Detailed characterization of alterations in lipid profiles during autophagic cell death of leukemia cells

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Table S1. Optimized MRM conditions for 23 lipids

Lipids	Ion mode	MRM transitions	MS/MS CE (eV)
TG	Positive	$[M+NH_4] > [M+NH_4-RCOONH_4]$	18
DG	Positive	$[M+NH_4] > [M+NH_4-35]$	8
ChE	Positive	$[M+NH_4] > 369$	8
PC	Positive	$[M+H] > 184$	26
PE	Positive	$[M+H] > [M+H-141]$	14
PG	Positive	$[M+NH_4] > [M+NH_4-189]$	14
LPC	Positive	$[M+H] > 184$	30
LPE	Positive	$[M+H] > [M+H-141]$	18
LPG	Positive	$[M+H] > [M+H-172]$	14
SM	Positive	$[M+H] > 184$	30
Cer	Positive	$[M+H] > 264$	26
dCer	Positive	$[M+H] > 266$	26
So	Positive	$[M+H] > [M+H-18]$	10
Sa	Positive	$[M+H] > [M+H-18]$	10
Methylated PS	Positive	$[M+H] > [M+H-213]$	20
Methylated PI	Positive	$[M+H] > [M+H-274]$	10
Methylated PA	Positive	$[M+H] > [M+H-126]$	0
Methylated LPS	Positive	$[M+H] > [M+H-213]$	20
Methylated LPI	Positive	$[M+H] > [M+H-274]$	12
Methylated LPA	Positive	$[M+H] > [M+H-126]$	14
Methylated Cer1P	Positive	$[M+H] > 264$	28
Methylated So1P	Positive	$[M+H] > 264$	12
Methylated Sa1P	Positive	$[M+H] > 266$	20

Table S2. Validation of analysis of 23 lipids based on MRM and the LODs of each lipid standard

Lipids[a]	RT[b] (min)	RSD (n=6) (%)[c]		Correlation (R^2)	Linear range (pg)	LOD (pg)
		RT[d]	Peak area[e]			
TG	3.47	1.1	5.7	0.9992	0.1 – 2000	0.1
DG	1.46	0.6	5.4	0.9986	0.2 – 2000	0.2
ChE	13.47	0.8	5.9	0.9894	1000 – 50000	1000
PC	1.66	1.1	4.9	0.9912	0.1 – 2000	0.1
PE	1.62	1.3	5.8	0.9954	0.2 – 2000	0.2
PG	1.46	0.8	8.9	0.9992	10 – 2000	10
LPC	1.36	1.0	4.8	0.9873	1 – 2000	1
LPE	1.38	1.2	5.7	0.9899	2 – 2000	2
LPG	1.27	0.9	3.5	0.9963	2 – 2000	2
SM	2.99	1.0	5.5	0.9956	1 – 2000	1
Cer	3.07	1.0	6.3	0.9962	1 – 2000	1
dCer	3.33	1.5	6.9	0.9984	1 – 2000	1
So	1.34	0.9	3.4	0.9803	10 – 2000	10
Sa	1.40	1.4	4.2	0.9984	10 – 2000	10
Methylated PS	1.88	0.2	4.2	0.9872	1 – 2000	1
Methylated PI	1.33	0.2	6.2	0.9954	100 – 50000	100
Methylated PA	2.14	0.3	4.8	0.9993	0.2 – 2000	0.2
Methylated LPS	1.57	0.2	5.4	0.9834	1 – 2000	1
Methylated LPI	1.32	0.2	6.5	0.9994	50 – 50000	50
Methylated LPA	2.04	0.8	7.3	0.9963	0.2 – 2000	0.2
Methylated Cer1P	3.75	0.2	4.8	0.9930	0.2 – 2000	0.2
Methylated So1P	1.39	0.1	4.5	0.9890	100 – 2000	100
Methylated Sa1P	1.44	0.2	4.4	0.9984	100 – 2000	100

a) Lipid standards used in this study were as follows: TG (11:1-11:1-11:1), DG (8:0-8:0), ChE (10:0), PC (10:0-10:0), PE (10:0-10:0), PG (10:0-10:0), LPC (13:0), LPE (14:0), LPG (14:0), SM (d18:1-12:0), Cer (d18:1-12:0), dCer (d18:1-12:0), So (d17:1), Sa (d17:0), PS (10:0-10:0), PI (8:0-8:0), PA (10:0-10:0), LPS (17:1), LPI (13:0), LPA (14:0), Cer1P (d18:1-12:0), So1P (d17:1), and Sa1P (d17:0).

