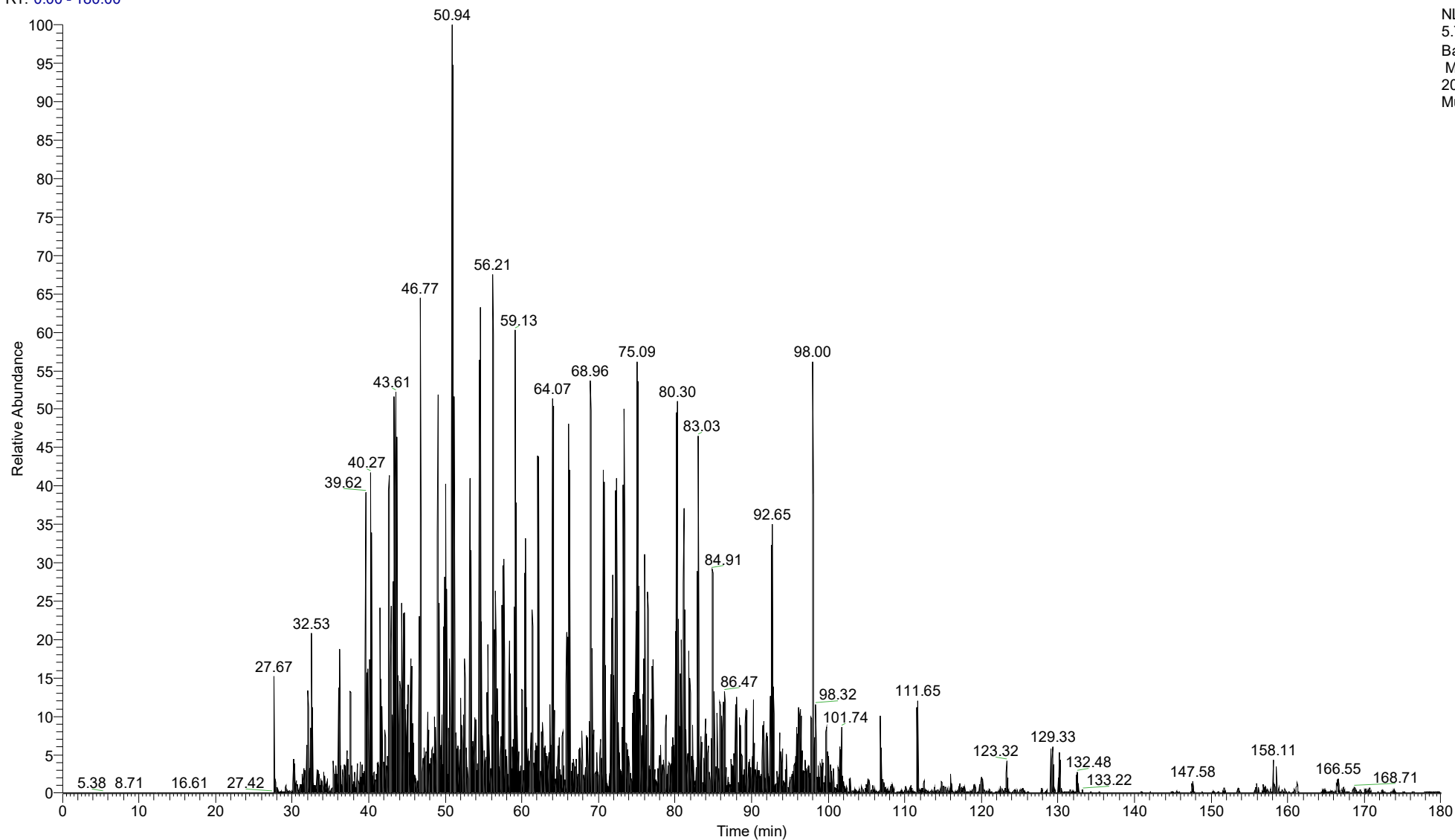
RT: 0.00 - 180.00



NL:
5.81E9
Base Peak
MS
20201109_
Multi_S1-3

(B)Chloroform/methanol + S-trap-1

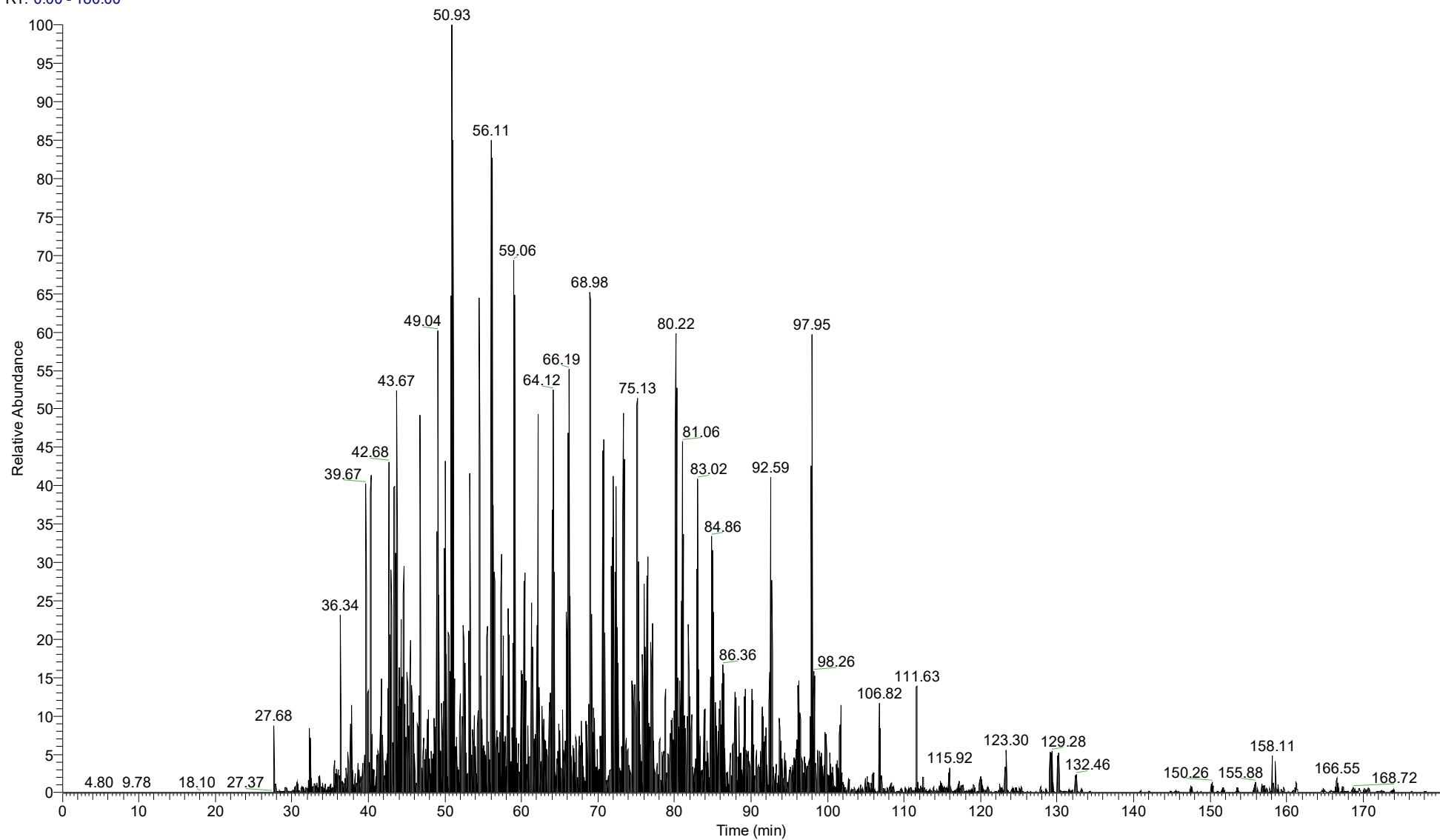
RT: 0.00 - 180.00



NL:
5.73E9
Base Peak
MS
20201109_
Multi_S2-1

(B)Chloroform/methanol + S-trap-2

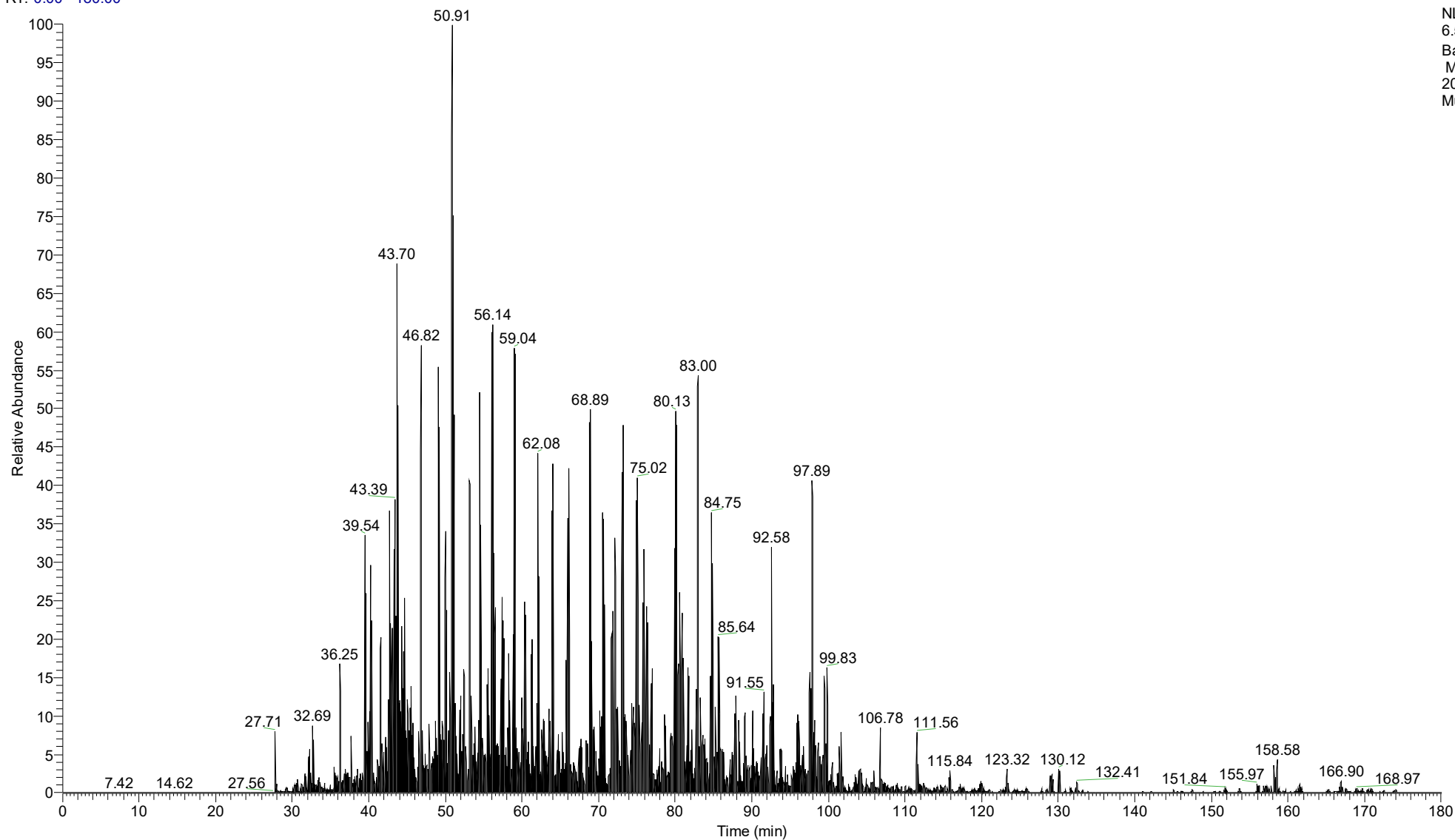
RT: 0.00 - 180.00



NL:
5.31E9
Base Peak
MS
20201109_
Multi_S2-2

(B)Chloroform/methanol + S-trap-3

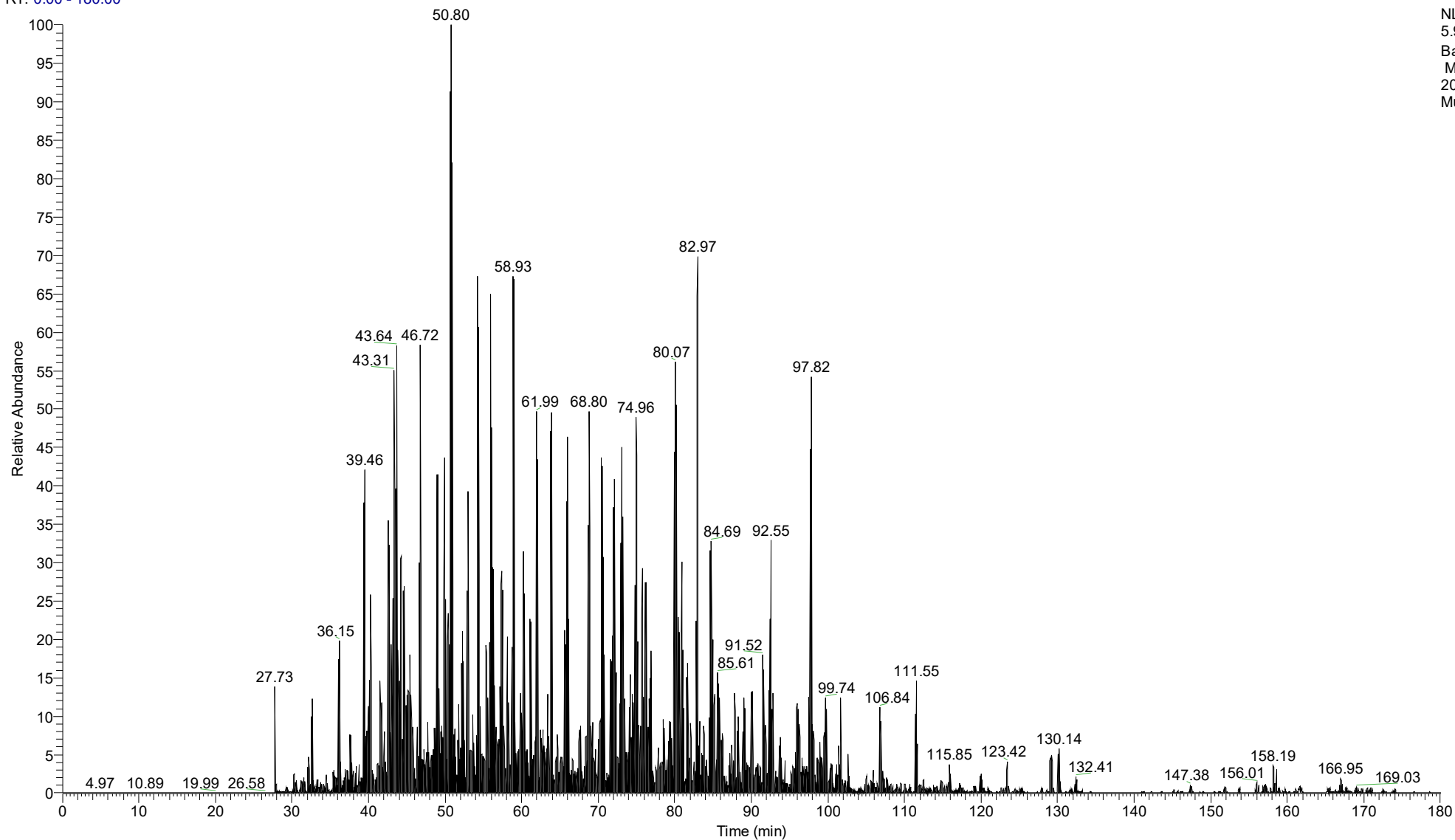
RT: 0.00 - 180.00



NL:
6.50E9
Base Peak
MS
20201109_
Multi_S2-3

(C)MTBE + S-trap-1

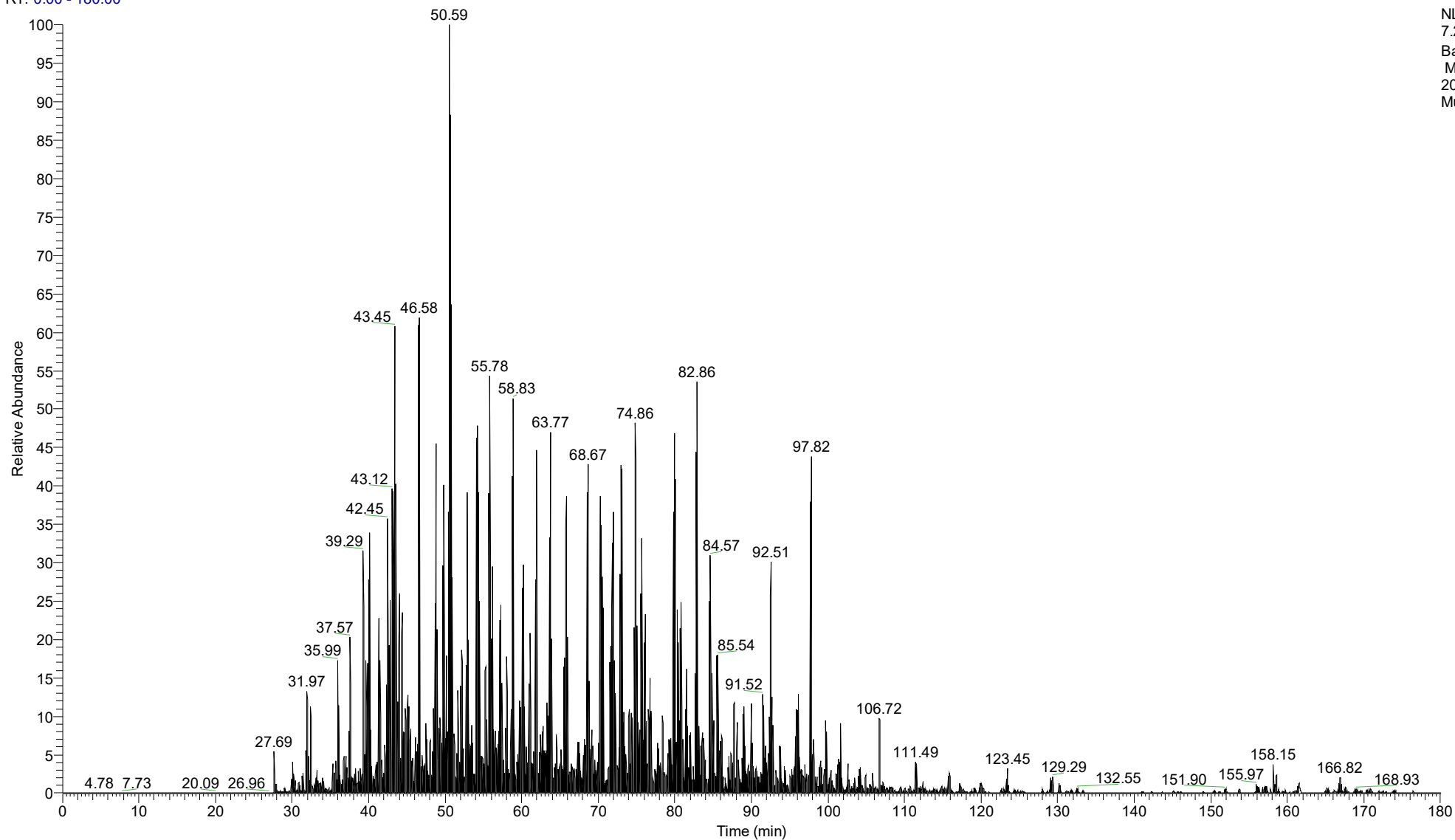
RT: 0.00 - 180.00



NL:
5.90E9
Base Peak
MS
20201109_
Multi_S3-1

(C)MTBE + S-trap-2

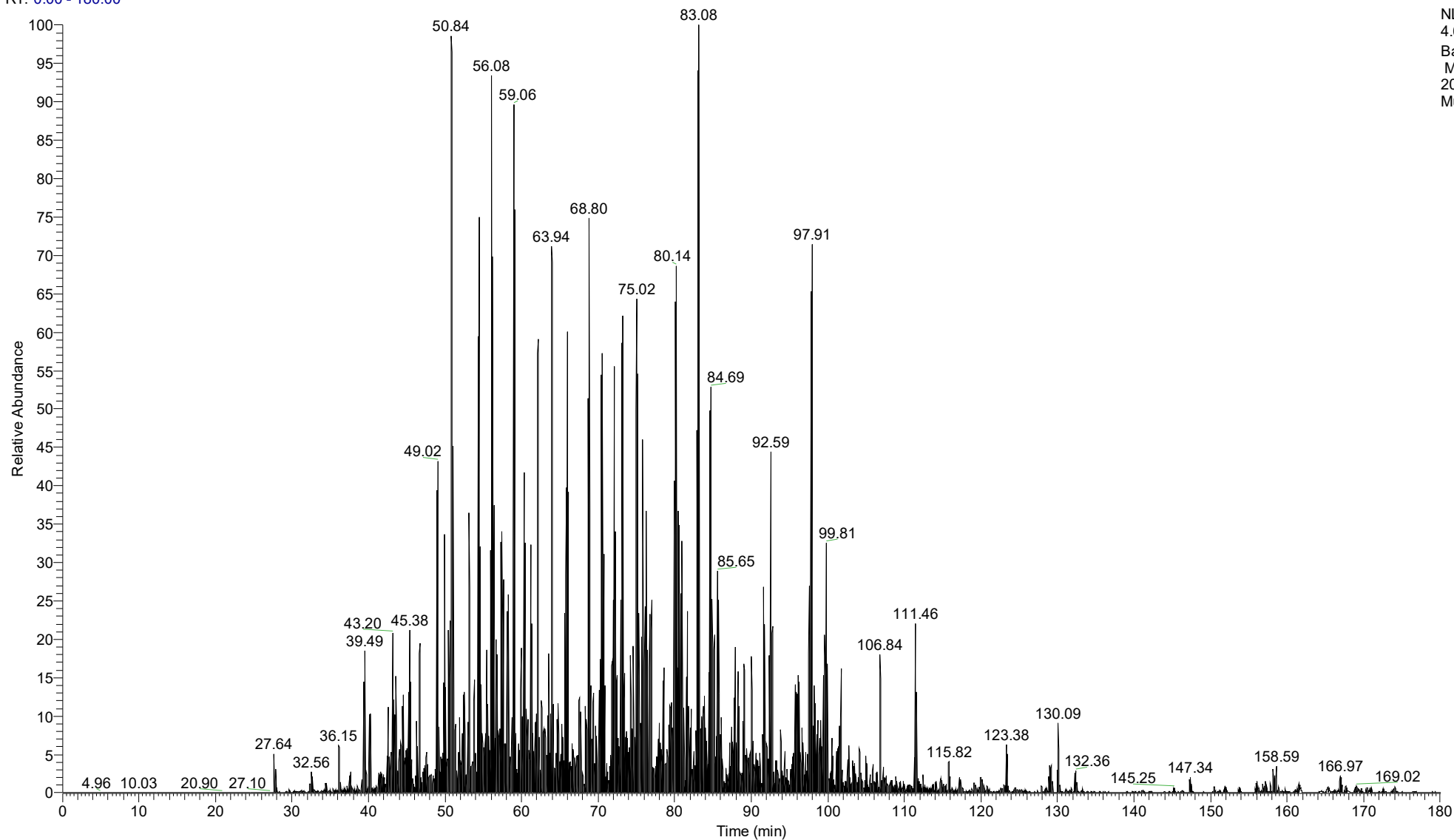
