

Acquisition Method Report

Acquisition Method Info

Method Name Metabolomics_method_4-15-19.m

Method Path D:\MassHunter\methods\Thomas\Metabolomics_method_4-15-19.m

Method Description ESI Positive MRM Reserpine Checkout Method

Device List

Sampler
Binary Pump
Column Oven
QQQ

MS QQQ Mass Spectrometer

Ion Source ESI **Tune File** D:\MassHunter\Tune\QQQ\G6470A\atunes.tune.xml

Stop Mode By StopTime **Stop Time (min)** 40

Time Filter On **Time Filter Width (min)** 0.07

Time Segments

Index	Start Time (min)	Scan Type	Ion Mode	Div Valve	Delta EMV (+)	Delta EMV (-)	Store
1	0	MRM	ESI	To MS	300	300	Yes

Time Segment 1

Scan Segments

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Succinyl-CoA 13-C	No	891	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Positive
	Malonyl-CoA 13-C	No	877	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Positive
	Succinyl-CoA	No	866	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Positive
	Malonyl-CoA	No	853	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Positive
	Acetyl-CoA 13-C	No	812	Unit/Enh (6490)	303	Unit/Enh (6490)	5	40	30	7	Positive
	FAD 13-C	No	811	Unit/Enh (6490)	454	Unit/Enh (6490)	5	100	42	7	Positive
	Acetyl-CoA	No	810	Unit/Enh (6490)	303	Unit/Enh (6490)	5	40	30	7	Positive
	FAD	No	784	Unit/Enh (6490)	437	Unit/Enh (6490)	5	100	42	7	Positive
	NADP 13-C	No	765	Unit/Enh (6490)	141	Unit/Enh (6490)	5	135	58	7	Positive
	NADP 13-C	No	763	Unit/Enh (6490)	635	Unit/Enh (6490)	5	135	30	7	Positive
	NADP	No	744	Unit/Enh (6490)	136	Unit/Enh (6490)	5	135	58	7	Positive
	NADP	No	744	Unit/Enh (6490)	136	Unit/Enh (6490)	5	100	42	7	Positive
	NAD 13-C	No	687	Unit/Enh (6490)	670	Unit/Enh (6490)	5	135	65	7	Positive
	NADH 13-C	No	685	Unit/Enh (6490)	418	Unit/Enh (6490)	5	135	65	7	Positive
	NAD 13-C	No	683	Unit/Enh (6490)	555	Unit/Enh (6490)	5	40	12	7	Positive
	NADH	No	666	Unit/Enh (6490)	649	Unit/Enh (6490)	5	135	65	7	Positive
	NAD	No	664	Unit/Enh (6490)	136	Unit/Enh (6490)	5	100	42	7	Positive
	GSSG 13-C	No	631	Unit/Enh (6490)	316	Unit/Enh (6490)	5	40	34	7	Positive