b) Retention time

c) Relative standard deviation; the concentration of each lipid was 0.1 mg/mL.

d) Relative retention time (compound/internal standard)

e) Relative peak area (compound/internal standard)

Table S3. Various lipids analyzed by UPLC/QqQ-MS

Lipids	RT	Lipids	RT	Lipids	RT	Lipids	RT
TG(64:9)	21.2	TG(56:2)	20.2	DG(34:3)	5.5	PC(44:12)	3.2
TG(64:11)	18.3	TG(56:3)	19.8	DG(36:0)	12.4	PC(42:1)	16.6
TG(64:12)	17.4	TG(56:4)	19.3	DG(36:4)	5.5	PC(42:2)	14.5
TG(62:2)	21.2	TG(56:5)	19.1	DG(36:5)	4.4	PC(42:3)	12.2
TG(62:3)	20.9	TG(56:6)	18.4	DG(40:1)	14.8	PC(42:4)	10.5
TG(62:4)	20.6	TG(56:7)	18	DG(40:2)	12.6	PC(42:5)	8.8
TG(62:6)	19.9	TG(54:0)	20.6	DG(40:3)	11.3	PC(42:6)	7.1
TG(62:7)	19.6	TG(54:1)	20.2	DG(40:4)	9.7	PC(42:7)	6.4
TG(62:8)	19.1	TG(54:2)	19.8	DG(40:6)	6.3	PC(42:8)	4.8
TG(62:9)	18.5	TG(54:3)	19.3	DG(40:7)	5.6	PC(42:9)	4
TG(62:10)	17.9	TG(54:4)	18.8	DG(42:11)	2.2	PC(42:10)	3.6
TG(62:11)	17.4	TG(54:5)	18.5	DG(42:3)	12.8	PC(42:11)	3
TG(62:12)	16.4	TG(54:6)	18	DG(42:5)	9.8	PC(40:1)	14.8
TG(62:13)	15.7	TG(54:7)	16.9	DG(42:6)	8.2	PC(40:2)	12.2
TG(60:1)	21.2	TG(52:0)	20.3	DG(42:5)	9.8	PC(40:3)	10.2
TG(60:2)	20.9	TG(52:1)	19.8	DG(42:6)	8.2	PC(40:4)	8.8
TG(60:3)	20.6	TG(52:2)	19.3	ChE(22:4)	18.3	PC(40:5)	7.1
TG(60:4)	20.3	TG(52:3)	18.8	ChE(22:6)	16.6	PC(40:6)	5.7
TG(60:5)	19.9	TG(52:4)	18	ChE(20:1)	19.7	PC(40:7)	4.9
TG(60:6)	19.5	TG(52:5)	17.6	ChE(20:3)	18.2	PC(40:8)	4
TG(60:7)	19	TG(52:6)	16.2	ChE(20:4)	17.3	PC(40:9)	3.3
TG(60:8)	18.8	TG(50:0)	19.8	ChE(20:5)	16.1	PC(38:1)	12.2
TG(60:9)	18.2	TG(50:1)	19.3	ChE(18:1)	19	PC(38:2)	9.8
TG(60:10)	17.4	TG(50:2)	18.8	ChE(18:2)	18.2	PC(38:3)	8.4
TG(60:11)	16.3	TG(50:3)	18.1	ChE(18:3)	17	PC(38:4)	7.3
TG(60:12)	15.7	TG(48:0)	19.3	ChE(16:0)	18.9	PC(38:5)	5.5
TG(58:0)	21.3	TG(48:1)	18.8	ChE(16:1)	18	PC(38:6)	4.9
TG(58:1)	20.9	TG(48:2)	18	PC(46:6)	11.6	PC(38:7)	3.8
TG(58:2)	20.6	TG(48:8)	7.9	PC(46:7)	9.2	PC(36:1)	10
TG(58:3)	20.2	TG(46:0)	18.7	PC(44:2)	16.8	PC(36:2)	7.9
TG(58:4)	19.9	TG(46:1)	17.9	PC(44:3)	14.5	PC(36:3)	6.2
TG(58:5)	19.5	TG(46:2)	17	PC(44:4)	12.9	PC(36:4)	5.6
TG(58:6)	19	TG(44:0)	17.9	PC(44:5)	10.8	PC(36:5)	4.6
TG(58:7)	18.7	TG(44:1)	16.9	PC(44:6)	9.2	PC(36:6)	3.8
TG(58:8)	18	DG(34:0)	10.5	PC(44:7)	7.7	PC(36:7)	3.5
TG(56:0)	21	DG(34:1)	9.1	PC(44:8)	6.1	PC(34:0)	10.2
TG(56:1)	20.6	DG(34:2)	6.8	PC(44:10)	4.3	PC(34:1)	7.8