RT: 0.00 - 180.00



NL:
7.24E9
Base Peak
MS
20201109_
Multi_S3-2

(C)MTBE + S-trap-3

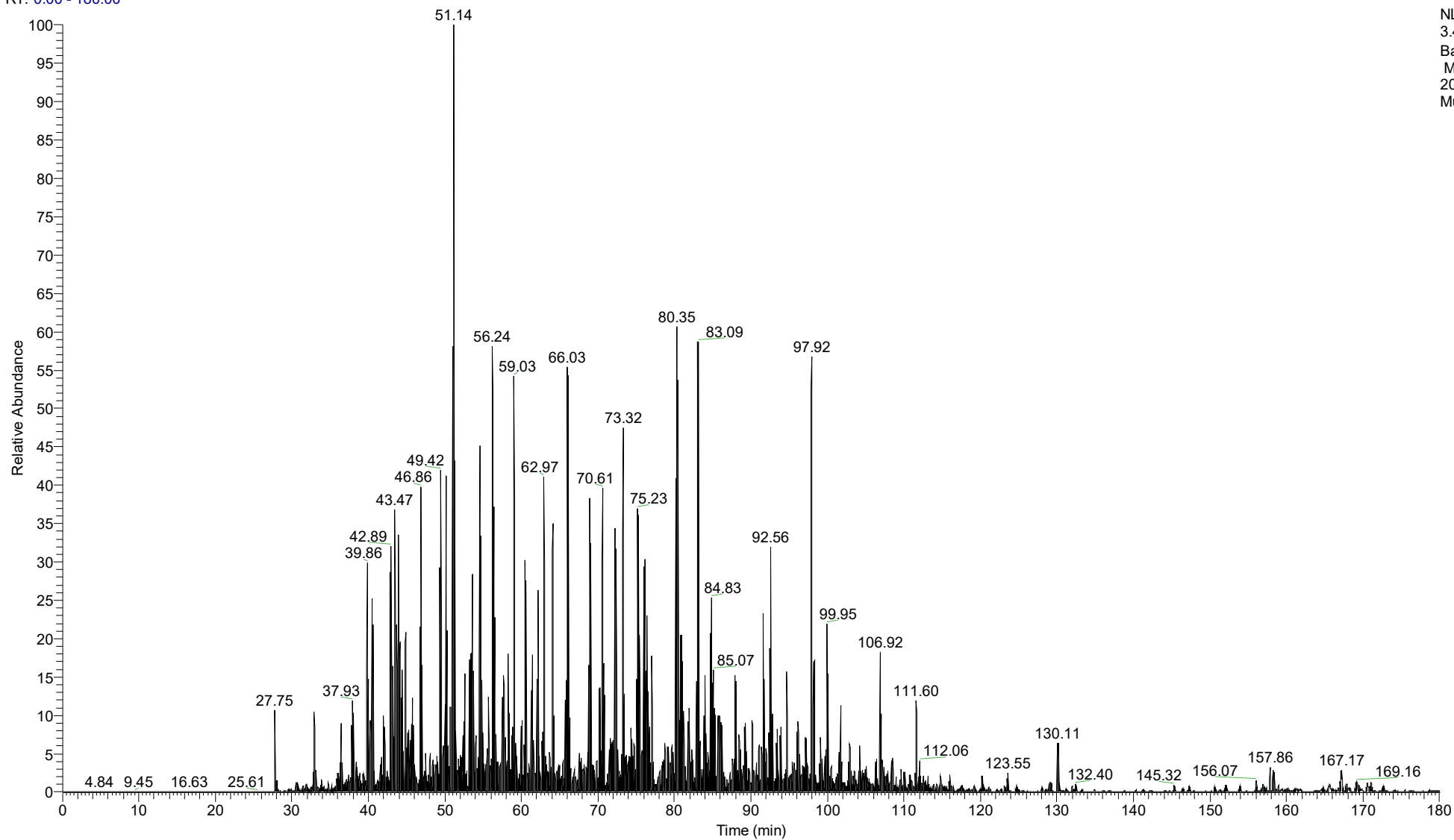
RT: 0.00 - 180.00



NL:
4.64E9
Base Peak
MS
20201109_
Multi_S3-3

(D)80%methanol + FASP-1

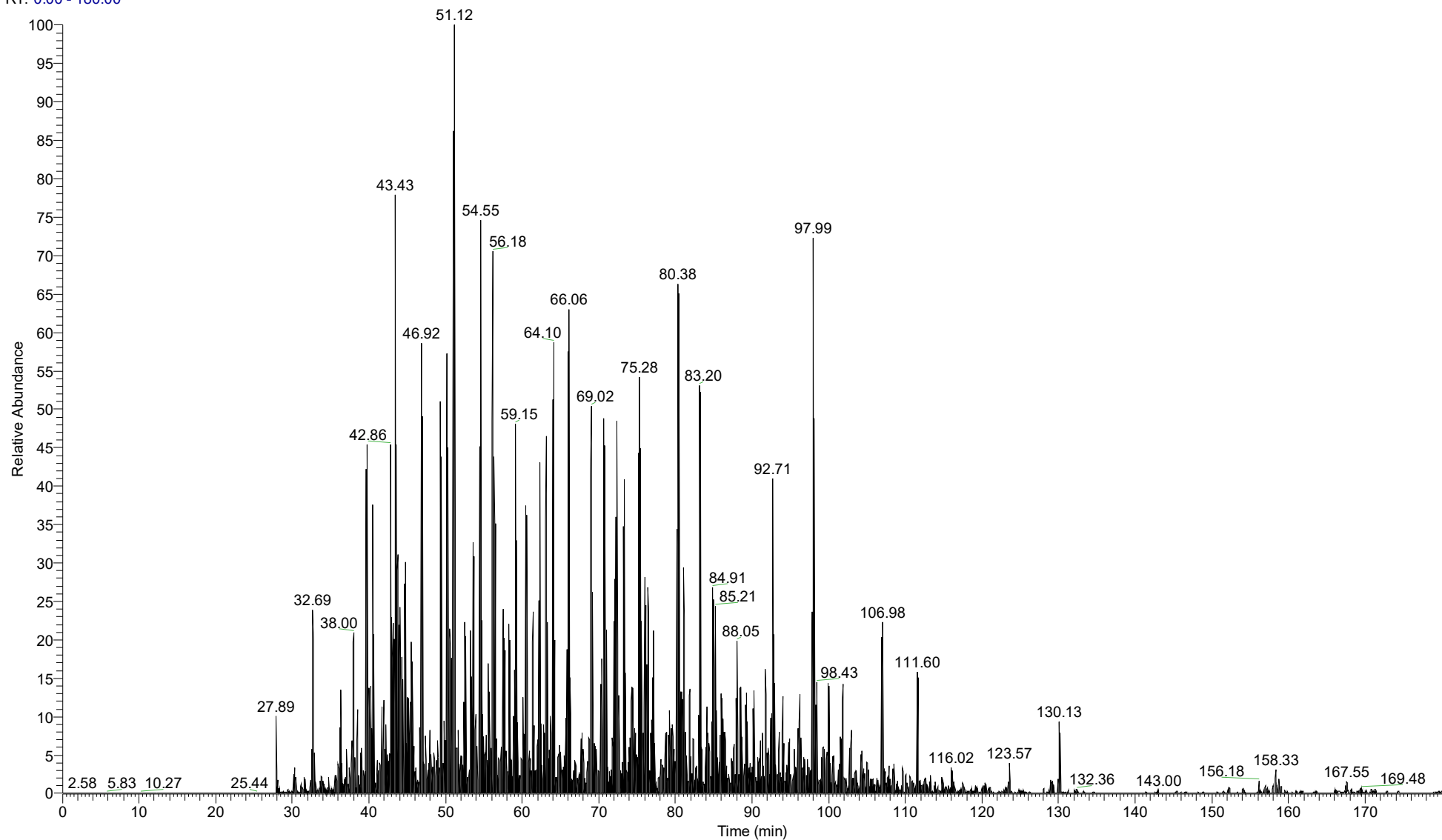
RT: 0.00 - 180.00



NL:
3.46E9
Base Peak
MS
20201109_
Multi_P1-1

(D)80%methanol + FASP-2

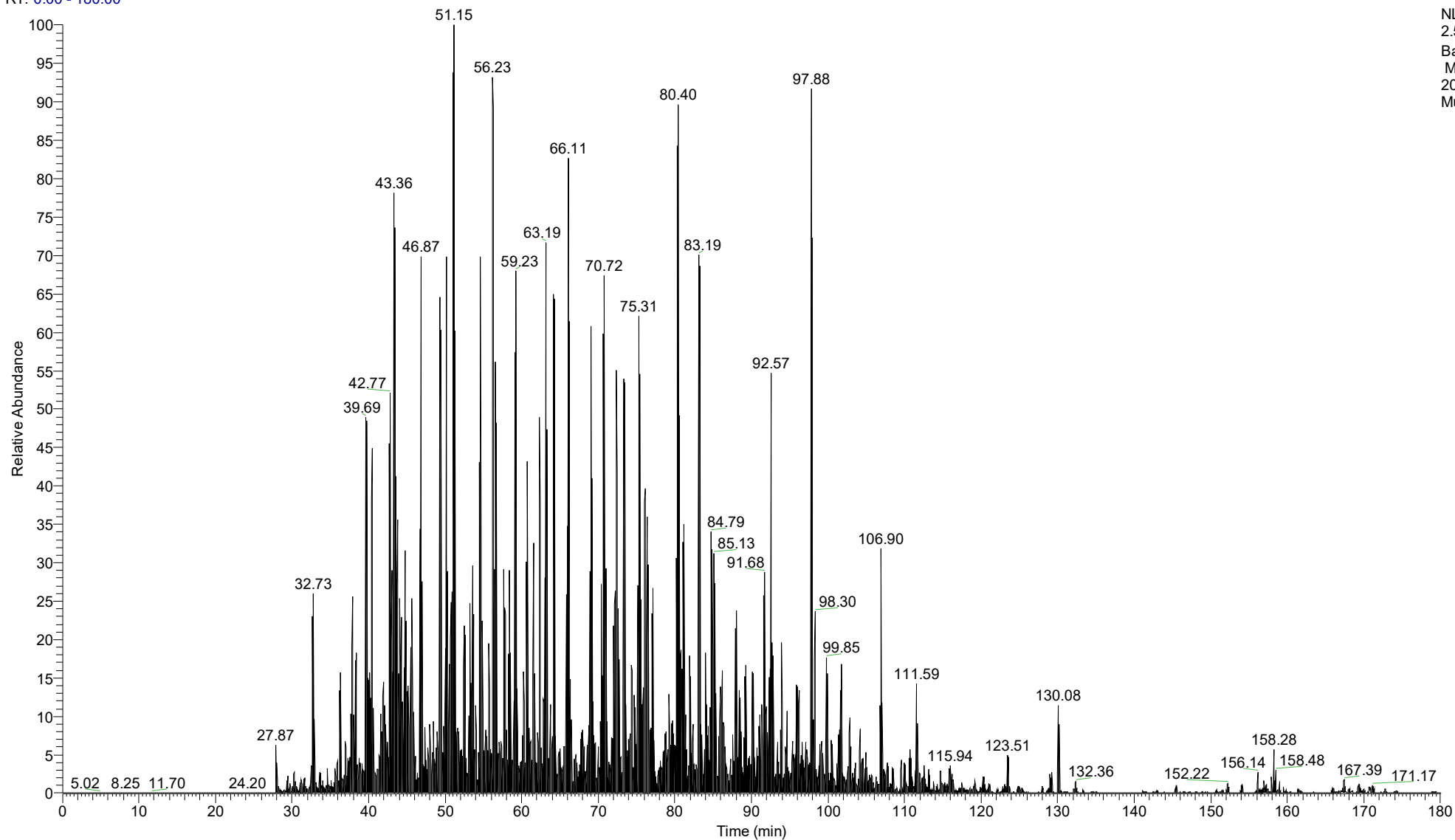
RT: 0.00 - 180.00



NL:
4.24E9
Base Peak
MS
20201109_
Multi_P1-2

(D)80%methanol + FASP-3

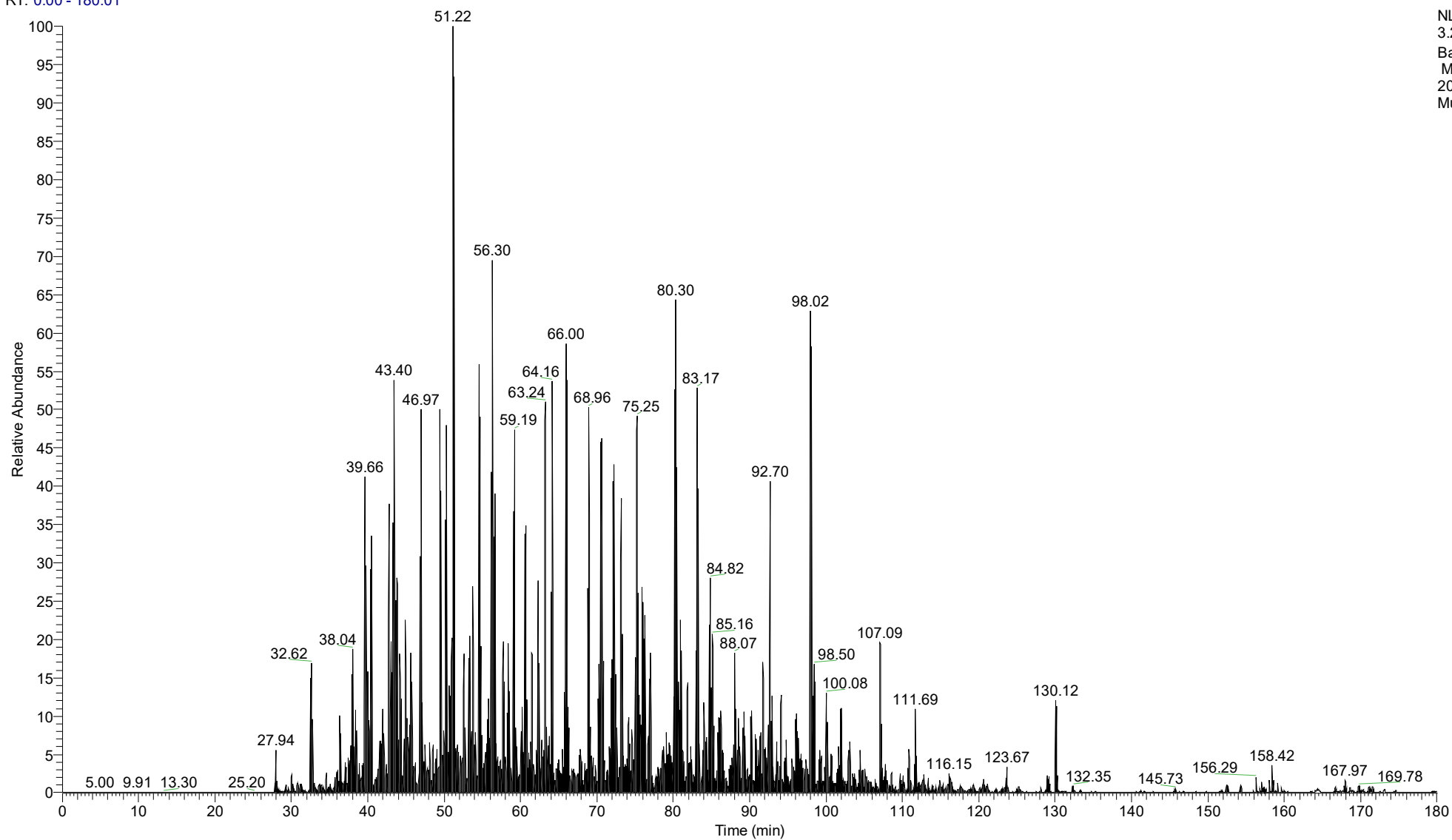
RT: 0.00 - 180.00



NL:
2.55E9
Base Peak
MS
20201109_
Multi_P1-3

(E)Chloroform/methanol + FASP-1

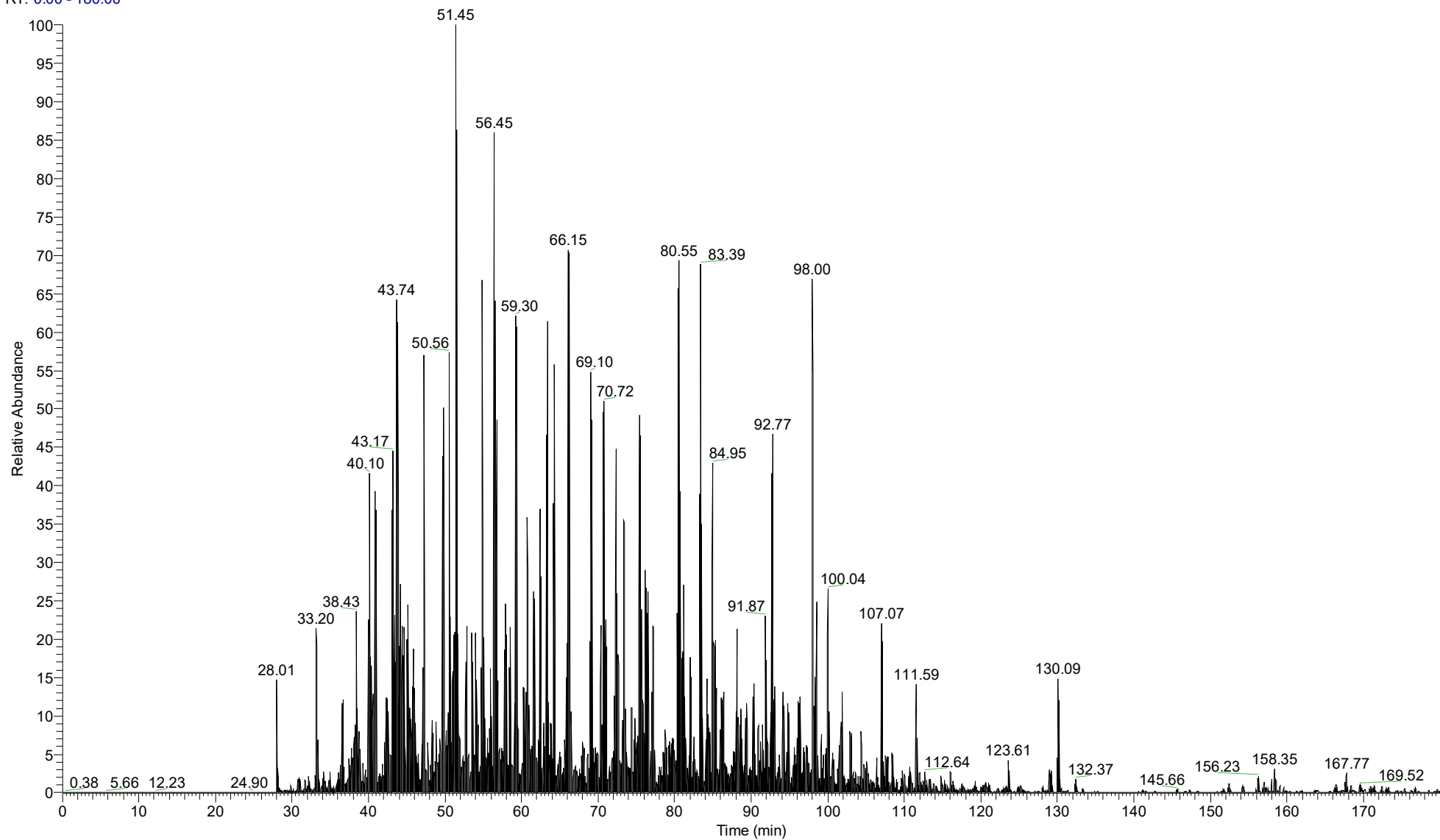
RT: 0.00 - 180.01



NL:
3.23E9