Acquisition Method Report



Agilent

Trusted Answers

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	GSSG	No	613	Unit/Enh (6490)	231	Unit/Enh (6490)	5	40	34	7	Positive
	GTP 13-C	No	532	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	GTP	No	522	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	ATP 13-C	No	516	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	ATP	No	506	Unit/Enh (6490)	408	Unit/Enh (6490)	5	40	40	7	Positive
	ATP	No	506	Unit/Enh (6490)	159	Unit/Enh (6490)	5	135	108	7	Positive
	GDP 13-C	No	452	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	GDP 13-C	No	452	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	GDP	No	442	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	108	7	Positive
	ADP 13-C	No	436	Unit/Enh (6490)	139	Unit/Enh (6490)	5	135	108	7	Positive
	ADP 13-C	No	436	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	98	7	Positive
	ADP	No	426	Unit/Enh (6490)	134	Unit/Enh (6490)	5	135	108	7	Positive
	SAM	No	399	Unit/Enh (6490)	250	Unit/Enh (6490)	5	40	13	7	Positive
	SAH	No	385	Unit/Enh (6490)	136	Unit/Enh (6490)	5	40	19	7	Positive
	GMP 13-C	No	372	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	60	7	Positive
	GMP	No	364	Unit/Enh (6490)	152	Unit/Enh (6490)	5	40	18	7	Positive
	IMP 13-C	No	357	Unit/Enh (6490)	140	Unit/Enh (6490)	5	40	19	7	Positive
	AMP 13-C	No	356	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	60	7	Positive
	IMP	No	349	Unit/Enh (6490)	137	Unit/Enh (6490)	5	40	19	7	Positive
	AMP	No	348	Unit/Enh (6490)	136	Unit/Enh (6490)	5	40	21	7	Positive
	CMP 13-C	No	331	Unit/Enh (6490)	79	Unit/Enh (6490)	5	135	60	7	Positive
	UMP	No	325	Unit/Enh (6490)	113	Unit/Enh (6490)	5	40	21	7	Positive
	CMP	No	324	Unit/Enh (6490)	112	Unit/Enh (6490)	5	40	21	7	Positive
	GSH	No	308	Unit/Enh (6490)	162	Unit/Enh (6490)	5	40	17	7	Positive
	Tryptophan	No	205	Unit/Enh (6490)	146	Unit/Enh (6490)	5	40	16	7	Positive
	Tyrosine 13-C	No	191	Unit/Enh (6490)	144	Unit/Enh (6490)	5	40	11	7	Positive
	Tyrosine	No	182.2	Unit/Enh (6490)	136	Unit/Enh (6490)	5	40	14	7	Positive
	Arginine 13-C	No	181	Unit/Enh (6490)	61	Unit/Enh (6490)	5	40	14	7	Positive
	Arginine	No	175.2	Unit/Enh (6490)	60	Unit/Enh (6490)	5	40	14	7	Positive
	Phenylalanine 13-C	No	175	Unit/Enh (6490)	128	Unit/Enh (6490)	5	40	11	7	Positive
	Phenylalanine	No	166	Unit/Enh (6490)	120	Unit/Enh (6490)	5	40	25	7	Positive
	Histidine 13-C	No	162	Unit/Enh (6490)	98	Unit/Enh (6490)	5	40	11	7	Positive
	Histidine	No	156	Unit/Enh (6490)	110	Unit/Enh (6490)	5	30	12	7	Positive
	Methionine 13-C	No	155	Unit/Enh (6490)	108	Unit/Enh (6490)	5	40	11	7	Positive