Table S3. Continued

Lipids	RT	Lipids	RT	Lipids	RT	Lipids	RT
PC(34:2)	6.2	PE(36:0)	10.8	PS(32:1)	6	PI(32:1)	18.7
PC(34:3)	5	PE(36:1)	8.8	PS(30:0)	6.2	PI(32:2)	18.1
PC(34:4)	4.2	PE(36:2)	7	PS(28:0)	5.3	PI(30:0)	18.7
PC(34:5)	3.6	PE(36:3)	5.4	PG(30:0)	4.1	PI(30:1)	18
PC(32:0)	8.4	PE(36:4)	4.9	PG(32:0)	5.3	PI(30:2)	16.9
PC(32:1)	6.4	PE(36:5)	4	PG(32:1)	4.1	PI(28:0)	17.8
PC(32:2)	5.2	PE(34:0)	8.8	PG(34:0)	6.9	PA(42:5)	12.5
PC(32:3)	4.4	PE(34:1)	6.9	PG(34:1)	5.3	PA(42:6)	11.3
PC(30:1)	6.6	PE(34:2)	5.4	PG(34:2)	4.1	PA(42:7)	9.6
PC(30:2)	5.3	PE(34:3)	4.6	PG(34:3)	3.3	PA(42:8)	8.1
PC(28:0)	7.3	PE(30:0)	5.2	PG(36:0)	8.8	PA(42:9)	7.3
PC(28:1)	5.5	PS(42:2)	13.2	PG(36:1)	6.9	PA(42:10)	5.5
PE(42:1)	14.7	PS(42:3)	11.4	PG(36:2)	5.4	PA(40:4)	12.5
PE(42:2)	12.8	PS(42:4)	10	PG(36:3)	4.3	PA(40:5)	10.6
PE(42:3)	10.9	PS(42:5)	8.5	PG(36:4)	3.9	PA(40:6)	9.2
PE(42:4)	9.5	PS(42:6)	7.1	PG(38:1)	8.9	PA(38:1)	15.1
PE(42:5)	8	PS(42:7)	6.2	PG(38:2)	7.1	PA(38:2)	13.6
PE(42:6)	6.2	PS(40:1)	13.2	PG(38:3)	5.8	PA(38:3)	12.4
PE(42:7)	5.4	PS(40:2)	11.3	PG(38:4)	4.6	PA(38:4)	10.6
PE(42:8)	4.5	PS(40:3)	10	PG(38:5)	3.8	PA(38:5)	8.7
PE(42:9)	3.4	PS(40:4)	8.4	PG(38:6)	3.5	PA(38:6)	7
PE(42:10)	3.2	PS(40:5)	6.9	PG(40:5)	4.7	PA(38:7)	6.2
PE(40:1)	12.8	PS(40:6)	6.2	PG(40:6)	4.5	PA(36:1)	13.3
PE(40:2)	10.8	PS(40:7)	4.7	PG(40:7)	3.5	PA(36:2)	11.5
PE(40:3)	9.3	PS(38:1)	11.3	PI(38:0)	20.6	PA(36:3)	10.5
PE(40:4)	7.8	PS(38:2)	9.4	PI(38:1)	20.2	PA(36:4)	8.6
PE(40:5)	6.4	PS(38:3)	8	PI(38:2)	19.8	PA(34:0)	10.5
PE(40:6)	5.7	PS(38:4)	7.3	PI(38:3)	19.4	PA(34:1)	8.6
PE(40:7)	4.2	PS(38:5)	5.6	PI(36:0)	20.2	PA(34:2)	6.8
PE(40:8)	3.6	PS(38:6)	4.5	PI(36:1)	19.8	PA(32:0)	8.6
PE(38:1)	10.8	PS(36:1)	9.3	PI(36:2)	19.3	PA(32:1)	6.8
PE(38:2)	8.9	PS(36:2)	7.5	PI(36:3)	18.7	PA(32:2)	6.1
PE(38:3)	7.6	PS(36:3)	6.1	PI(36:4)	17.9	PA(32:3)	4.9
PE(38:4)	6.5	PS(34:0)	9.2	PI(34:0)	19.8	PA(30:0)	6.2
PE(38:5)	5	PS(34:1)	7.4	PI(34:1)	19.3	PA(30:1)	5.1
PE(38:6)	4.4	PS(34:2)	5.9	PI(34:2)	18.6	PA(30:2)	4.3
PE(38:7)	3.3	PS(32:0)	7.3	PI(32:0)	19.3	PA(28:0)	4.7