Base Peak
MS
20201109_
Multi_P2-1

(E)Chloroform/methanol + FASP-2

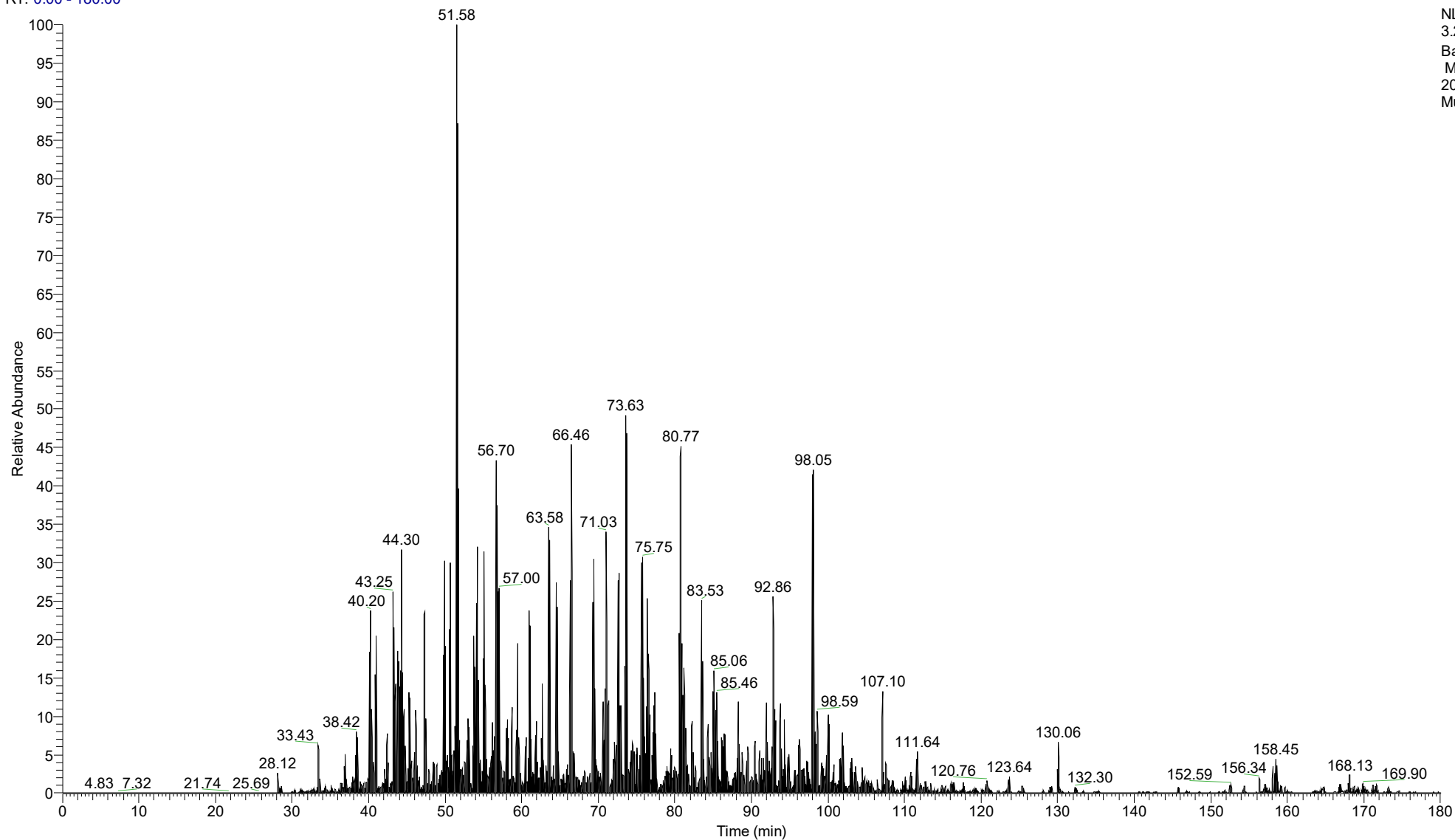
RT: 0.00 - 180.00



NL:
2.99E9
Base Peak
MS
20201109_
Multi_P2-2

(E)Chloroform/methanol + FASP-3

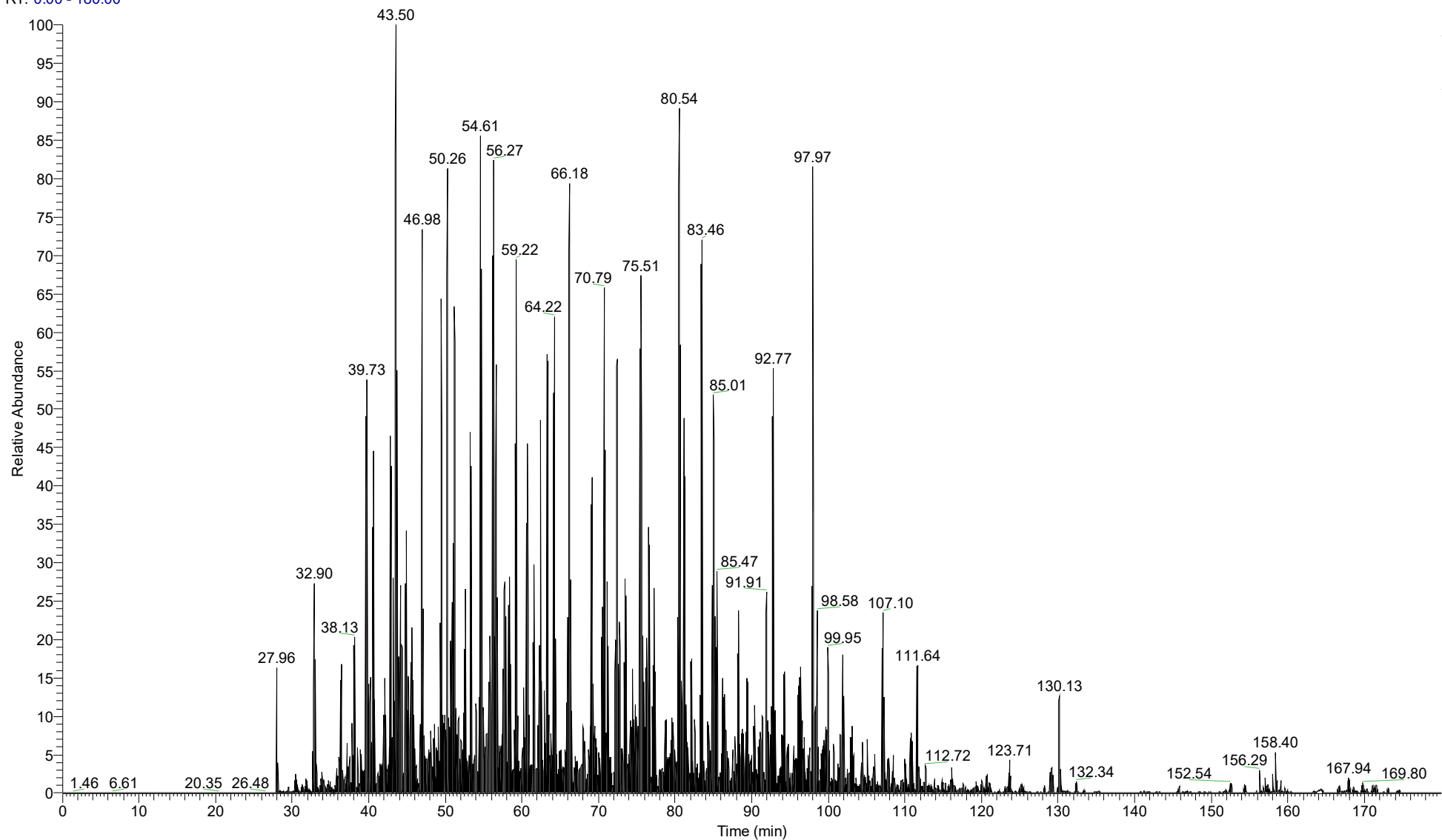
RT: 0.00 - 180.00



NL:
3.23E9
Base Peak
MS
20201109_
Multi_P2-3

(F)MTBE + FASP-1

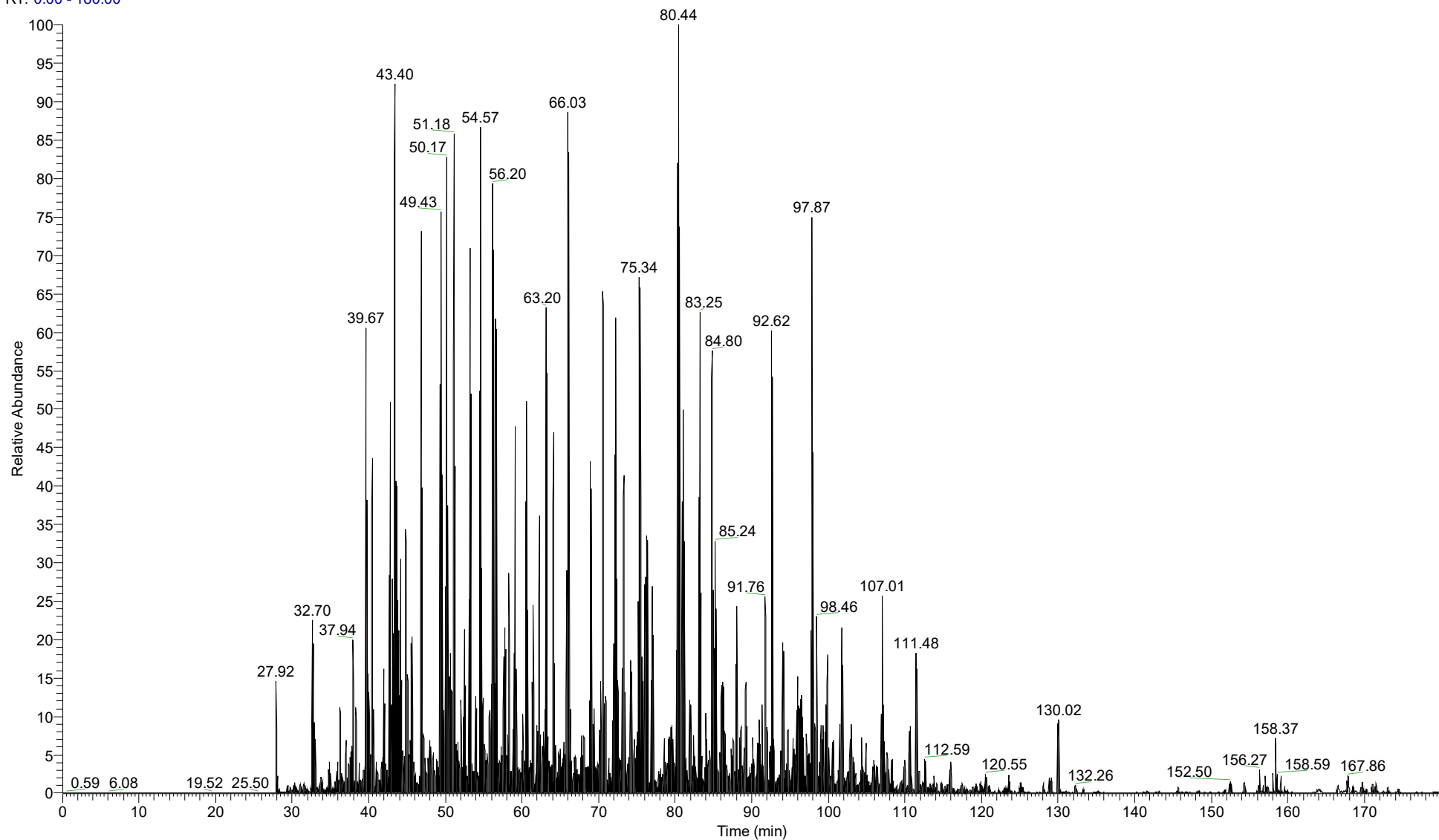
RT: 0.00 - 180.00



NL:
2.45E9
Base Peak
MS
20201109_
Multi_P3-1

(F)MTBE + FASP-2

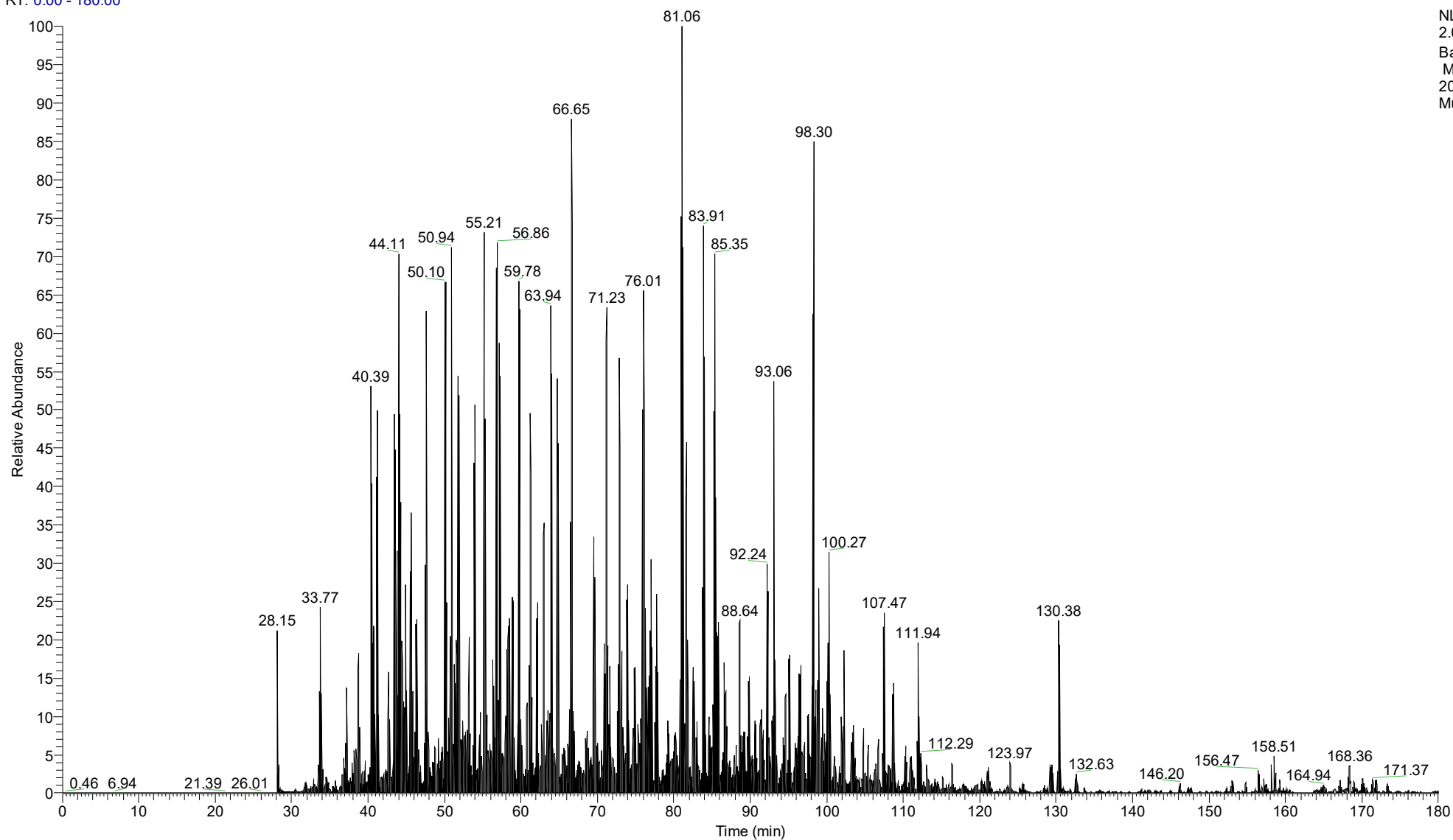
RT: 0.00 - 180.00



NL:
1.93E9
Base Peak
MS
20201109_
Multi_P3-2

(F)MTBE + FASP-3

RT: 0.00 - 180.00



NL:
2.06E9
Base Peak
MS
20201109_
Multi_P3-3

Figure S1 Chromatogram of proteomics data of each method.