Acquisition Method Report

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Lysine 13-C	No	153	Unit/Enh (6490)	89	Unit/Enh (6490)	5	40	11	7	Positive
	Glutamine 13-C	No	153	Unit/Enh (6490)	88	Unit/Enh (6490)	5	40	16	7	Positive
	Methionine	No	150	Unit/Enh (6490)	56	Unit/Enh (6490)	5	40	15	7	Positive
	Glutamate	No	148	Unit/Enh (6490)	84.1	Unit/Enh (6490)	5	40	16	7	Positive
	Glutamine	No	147	Unit/Enh (6490)	84.1	Unit/Enh (6490)	5	40	16	7	Positive
	Lysine	No	147	Unit/Enh (6490)	84.1	Unit/Enh (6490)	5	30	16	7	Positive
	Isoleucine 13-C	No	138	Unit/Enh (6490)	91	Unit/Enh (6490)	5	40	11	7	Positive
	Leucine 13-C	No	138	Unit/Enh (6490)	91	Unit/Enh (6490)	5	40	11	7	Positive
	Aspartate 13-C	No	137	Unit/Enh (6490)	76	Unit/Enh (6490)	5	40	15	7	Positive
	Leucine	No	136	Unit/Enh (6490)	89	Unit/Enh (6490)	5	40	11	7	Positive
	Asparagine 13-C	No	135	Unit/Enh (6490)	118	Unit/Enh (6490)	5	40	15	7	Positive
	Aspartate	No	134	Unit/Enh (6490)	74	Unit/Enh (6490)	5	40	15	7	Positive
	Asparagine	No	133.1	Unit/Enh (6490)	74	Unit/Enh (6490)	5	40	15	7	Positive
	d2_ND	No	127	Unit/Enh (6490)	84	Unit/Enh (6490)	5	100	20	7	Positive
	Cysteine 13-C	No	125	Unit/Enh (6490)	78	Unit/Enh (6490)	5	40	27	7	Positive
	Nicotinic acid	No	124	Unit/Enh (6490)	80	Unit/Enh (6490)	5	40	20	7	Positive
	Threonine 13-C	No	124	Unit/Enh (6490)	77	Unit/Enh (6490)	5	40	11	7	Positive
	Nicotinamide	No	123	Unit/Enh (6490)	80	Unit/Enh (6490)	5	40	20	7	Positive
	Valine 13-C	No	123	Unit/Enh (6490)	76	Unit/Enh (6490)	5	40	11	7	Positive
	Cysteine	No	122	Unit/Enh (6490)	59	Unit/Enh (6490)	5	40	27	7	Positive
	Threonine	No	120	Unit/Enh (6490)	56	Unit/Enh (6490)	5	40	30	7	Positive
	Valine	No	118	Unit/Enh (6490)	72	Unit/Enh (6490)	5	40	15	7	Positive
	Proline 13-C	No	118	Unit/Enh (6490)	70	Unit/Enh (6490)	5	40	11	7	Positive
	Proline	No	116	Unit/Enh (6490)	70	Unit/Enh (6490)	5	40	11	7	Positive
	Serine 13-C	No	109	Unit/Enh (6490)	91	Unit/Enh (6490)	5	40	11	7	Positive
	Serine	No	106	Unit/Enh (6490)	60	Unit/Enh (6490)	5	40	13	7	Positive
	Alanine 13-C	No	91	Unit/Enh (6490)	45	Unit/Enh (6490)	5	40	11	7	Positive
	Alanine	No	90	Unit/Enh (6490)	44	Unit/Enh (6490)	5	40	11	7	Positive
	Glycine 13-C	No	78	Unit/Enh (6490)	31	Unit/Enh (6490)	5	40	11	7	Positive
	Glycine	No	76	Unit/Enh (6490)	29	Unit/Enh (6490)	5	40	11	7	Positive
	glyoxylate 13-C	No	75	Unit/Enh (6490)	46	Unit/Enh (6490)	5	40	12	7	Positive
	glyoxylate	No	73	Unit/Enh (6490)	45	Unit/Enh (6490)	5	40	12	7	Positive
	Trehalose	No	341.3	Unit/Enh (6490)	179.3	Unit/Enh (6490)	5	40	17	7	Negative
	GSH 13-C	No	316	Unit/Enh (6490)	148	Unit/Enh (6490)	5	40	48	7	Negative

Acquisition Method Report



Agilent

Trusted Answers

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	S7P 13-C	No	296	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	20	7	Negative
	S7P	No	289	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	20	7	Negative
	6PG 13-C	No	281	Unit/Enh (6490)	97	Unit/Enh (6490)	5	100	12	7	Negative
	6PG	No	275	Unit/Enh (6490)	97	Unit/Enh (6490)	5	100	12	7	Negative
	F6P 13-C	No	265	Unit/Enh (6490)	97	Unit/Enh (6490)	5	100	10	7	Negative
	G6P 13-C	No	265	Unit/Enh (6490)	97	Unit/Enh (6490)	5	100	12	7	Negative
	Glucosamine 6-phosphate 13-C	No	264	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	63	7	Negative
	F6P	No	259	Unit/Enh (6490)	169	Unit/Enh (6490)	5	100	16	7	Negative
	G6P	No	259	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	20	7	Negative
	Glucosamine 6-phosphate	No	258	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	63	7	Negative
	R5P 13-C	No	234	Unit/Enh (6490)	97	Unit/Enh (6490)	5	90	6	7	Negative
	Xylulose-5-phosphate 13-C	No	234	Unit/Enh (6490)	97	Unit/Enh (6490)	5	70	4	7	Negative
	R5P	No	229	Unit/Enh (6490)	97	Unit/Enh (6490)	5	90	6	7	Negative
	Xylulose-5-phosphate	No	229	Unit/Enh (6490)	97	Unit/Enh (6490)	5	70	4	7	Negative
	isocitrate 13-C	No	197	Unit/Enh (6490)	179	Unit/Enh (6490)	5	90	6	5	Negative
	Citric acid 13-C	No	197	Unit/Enh (6490)	116	Unit/Enh (6490)	5	90	10	4	Negative
	Citrate 13-C	No	197	Unit/Enh (6490)	90	Unit/Enh (6490)	5	40	27	7	Negative
	Isocitric acid	No	191	Unit/Enh (6490)	155	Unit/Enh (6490)	5	40	10	5	Negative
	Citric acid	No	191	Unit/Enh (6490)	111	Unit/Enh (6490)	5	90	10	5	Negative
	Citric acid 2	No	191	Unit/Enh (6490)	87	Unit/Enh (6490)	5	40	18	5	Negative
	3PG 13-C	No	188	Unit/Enh (6490)	97	Unit/Enh (6490)	5	80	14	7	Negative
	3PG	No	185	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	20	7	Negative
	Glycerol 3-Phosphate 13-C	No	174	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Negative
	Glyceraldehyde 3-phosphate 13-C	No	172	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	25	7	Negative
	DHAP 13-C	No	172	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	15	7	Negative
	Glycerol 3-Phosphate	No	171	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	30	7	Negative
	Glyceraldehyde 3-phosphate	No	169	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	25	7	Negative
	G3P	No	169	Unit/Enh (6490)	97	Unit/Enh (6490)	5	40	20	7	Negative
	DHAP	No	169	Unit/Enh (6490)	79	Unit/Enh (6490)	5	40	15	7	Negative
	Glutamic acid 13-C	No	151	Unit/Enh (6490)	133	Unit/Enh (6490)	5	40	8	4	Negative
	alpha-ketoglutarate 13-C	No	150	Unit/Enh (6490)	105	Unit/Enh (6490)	5	40	17	7	Negative