Table S3. Continued

Lipids	RT	Lipids	RT	Lipids	RT	Lipids	RT
PA(28:1)	4.2	LPE(22:4)	1.57	LPA(20:5)	1.27	Cer(d18:1-16:0)	5.8
PA(28:2)	3.4	LPE(22:6)	1.38	LPA(18:0)	2.15	Cer(d18:1-18:0)	7.6
LPC(14:0)	1.56	LPS(18:0)	2	LPA(18:1)	1.83	Cer(d18:1-20:0)	9.6
LPC(16:0)	1.88	LPS(18:1)	1.69	LPA(18:2)	1.59	Cer(d18:1-20:1)	7.6
LPC(16:1)	1.63	LPG(16:0)	1.45	LPA(18:3)	1.29	Cer(d18:1-22:0)	11.7
LPC(18:0)	2.3	LPG(18:1)	1.47	LPA(16:0)	1.82	Cer(d18:1-22:1)	9.6
LPC(18:1)	1.8	LPG(20:1)	1.79	LPA(16:1)	1.56	Cer(d18:1-24:0)	13.7
LPC(18:2)	1.69	LPG(20:4)	1.36	SM(d18:1-24:0)	14.9	Cer(d18:1-24:1)	11.7
LPC(18:3)	1.57	LPG(20:5)	1.26	SM(d18:1-24:1)	12.6	dCer(d18:0-24:0)	13.6
LPC(20:1)	1.79	LPG(22:6)	1.28	SM(d18:1-22:0)	7.8	dCer(d18:0-24:1)	11.7
LPC(20:3)	1.69	LPI(22:4)	1.48	SM(d18:1-22:1)	6.4	dCer(d18:0-16:0)	5.8
LPC(20:4)	1.53	LPI(22:6)	1.47	SM(d18:1-22:4)	3.7	Cer1P(d18:1-24:0)	13.3
LPC(20:5)	1.4	LPI(20:4)	1.45	SM(d18:1-20:0)	9.8	Cer1P(d18:1-24:1)	11.4
LPC(22:4)	1.56	LPI(18:1)	1.47	SM(d18:1-20:1)	8	Cer1P(d18:1-22:0)	11.5
LPC(22:6)	1.5	LPI(18:2)	1.3	SM(d18:1-20:3)	5.6	Cer1P(d14:1-24:1)	9.3
LPC(24:0)	2.1	LPI(16:0)	1.44	SM(d18:1-20:4)	3.7	Cer1P(d18:1-18:0)	7.3
LPC(24:1)	1.9	LPA(24:0)	4.23	SM(d18:1-18:0)	8.1	Cer1P(d18:1-16:0)	5.6
LPE(16:0)	1.62	LPA(24:1)	3.33	SM(d18:1-18:1)	6.3	Cer1P(d18:1-14:0)	4.3
LPE(16:1)	1.46	LPA(22:0)	3.29	SM(d18:1-18:2)	4.8	So(d16:1)	1.2
LPE(18:0)	1.94	LPA(22:1)	2.66	SM(d18:1-16:0)	6.3	So(d14:1)	1.16
LPE(18:1)	1.64	LPA(22:4)	1.65	SM(d18:1-16:1)	5	Sa(d18:0)	1.62
LPE(18:2)	1.48	LPA(22:6)	1.49	Cer(d16:1-16:0)	4.4	So1P(d18:1)	1.43
LPE(20:1)	1.65	LPA(20:0)	2.63	Cer(d16:1-22:0)	9.7	Sa1P(d18:0)	1.49
LPE(20:3)	1.54	LPA(20:1)	2.18	Cer(d16:1-24:0)	11.8		
LPE(20:4)	1.42	LPA(20:3)	1.61	Cer(d16:1-24:1)	9.7		
LPE(20:5)	1.34	LPA(20:4)	1.54	Cer(d18:1-14:0)	4.4		

Figure S1. Total ion chromatogram of various lipids in cancer cells