	Label	Feature	ID(compound) Level of Confidence : 3	ID(compound) Level of Confidence : 2
80%methanol	1-1	3179	568	61
	1-2	3108	543	63
	1-3	3158	545	86
Chloroform/methanol	2-1	2306	434	64
	2-2	2126	418	69
	2-3	2360	458	61
MTBE	3-1	2680	496	74
	3-2	2549	480	66
	3-3	2510	460	74

Figure S2 List of the number of metabolite features, compounds identified as level of confidence 2,3 for each extraction method

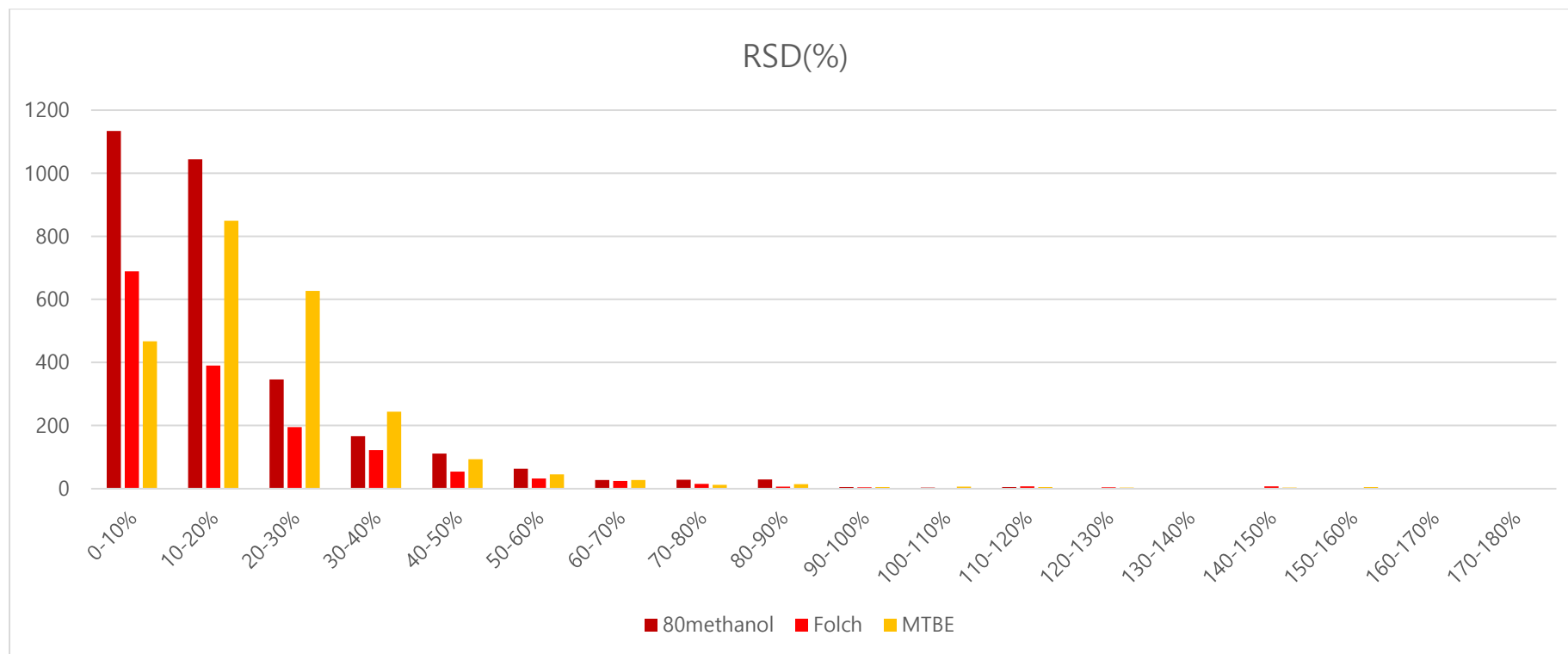
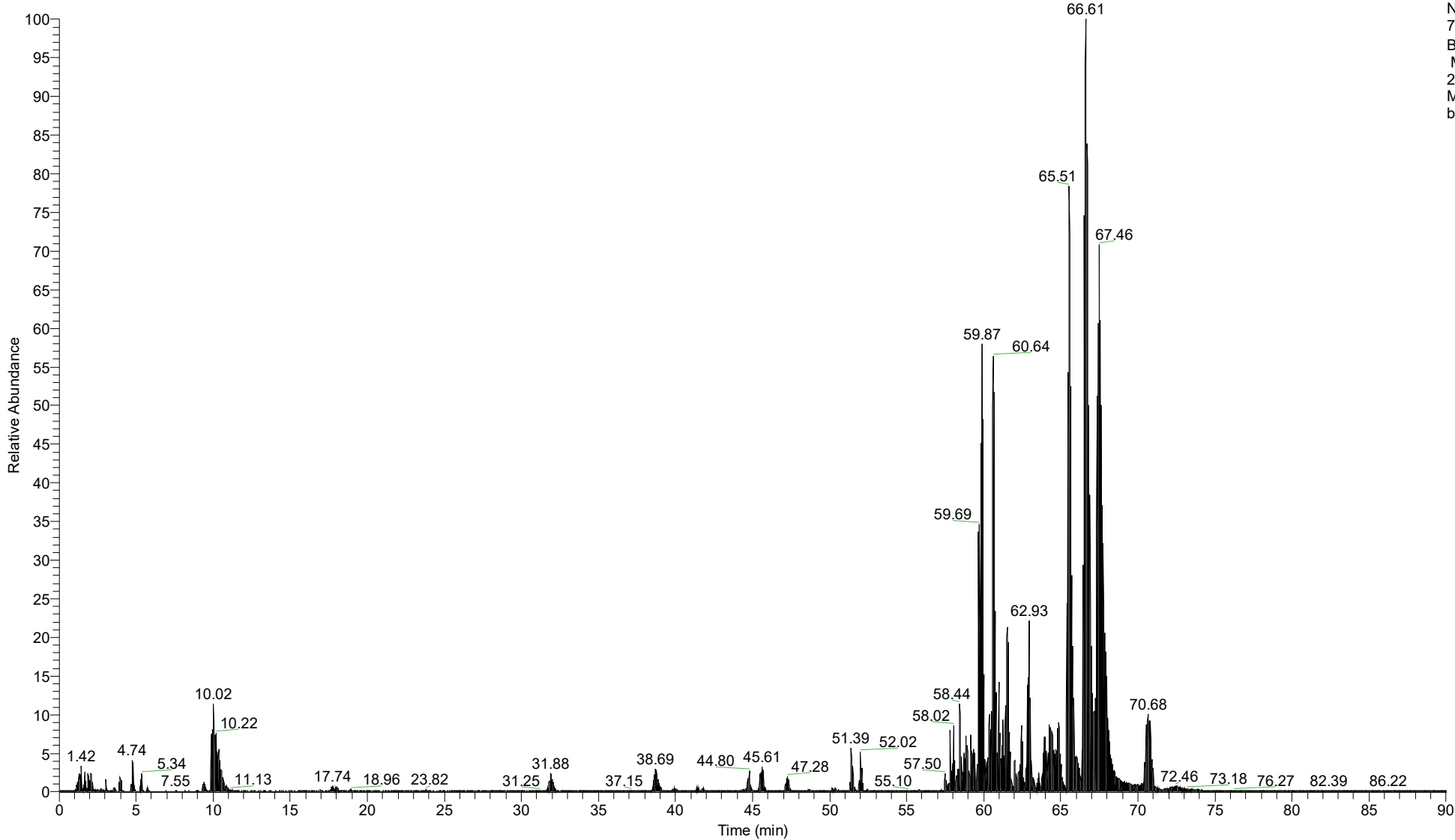


Figure S3 Histogram for RSD of each method(metabolite).