Acquisition Method Report



Agilent

Trusted Answers

Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Glutamic acid	No	148	Unit/Enh (6490)	130	Unit/Enh (6490)	5	40	8	4	Negative
	Glutamic acid 2	No	148	Unit/Enh (6490)	84	Unit/Enh (6490)	5	40	12	4	Negative
	alpha-ketoglutarate	No	145	Unit/Enh (6490)	101	Unit/Enh (6490)	5	40	10	5	Negative
	alpha-ketoglutarate 2	No	145	Unit/Enh (6490)	57	Unit/Enh (6490)	5	40	10	5	Negative
	Apartate 13-C	No	136	Unit/Enh (6490)	91	Unit/Enh (6490)	5	40	20	7	Negative
	Oxaloacetate 13-C	No	135	Unit/Enh (6490)	90	Unit/Enh (6490)	5	40	12	7	Negative
	Malic acid	No	133	Unit/Enh (6490)	115	Unit/Enh (6490)	5	40	10	5	Negative
	Malate 13-C	No	133	Unit/Enh (6490)	115	Unit/Enh (6490)	5	80	7	5	Negative
	Malic acid 2	No	133	Unit/Enh (6490)	71	Unit/Enh (6490)	5	40	14	5	Negative
	Apartate	No	131.9	Unit/Enh (6490)	88.1	Unit/Enh (6490)	5	40	20	7	Negative
	Oxaloacetic acid	No	131	Unit/Enh (6490)	87	Unit/Enh (6490)	5	40	10	5	Negative
	Oxaloacetic acid 2	No	131	Unit/Enh (6490)	41	Unit/Enh (6490)	5	40	54	5	Negative
	Succinic acid 13-C	No	121	Unit/Enh (6490)	76	Unit/Enh (6490)	5	82	9	5	Negative
	fumaric acid 13-C	No	119	Unit/Enh (6490)	74	Unit/Enh (6490)	5	70	3	5	Negative
	Succinic acid	No	117	Unit/Enh (6490)	99	Unit/Enh (6490)	5	40	10	5	Negative
	Succinic acid 2	No	117	Unit/Enh (6490)	73	Unit/Enh (6490)	5	40	10	5	Negative
	Fumaric acid	No	115	Unit/Enh (6490)	71	Unit/Enh (6490)	5	40	10	5	Negative
	Fumaric acid 2	No	115	Unit/Enh (6490)	41	Unit/Enh (6490)	5	40	18	5	Negative
	Lactate 13-C	No	92	Unit/Enh (6490)	45	Unit/Enh (6490)	5	40	16	7	Negative
	Pyruvate 13-C	No	90	Unit/Enh (6490)	45	Unit/Enh (6490)	5	40	12	7	Negative
	Pyruvate 13-C	No	90	Unit/Enh (6490)	45	Unit/Enh (6490)	5	40	12	7	Negative
	Oxaloacetate	No	89	Unit/Enh (6490)	61	Unit/Enh (6490)	5	40	12	7	Negative
	Lactate	No	89	Unit/Enh (6490)	43	Unit/Enh (6490)	5	40	16	7	Negative
	Lactic acid	No	89	Unit/Enh (6490)	43	Unit/Enh (6490)	5	40	10	4	Negative
	Pyruvate	No	86.8	Unit/Enh (6490)	42.8	Unit/Enh (6490)	5	40	12	7	Negative