(A)80%methanol + S-trap-1

(A)80%methanol-1

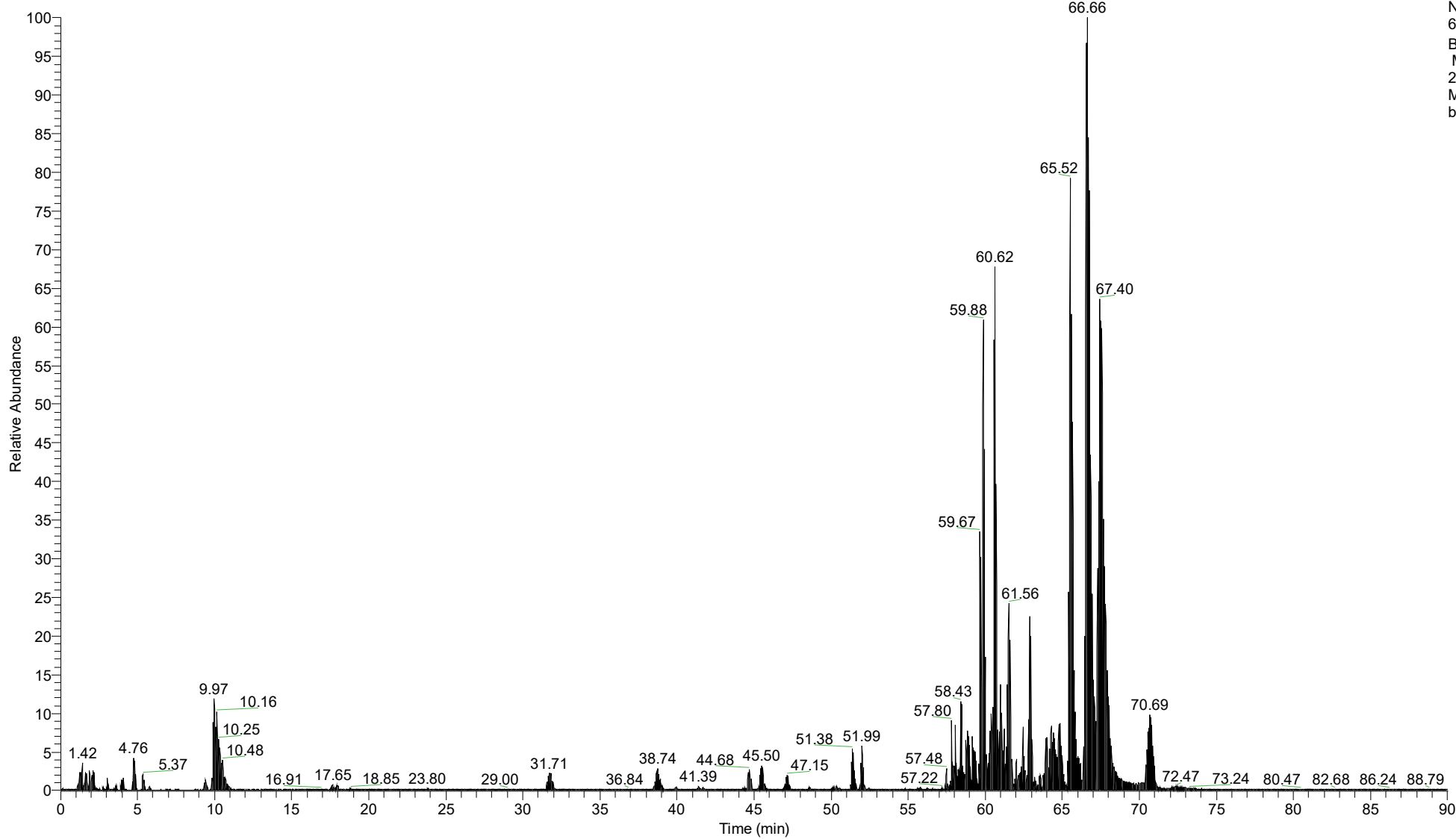
RT: 0.00 - 90.01



NL:
7.29E9
Base Peak
MS
20201008_
Multi_meta
bolite1-1

(A)80%methanol-2

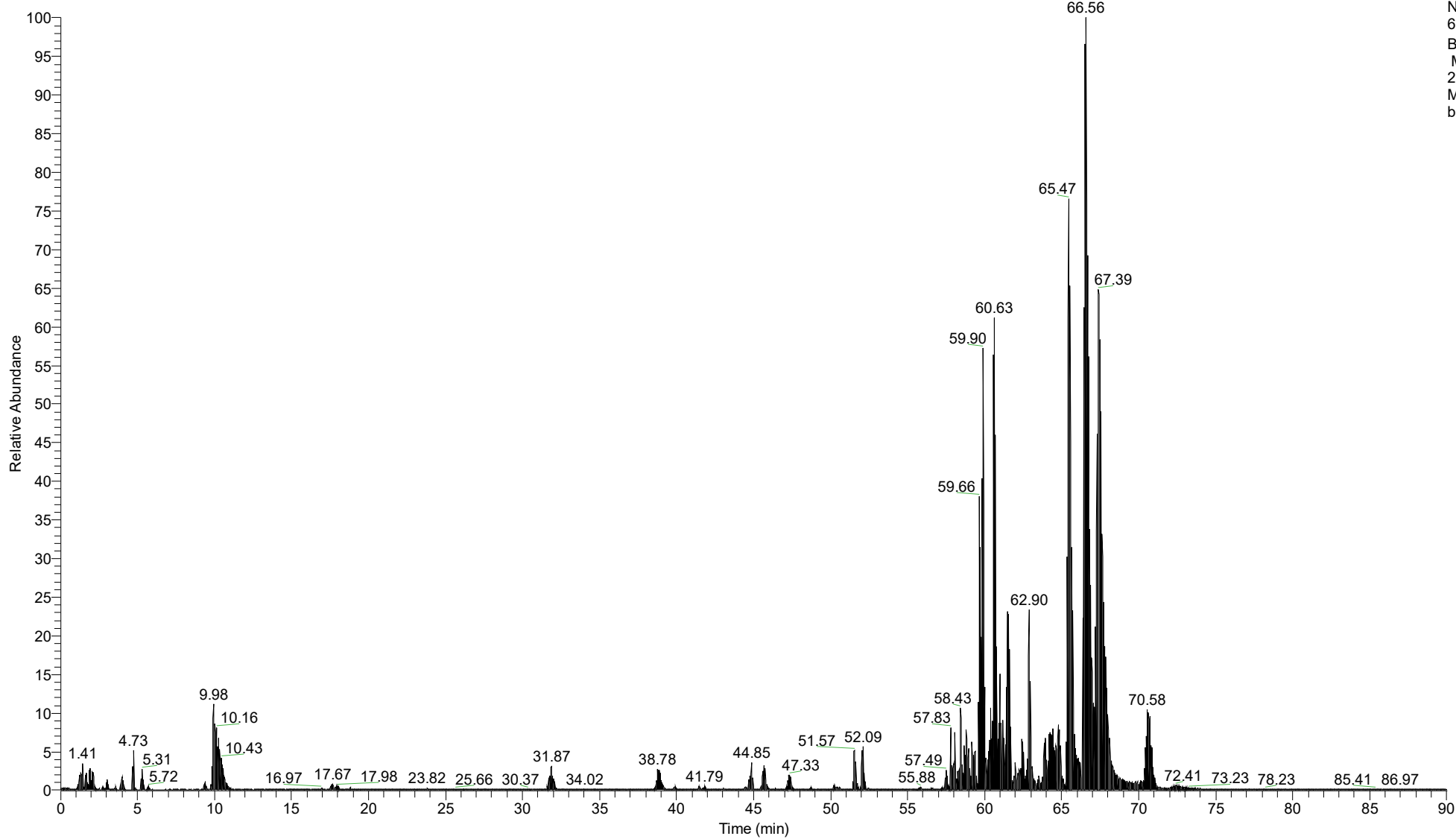
RT: 0.00 - 90.01



NL:
6.68E9
Base Peak
MS
20201008_
Multi_meta
bolite1-2

(A)80%methanol-3

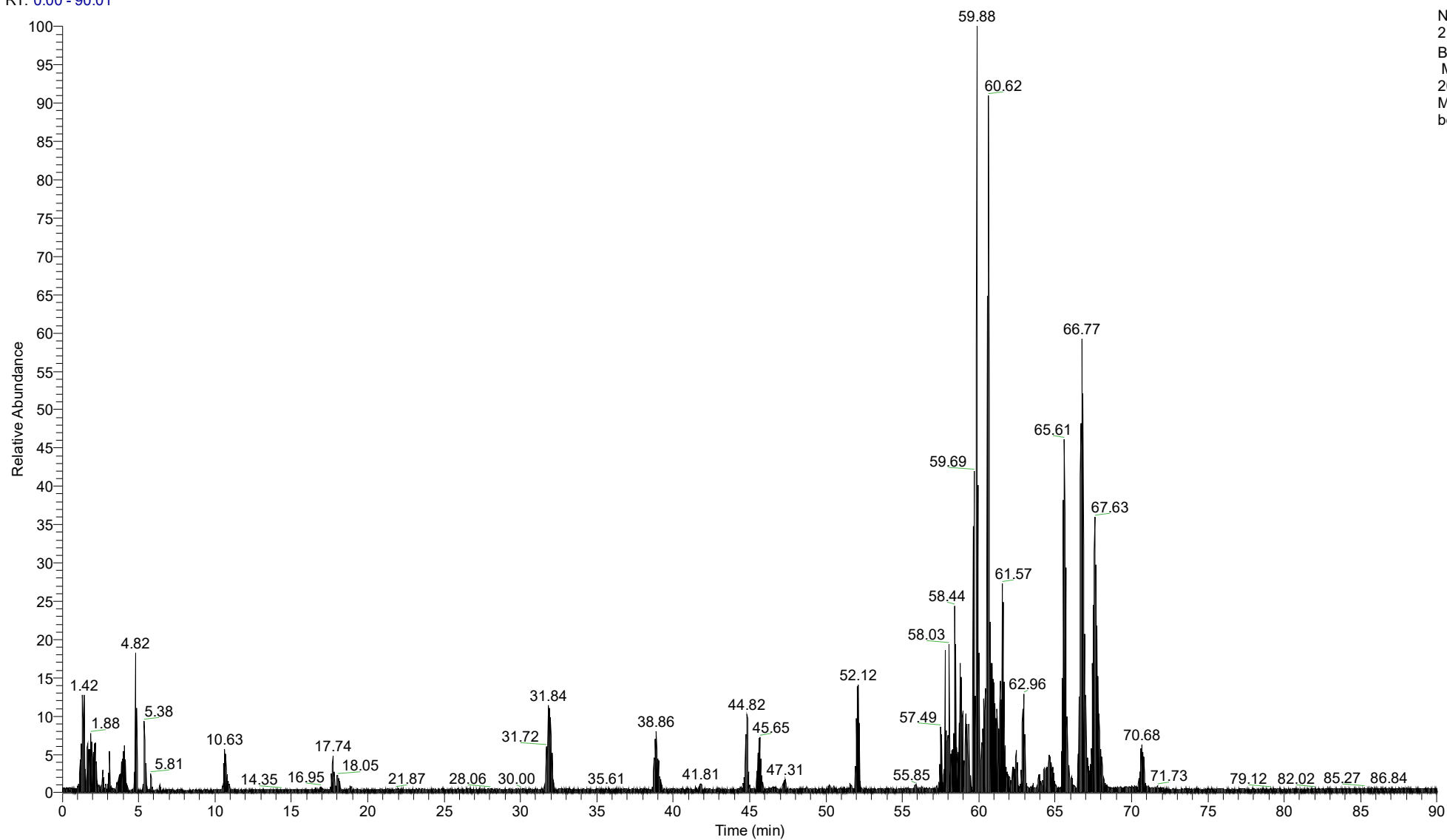
RT: 0.00 - 90.01



NL:
6.90E9
Base Peak
MS
20201008_
Multi_meta
bolite1-3

(B)Chloroform/methanol-1

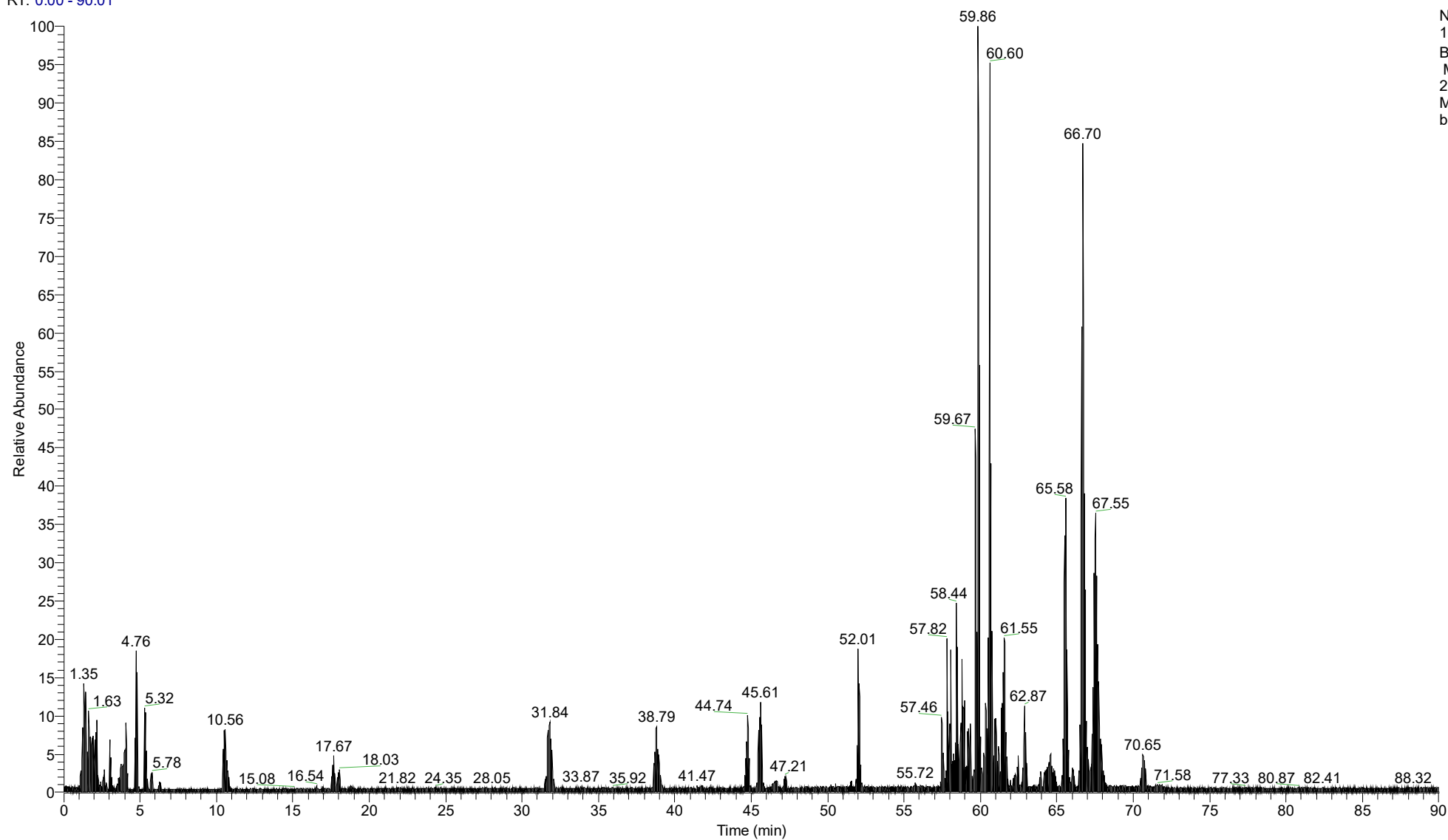
RT: 0.00 - 90.01



NL:
2.15E9
Base Peak
MS
20201008_
Multi_meta
bolite2-1

(B)Chloroform/methanol-2

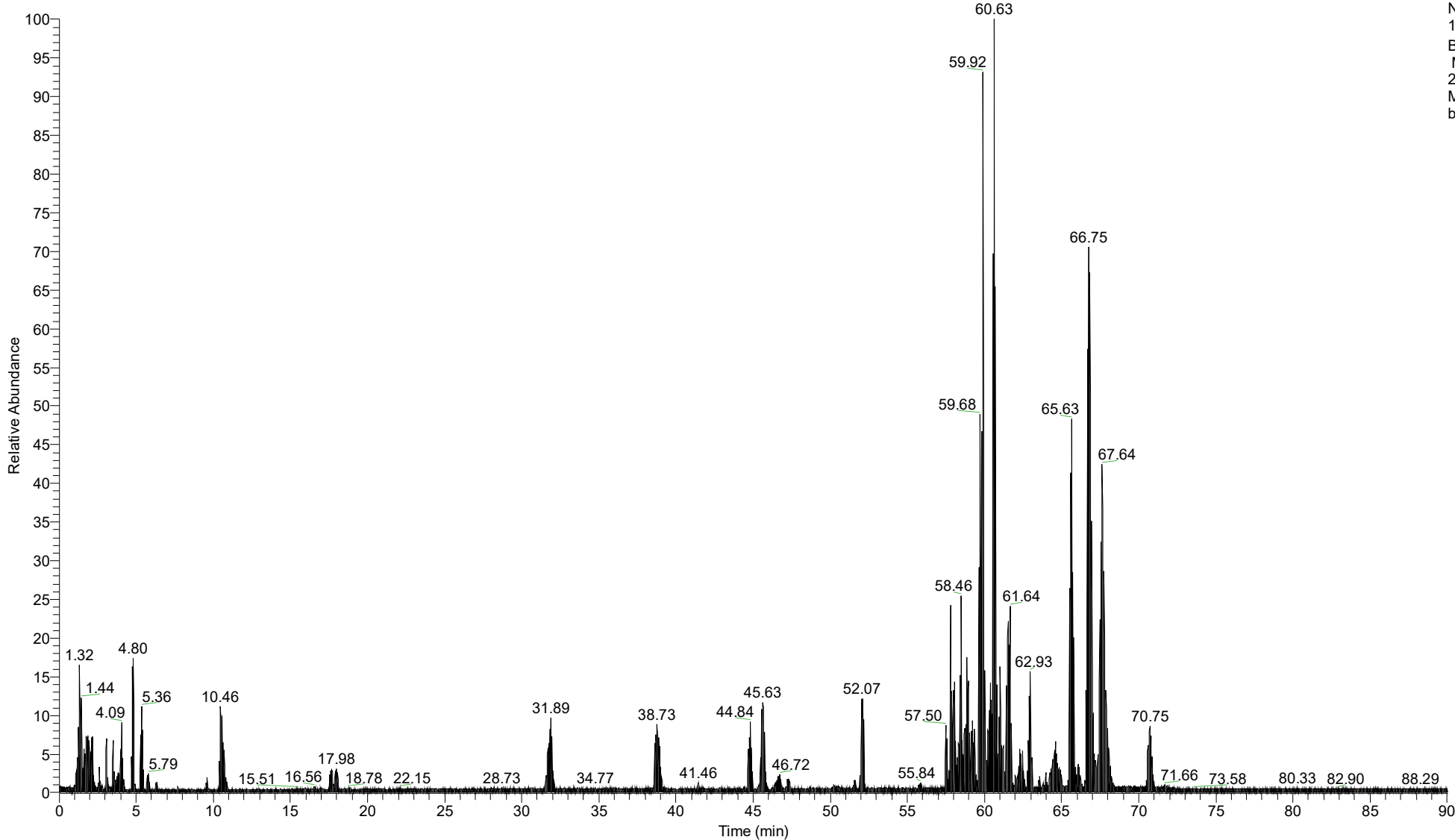
RT: 0.00 - 90.01



NL:
1.89E9
Base Peak
MS
20201008_
Multi_meta
bolite2-2

(B)Chloroform/methanol-3

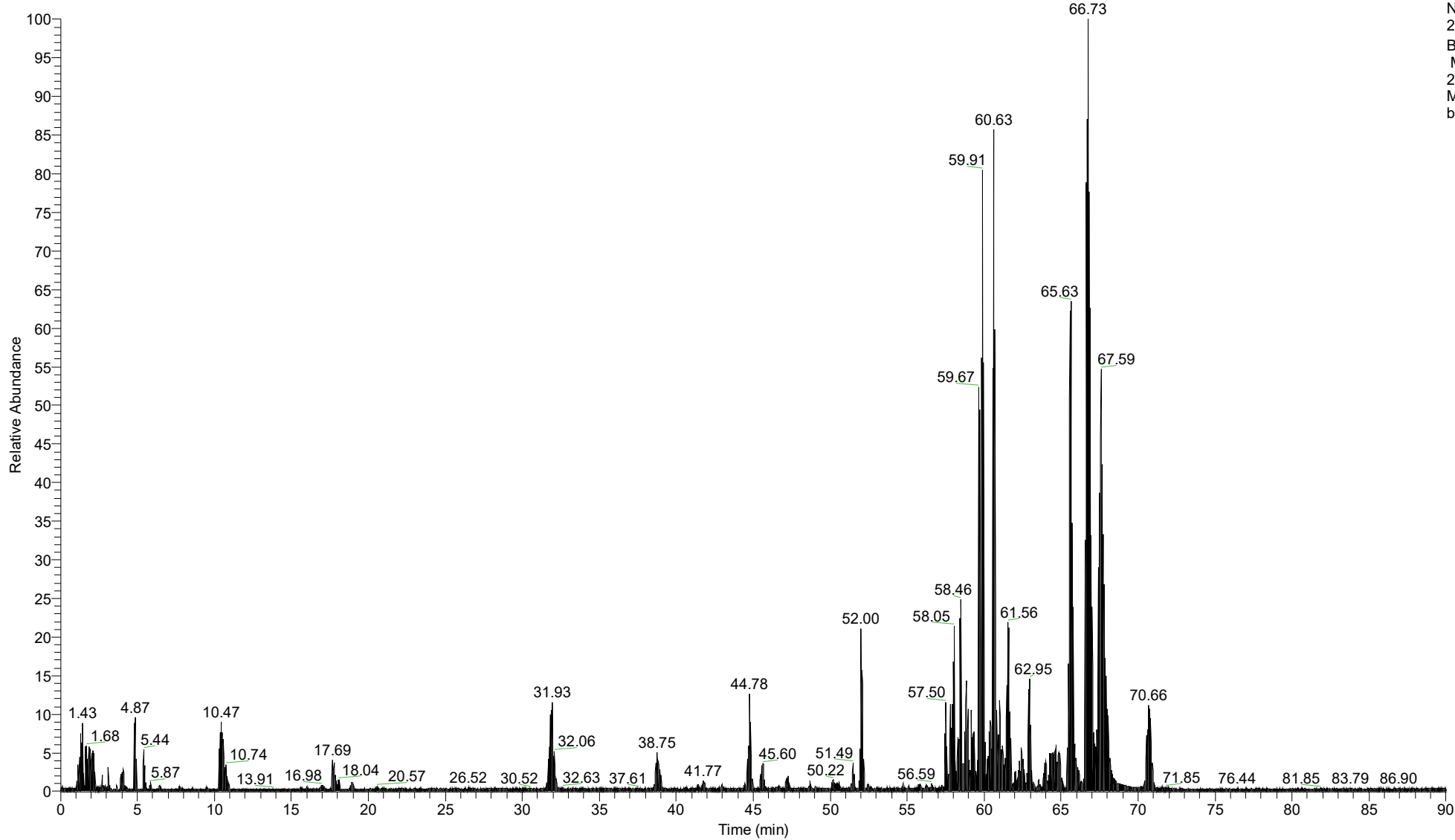
RT: 0.00 - 90.01



NL:
1.99E9
Base Peak
MS
20201008_
Multi_meta
bolite2-3

(C)MTBE-1

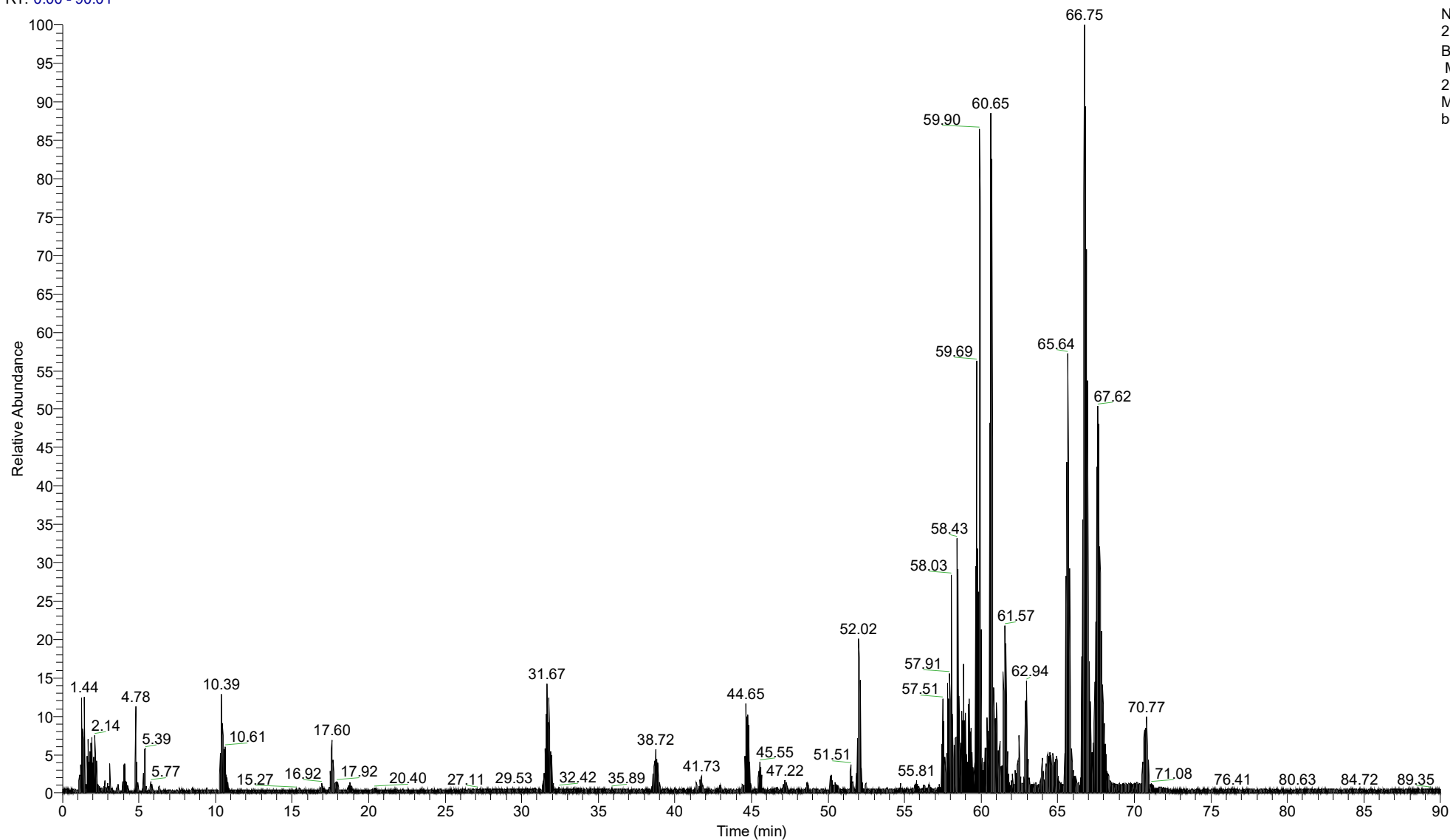
RT: 0.00 - 90.01



NL:
2.88E9
Base Peak
MS
20201008_
Multi_meta
bolite3-1

(C)MTBE-2

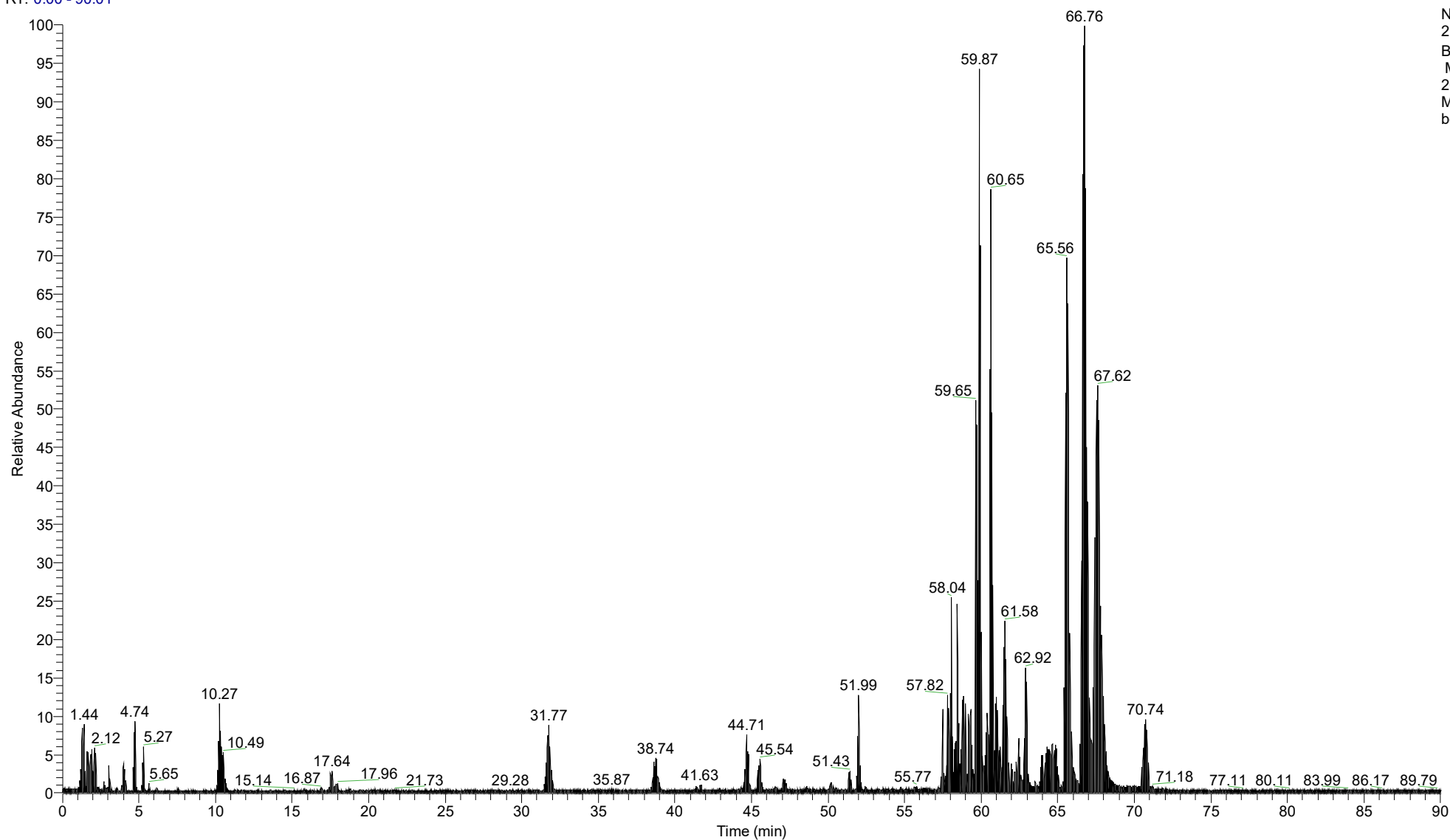
RT: 0.00 - 90.01



NL:
2.21E9
Base Peak
MS
20201008_
Multi_meta
bolite3-2

(C)MTBE-3

RT: 0.00 - 90.01



NL:
2.79E9
Base Peak
MS
20201008_
Multi_meta
bolite3-3

Figure S4 Chromatogram of metabolomics data of each method.

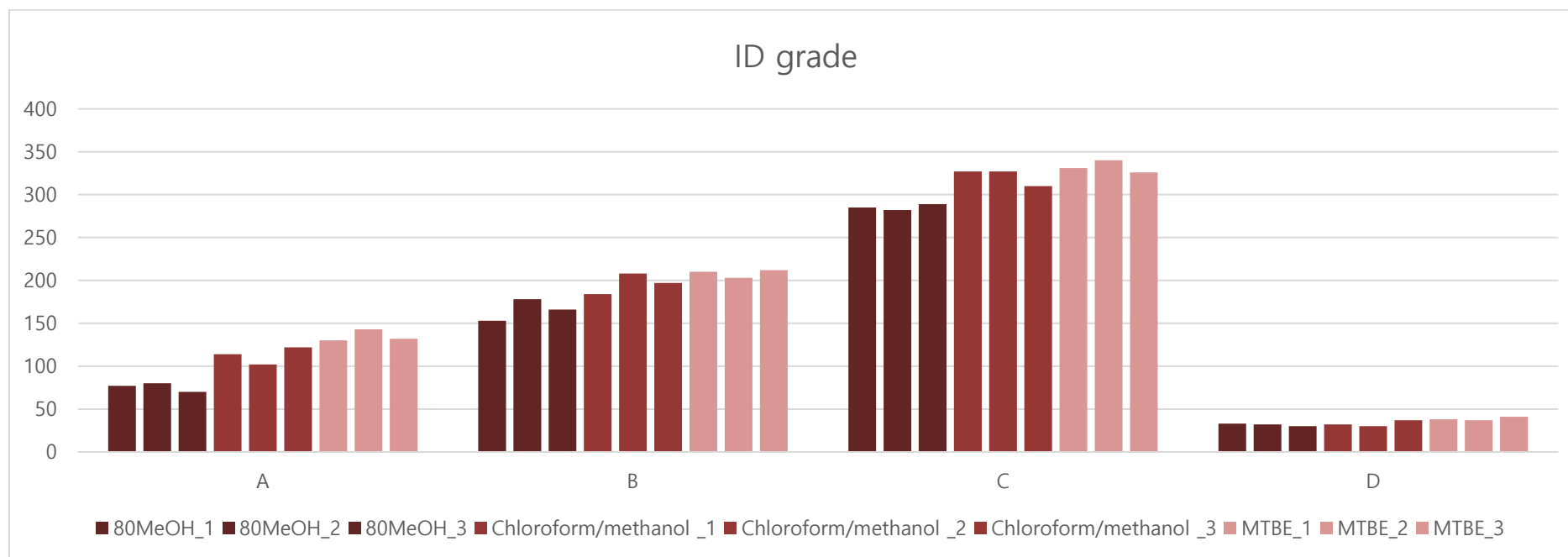
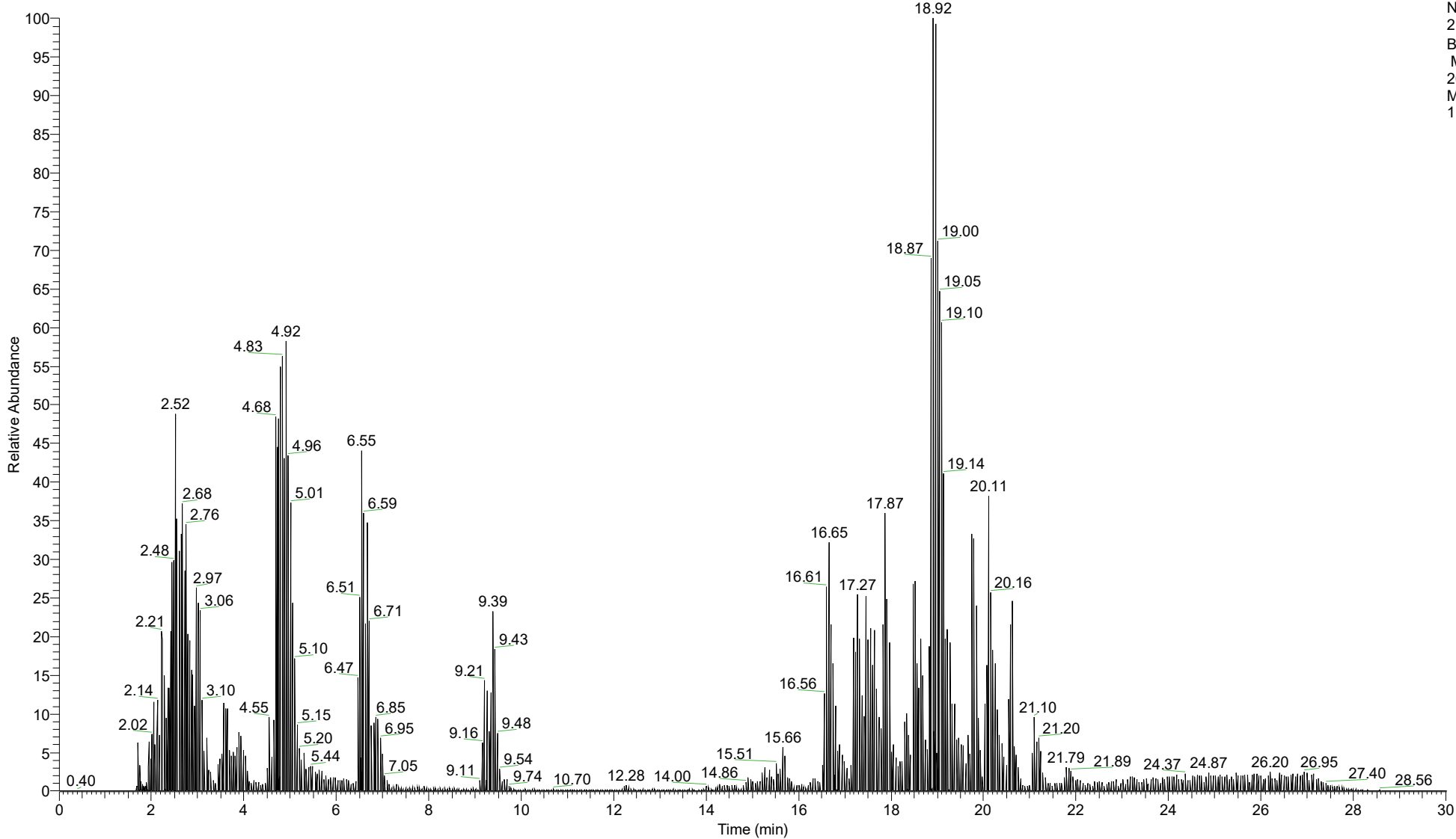


Figure S5. ID grade graph for each extraction method of lipids identified by lipid search. (ID Quality filter- Grade A : Lipid of which fatty acid chains and class were identified completely./ Grade B : Lipid of which class and some fatty acid chains were identified./Grade C : Lipid of which class or fatty acid was identified./Grade D : other)