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	350	350
Gas Flow (l/min)	10	10
Nebulizer (psi)	35	35
Capillary (V)	4000	4000

Scan Parameters

Data Stg	Threshold
Centroid	0

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	TIC	0	10000000



Instrument Curves

Actual

Name: Sampler

Module: G7129B

Auxiliary

Draw Speed	100 µL/min
Eject Speed	400 µL/min
Wait Time After Draw	1.2 s
Needle Height Offset	0.0 mm

Injection

Injection Mode	Injection with needle wash
Injection Volume	5.00 µL

Needle Wash

Needle Wash Location	Flush Port
Wash Time	3 s

High throughput

Sample Flush-Out Factor	5.0
Injection Valve to Bypass for Delay Volume Reduction	No

Overlapped Injection

Overlapped Injection Mode	Off
---------------------------	-----

Stop Time

Stoptime Mode	As pump/No limit
---------------	------------------

Post Time

Posttime Mode	Off
---------------	-----

Name: Binary Pump

Module: G7120A

Flow	1.000 mL/min
Use Solvent Types	No
Stroke Mode	Synchronized
Low Pressure Limit	0.00 bar
High Pressure Limit	400.00 bar
Max. Flow Ramp Up	100.000 mL/min ²
Max. Flow Ramp Down	100.000 mL/min ²
Expected Mixer	No check

Stroke A

Automatic Stroke Calculation A	Yes
--------------------------------	-----

Compress A

Compressibility Mode A	Compressibility Value Set
Compressibility A	50 10e-6/bar

Compress B

Compressibility Mode B	Compressibility Value Set
Compressibility B	115 10e-6/bar

Stop Time

Stoptime Mode	Time set
Stoptime	40.00 min

Post Time

Posttime Mode	Off
---------------	-----

Solvent Composition

	Channel	Name 1	Name 2	Selected	Used	Percent (%)
1	A	100 Water		Ch. 1	Yes	100.00 %
2	B	100 ACN		Ch. 1	Yes	0.00 %

Timetable

	Time (min)	A (%)	B (%)	Flow (mL/min)
1	5.00 min	100.00 %	0.00 %	1.000 mL/min



	Pressure (bar)
1	400.00 bar

Acquisition Method Report



Agilent

Trusted Answers

	Time (min)	A (%)	B (%)	Flow (mL/min)
2	25.00 min	95.00 %	5.00 %	1.000 mL/min
3	30.00 min	0.00 %	100.00 %	1.000 mL/min
4	40.00 min	0.00 %	100.00 %	1.000 mL/min
5	45.00 min	100.00 %	0.00 %	1.000 mL/min
6	50.00 min	100.00 %	0.00 %	1.000 mL/min

Name: Column Oven

Module: G7130A

Temperature Control

Temperature Control Mode	Temperature Set
Temperature	25.0 °C
Temperature Not Ready Limit	
Temperature Not Ready Limit On	Yes
Temperature Not Ready Limit Value	0.8 °C
Temperature Equilibration Time	0.0 min

Enforce column for run

Enforce column for run enabled	No
--------------------------------	----

Stop Time

Stoptime Mode	As pump/injector
---------------	------------------

Post Time

Posttime Mode	Off
---------------	-----

Timetable



	Pressure (bar)
2	400.00 bar
3	400.00 bar
4	400.00 bar
5	400.00 bar
6	400.00 bar