(A)80%methanol-1

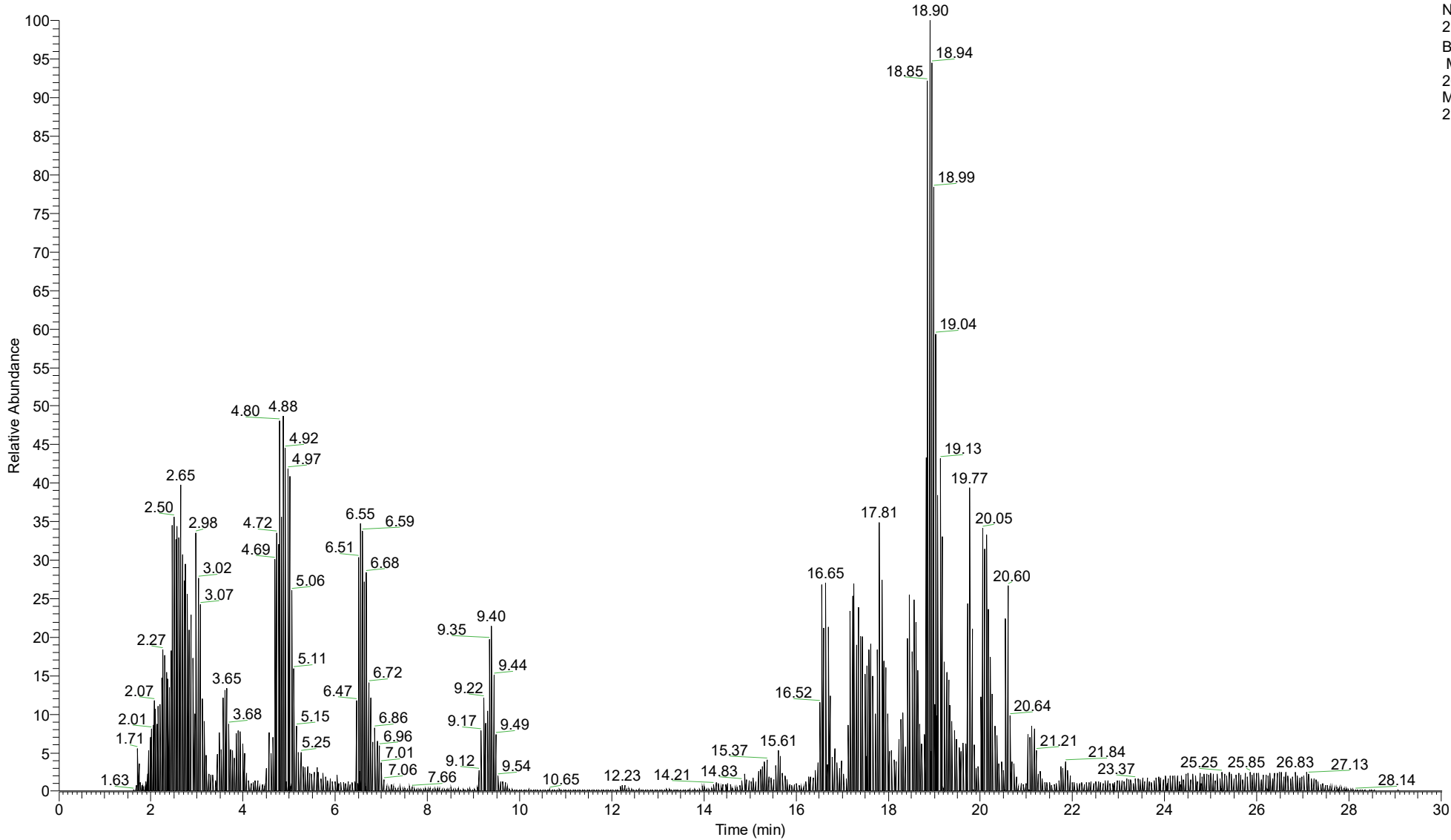
RT: 0.00 - 30.01



NL:
2.91E9
Base Peak
MS
20201007_
Multi_lipid1-
1

(A)80%methanol-2

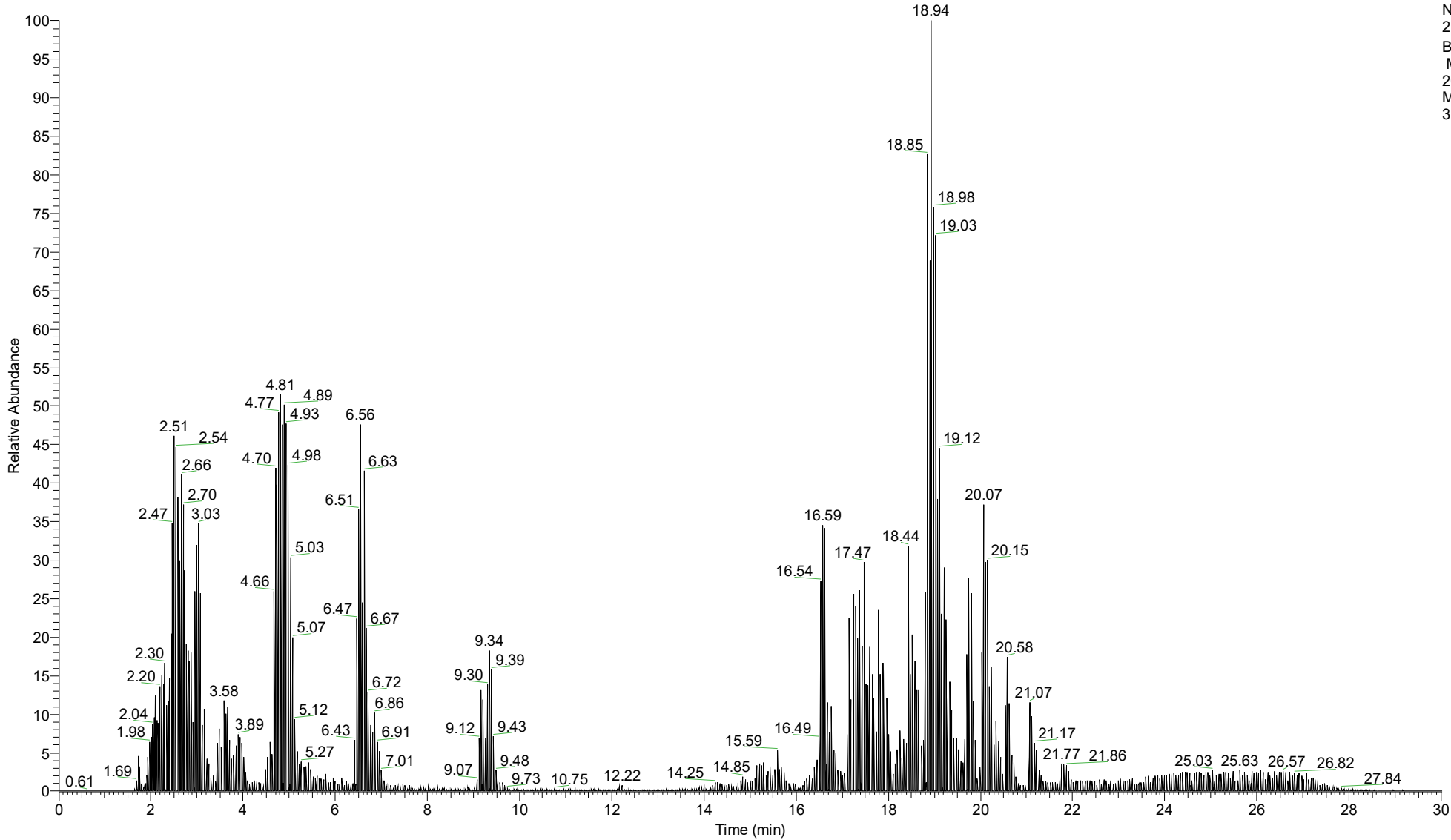
RT: 0.00 - 30.01



NL:
2.85E9
Base Peak
MS
20201007_
Multi_lipid1-
2

(A)80%methanol-3

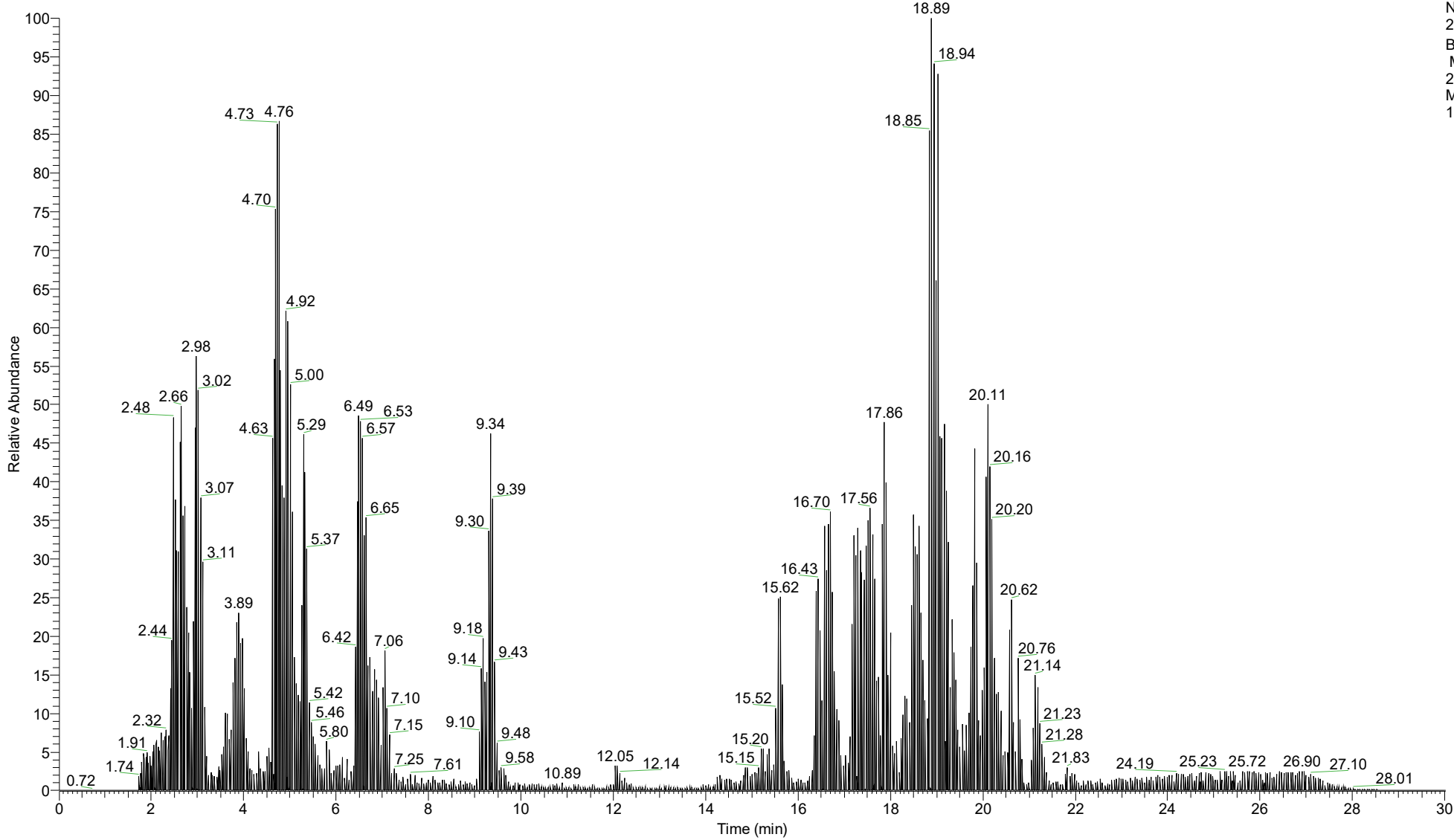
RT: 0.00 - 30.01



NL:
2.81E9
Base Peak
MS
20201007_
Multi_lipid1-
3

(B)Chloroform/methanol-1

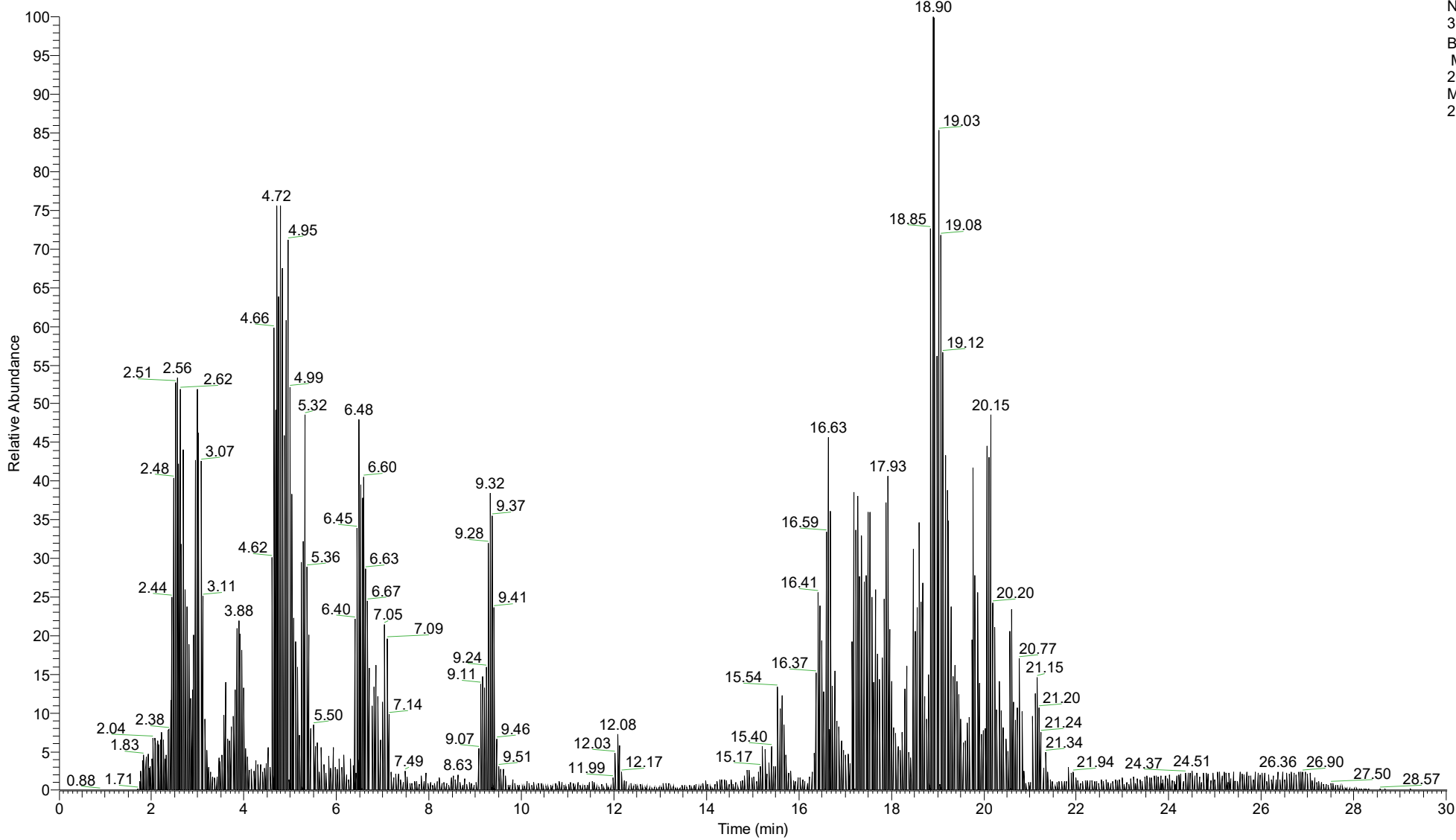
RT: 0.00 - 30.01



NL:
2.88E9
Base Peak
MS
20201007_
Multi_lipid2-
1

(B)Chloroform/methanol-2

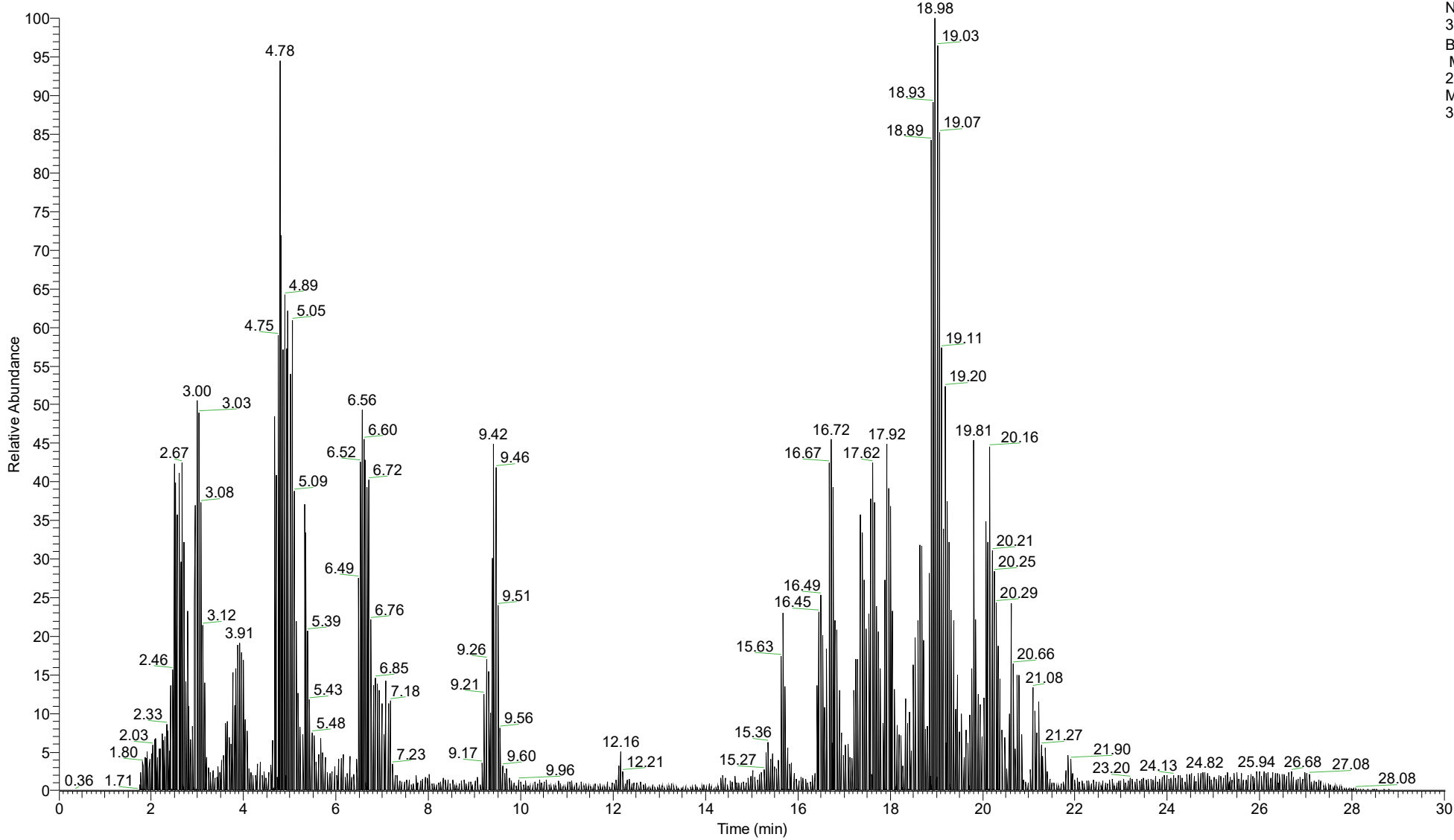
RT: 0.00 - 30.01



NL:
3.00E9
Base Peak
MS
20201007_
Multi_lipid2-
2

(B)Chloroform/methanol-3

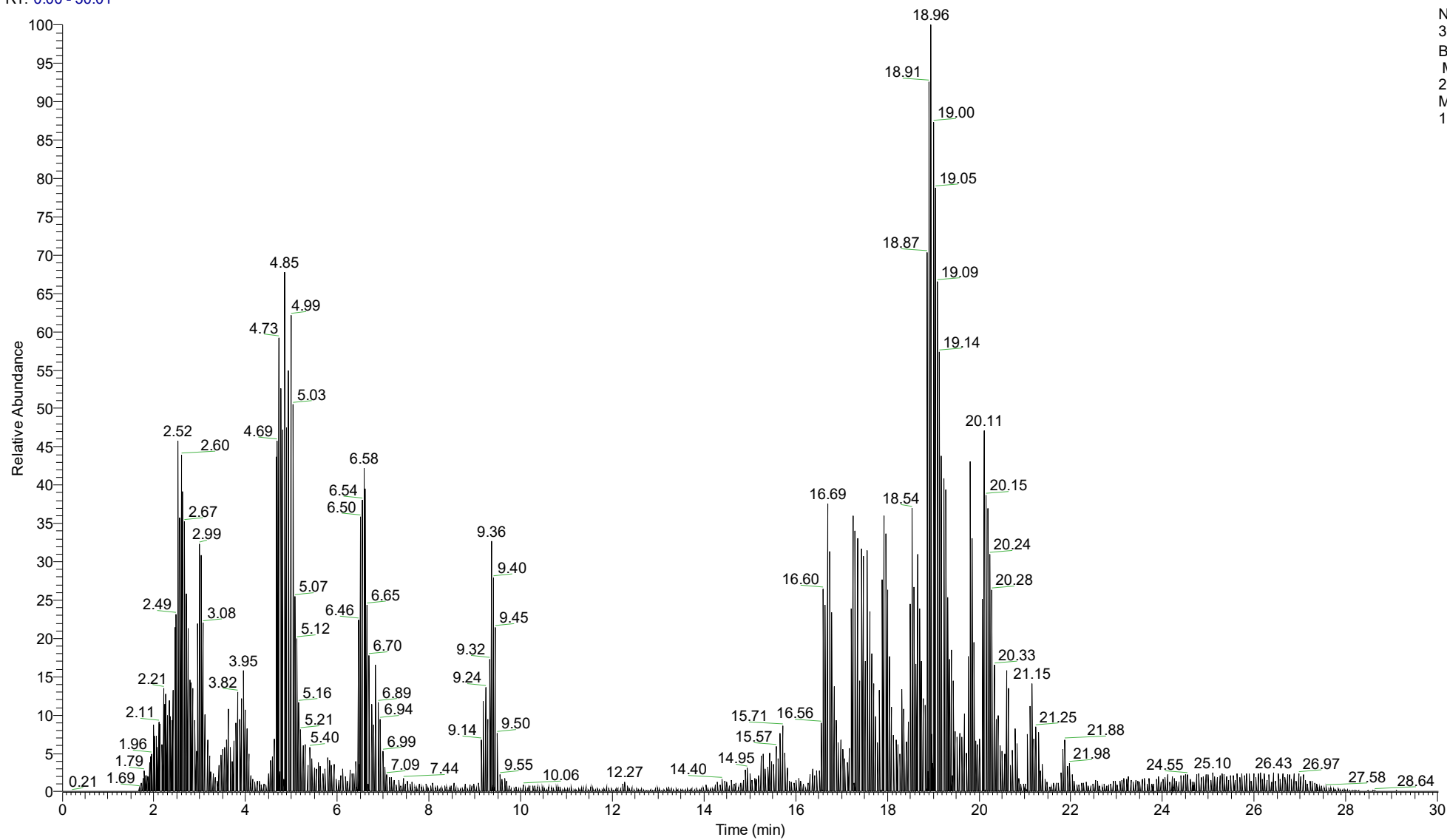
RT: 0.00 - 30.01



NL:
3.09E9
Base Peak
MS
20201007_
Multi_lipid2-
3

(C)MTBE-1

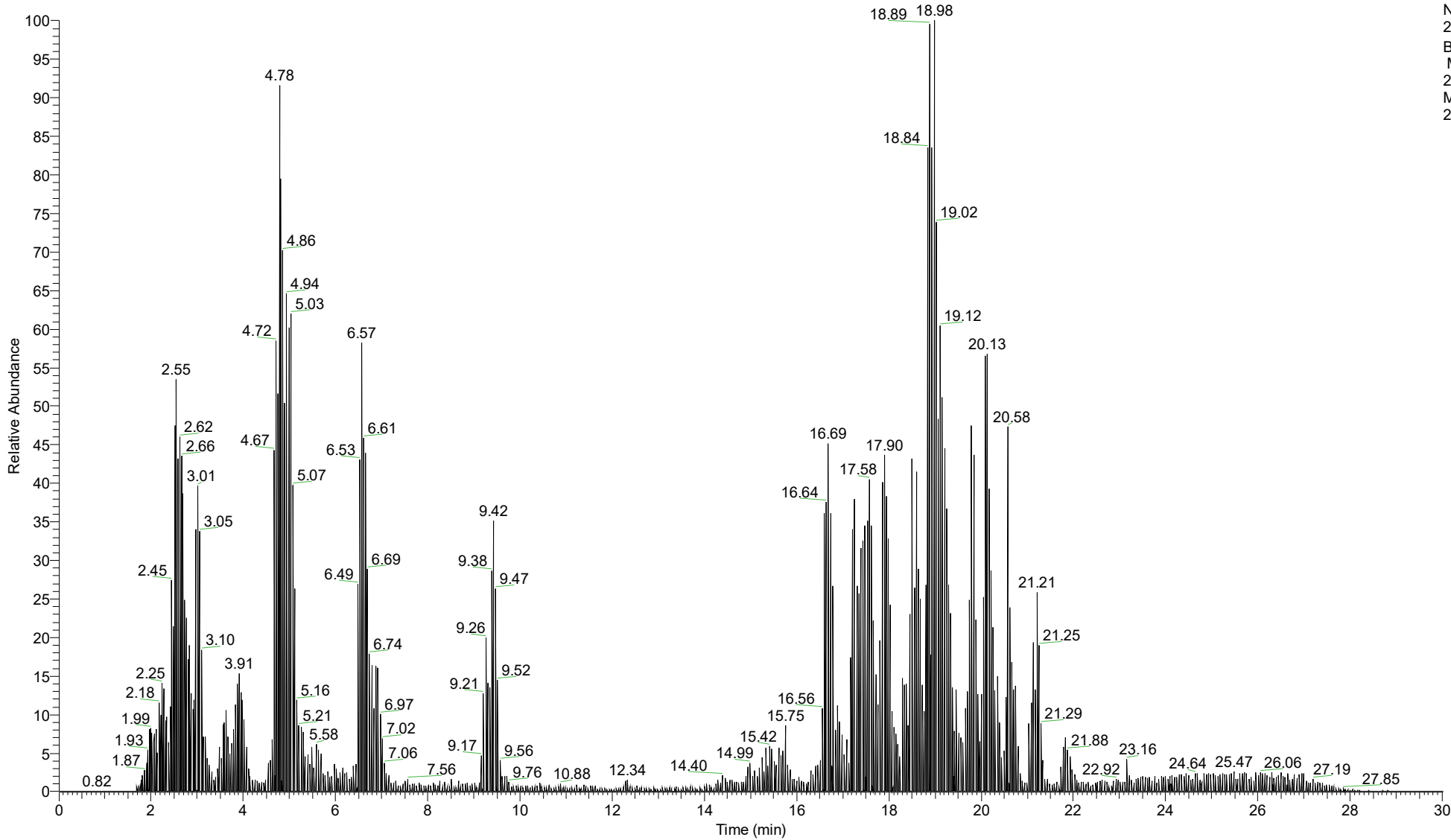
RT: 0.00 - 30.01



NL:
3.08E9
Base Peak
MS
20201007_
Multi_lipid3-
1

(C)MTBE-2

RT: 0.00 - 30.01



NL:
2.86E9
Base Peak
MS
20201007_
Multi_lipid3-
2

(C)MTBE-3

RT: 0.00 - 30.01

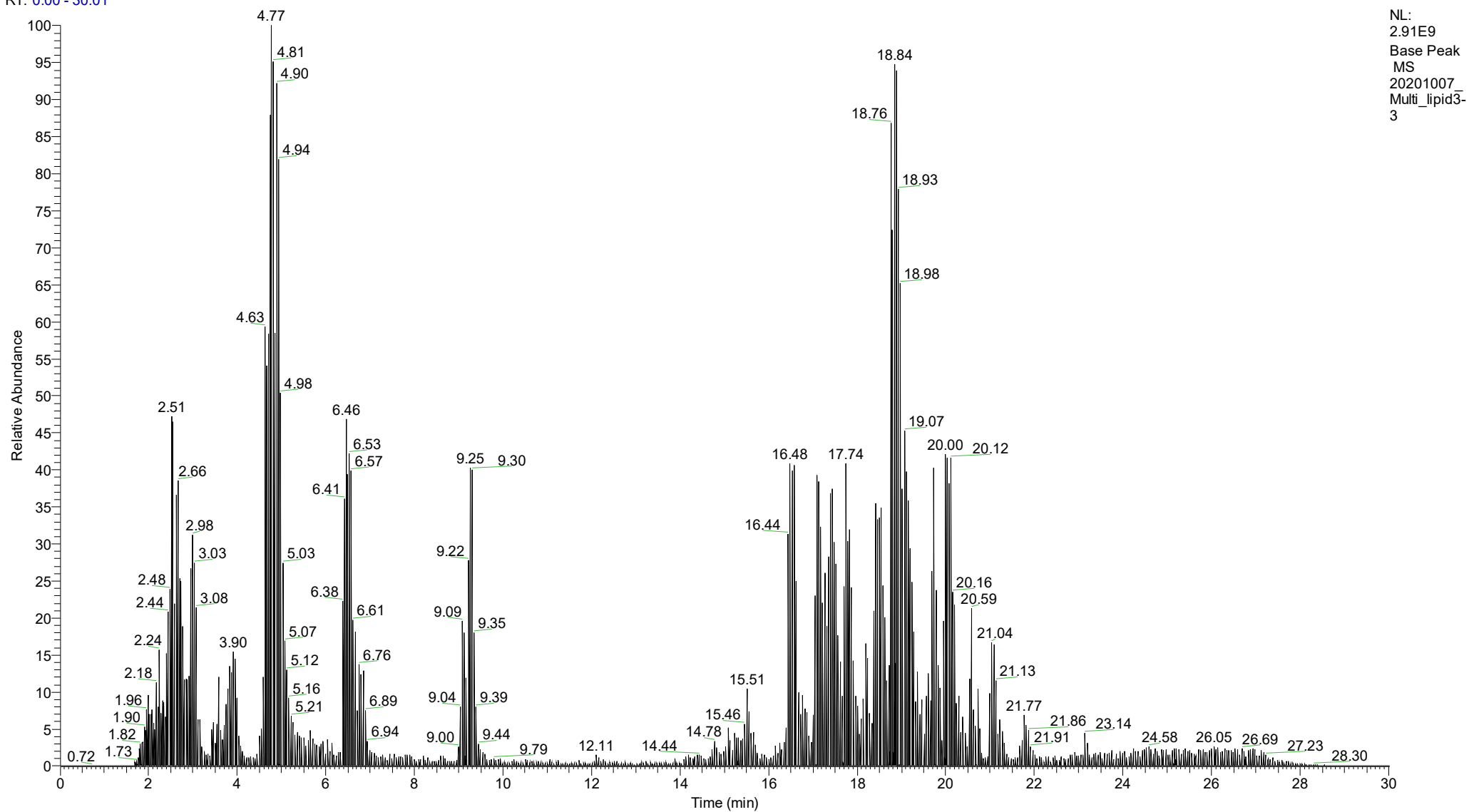
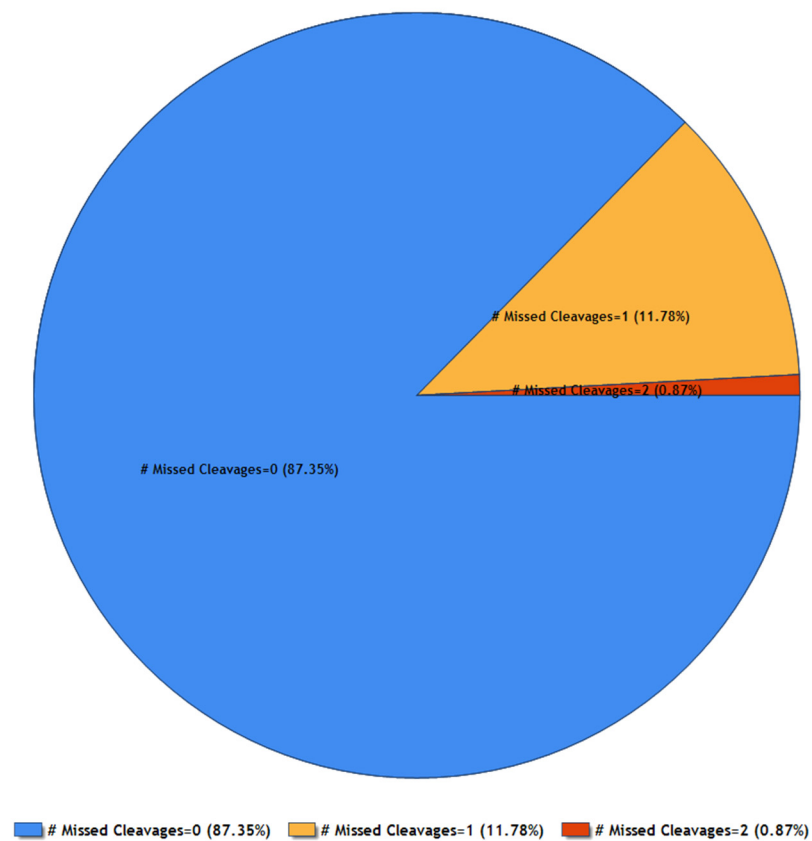
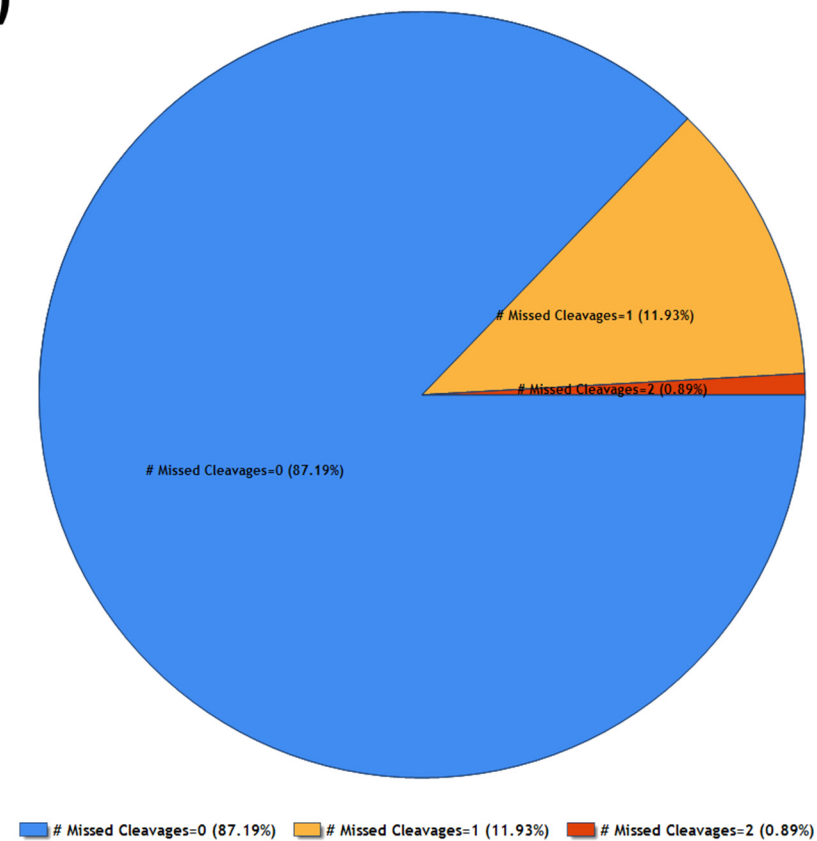


Figure S6 Chromatogram of lipidomics data of each method.

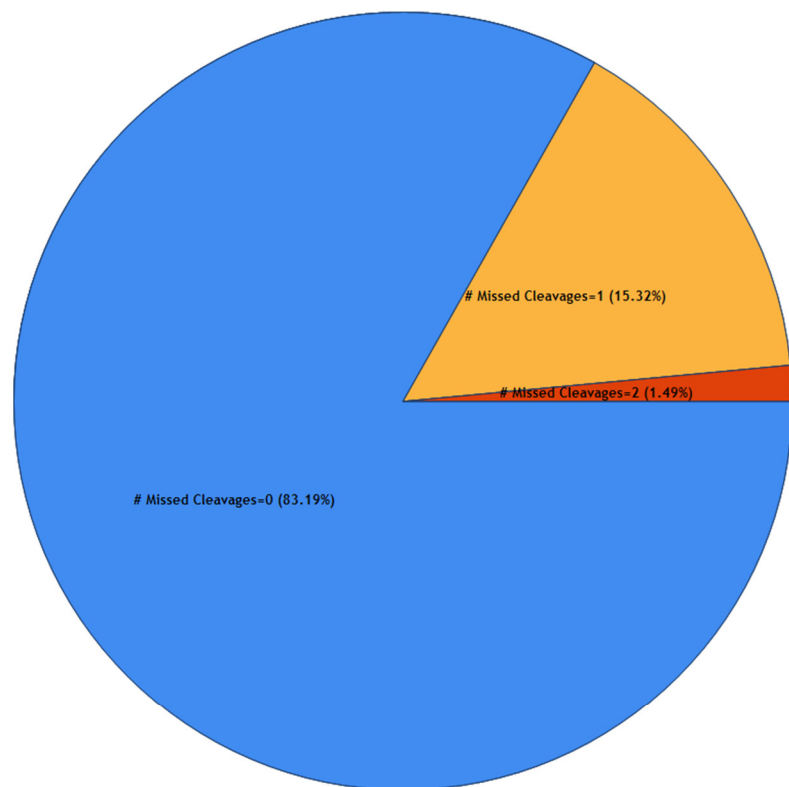
(A)



(B)

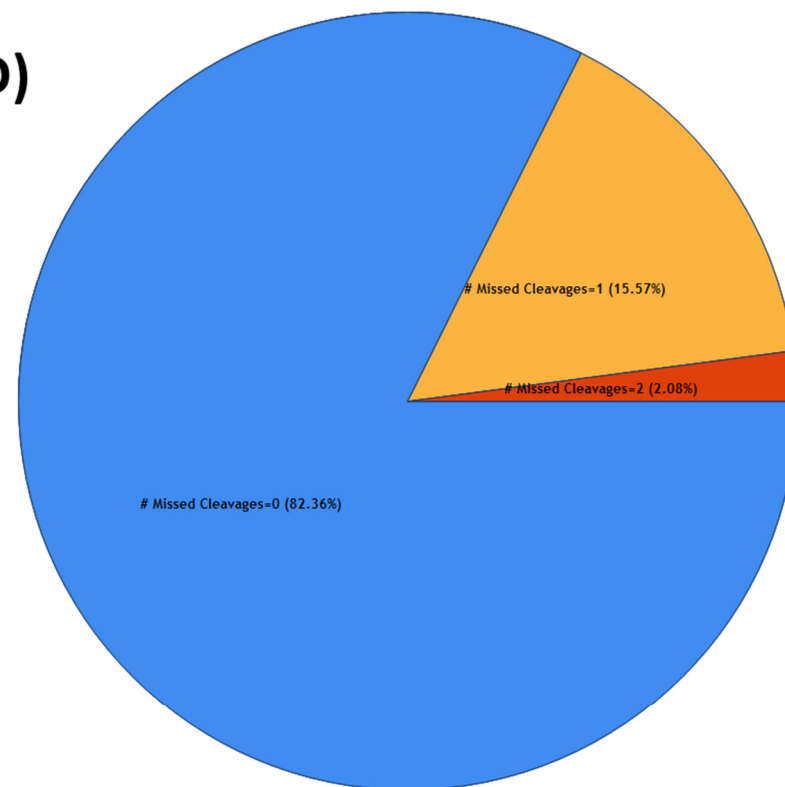


(C)



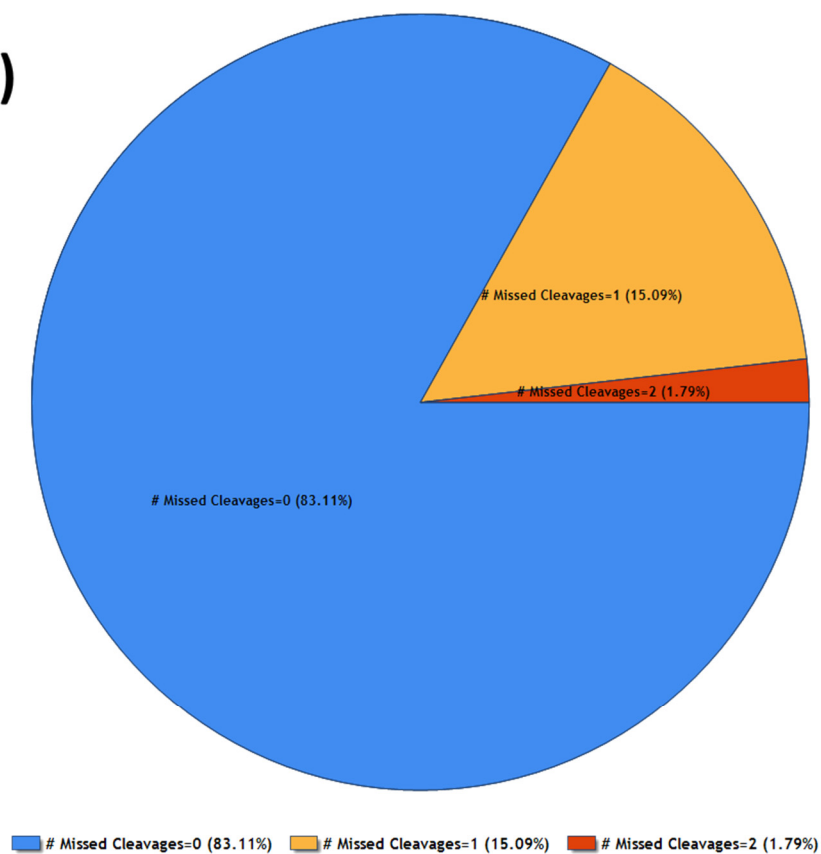
Missed Cleavages=0 (83.19%) # Missed Cleavages=1 (15.32%) # Missed Cleavages=2 (1.49%)

(D)



Missed Cleavages=0 (82.36%) # Missed Cleavages=1 (15.57%) # Missed Cleavages=2 (2.08%)

(E)



(F)

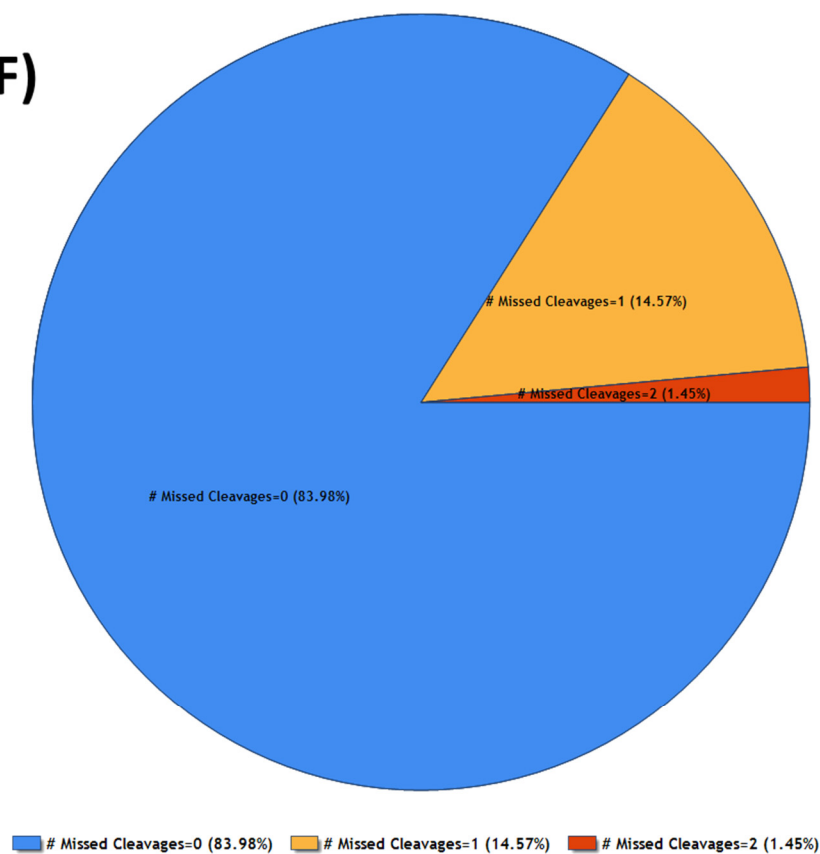


Figure S7 Number of missed cleavages in identified peptides. (A) FASP_80methanol, (B) FASP_Chloroform/methanol, (C) FASP_MTBE, (D) S-trap_80methanol, (E) S-trap_Chloroform/methanol, (F) S-trap_MTBE

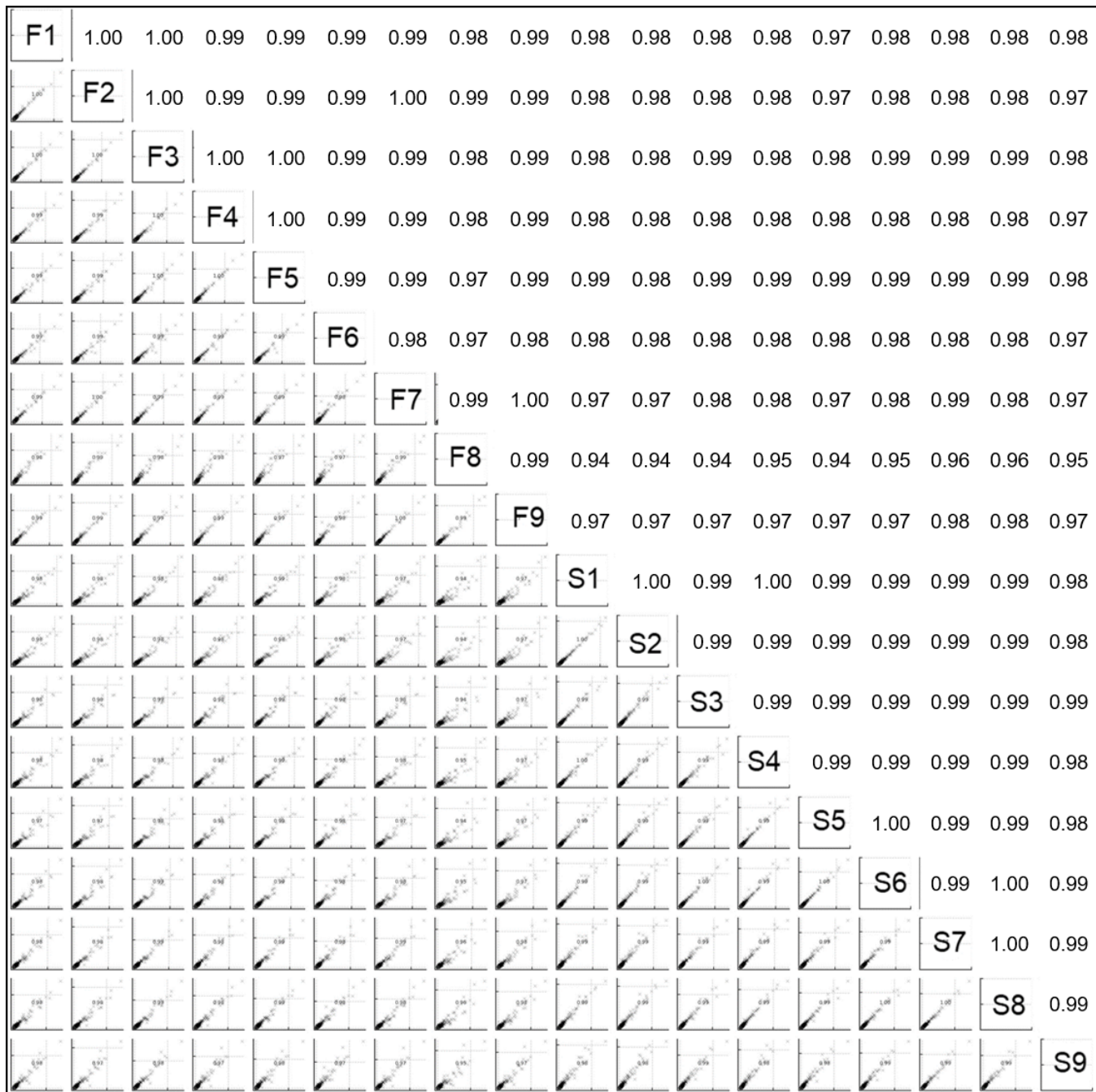


Figure S8 Correlation scatter plot in proteomics data

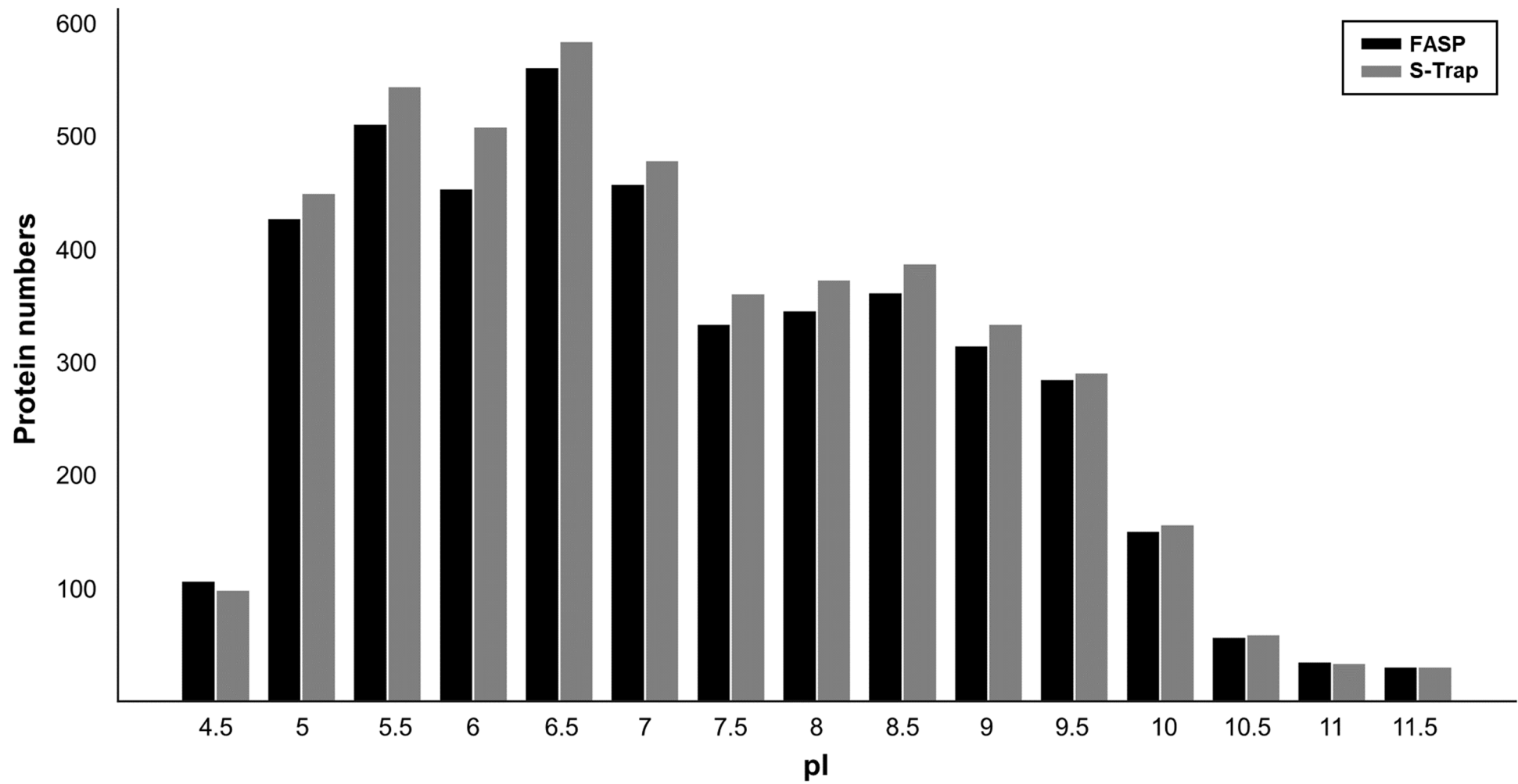


Figure S9. Histogram of pI(isoelectric points)

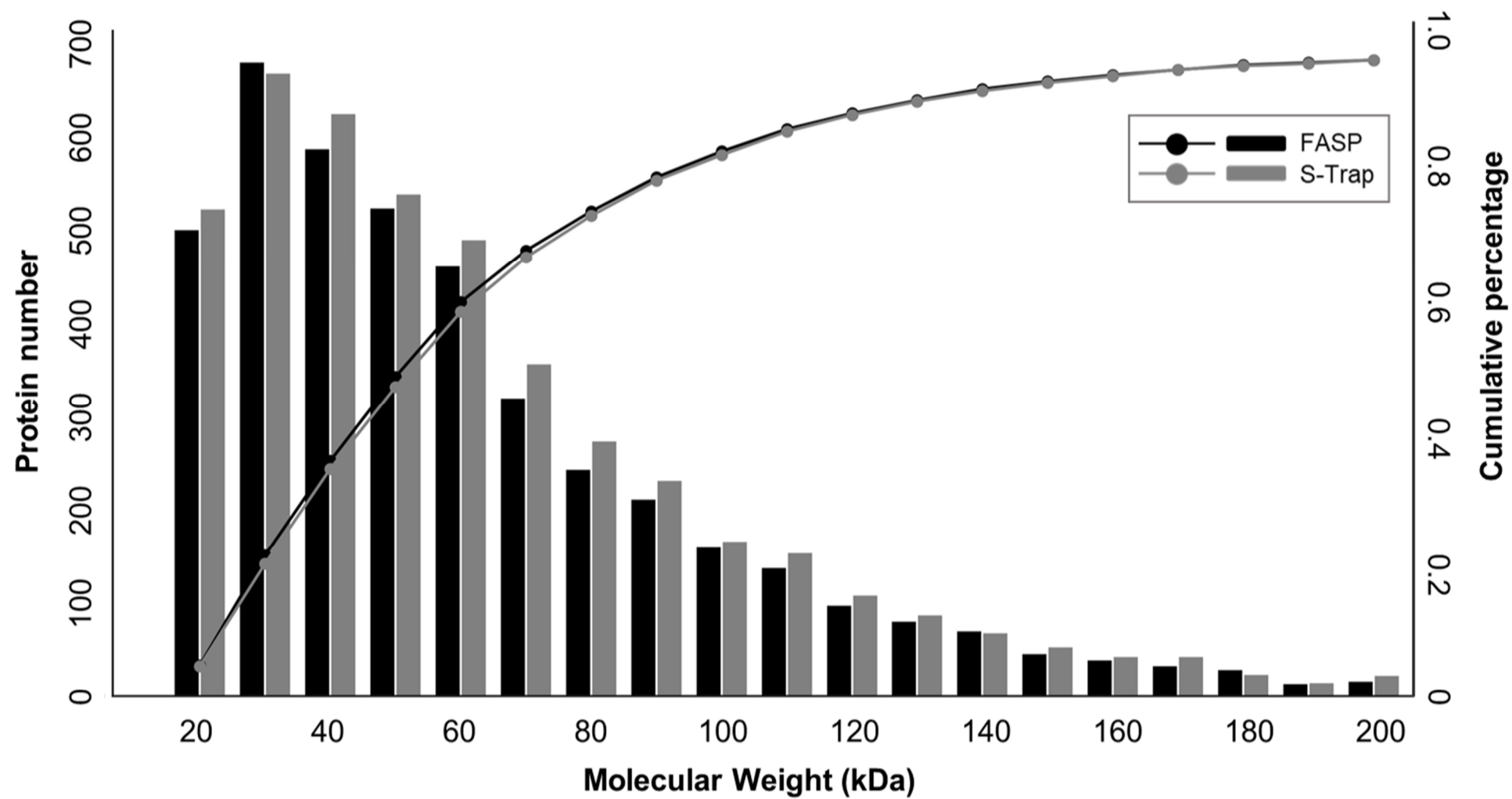


Figure S10. Histograms and cumulative distributions of molecular weight(MW)

FASP/S-Trap	log2(FC)	raw.pval	Gene name	Discription
Q71DI3	2.079	1.58E-07	H3C15	Histone H3.2
Q9BW91	-1.0016	0.00020524	NUDT9	ADP-ribose pyrophosphatase mitochondrial
Q7Z417	-1.075	0.0067655	NUDT9	FMR1-interacting protein NUFIP2

Table S2. Fold change and p-value of Q71DI3, Q9BW91, Q7Z417