

Supplementary Table S3: List of multiple reaction monitoring (MRM) for all the identified metabolites and LC-MS parameters in positive mode

Elevated Dimethylarginine, ATP, cytokines, metabolic remodeling involving tryptophan metabolism and potential microglial inflammation characterize Primary Open Angle Glaucoma

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MRM
details

Compound Name	ISTD	Precursor ion	Product ion	Dwell	Frag(V)	CE(V)	Cell	Polarity
(L)-arginino-succinate	No	291.1299	70	3	380	37	2	Positive
1-Methyl-Histidine	No	170.0924	124	3	380	20	2	Positive
2-Aminobutyraldehyde	No	88.0757	70.1	3	380	9	2	Positive
2-Aminoheptanoic acid	No	146.1176	100.1	3	380	5	2	Positive
2-Aminooctanoic acid	No	160.1332	55.3	3	380	21	2	Positive
2-Hydroxypyridine	No	96.0444	78.1	3	380	17	2	Positive
2-Methyl glutamic acid	No	162.0761	116.1	3	380	9	2	Positive
2-Methylbutyroylcarnitine	No	246.17	187	3	380	15	2	Positive
3-Hydroxykynurenine	No	225.087	162.1	3	380	17	2	Positive
3-PHOSPHOGLYCERATE	No	187	141	3	380	15	2	Positive
3-phospho-serine	No	186.0162	88	3	380	12	2	Positive
4 Acetamidobutanoic acid	No	146.08	86.1	3	380	9	2	Positive
4 Hydroxybutyric acid	No	105.0546	45	3	380	5	2	Positive
4-Coumarate	No	165.0446	119	3	380	10	2	Positive
4-Methyl-2-oxo pentanoic acid	No	131.0703	71	3	380	10	2	Positive
5-Hydroxyindoleacetic acid	No	192.0655	146	3	380	10	2	Positive
5-oxo-proline	No	130.0499	84	3	380	10	2	Positive
7-methylguanosine	No	299.1224	166	3	380	24	2	Positive
Acetyl Carnitine	No	204.123	85	3	380	17	2	Positive
Acetylcholine	No	146.1176	43.02	3	380	10	2	Positive
Adenine	No	136.6	119	3	380	10	5	Positive
Allo-Threonine	No	120.0655	74.1	3	380	5	2	Positive
Aminobutyric acid	No	104.0706	44.1	3	380	9	2	Positive
Arginine	No	175.119	70.1	3	380	25	2	Positive
Asparagine	No	133.0608	87.1	3	380	9	2	Positive
Asparanine-15N2	yes	135	117	3	380	15	2	Positive
Aspartame	No	295.1288	180.1	3	380	5	2	Positive
ASP-PH	No	281.1132	120.1	3	380	10	2	Positive
Betaine	No	118.0863	59.2	3	380	17	2	Positive
betaine aldehyde	No	103.0992	58	3	380	21	2	Positive
Carnitine	No	162.1125	60.1	3	380	12	2	Positive

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Choline	No	105.1148	45	3	380	21	2	Positive
citrulline	No	176.103	159	3	380	5	2	Positive
Creatinine	No	114.0662	44	3	380	17	2	Positive
Cystathionine	No	223.0747	134.1	3	380	8	2	Positive
Cysteine 15N	Yes	123	95	3	380	10	2	Positive
Cystine	No	241.03	152	3	380	9	2	Positive
Cytosine	No	112.1	95.1	3	380	17	5	Positive
Deoxy carnitine	No	146.1176	60.1	3	380	13	2	Positive
Dimethyl Arginine	No	203.1503	70.1	3	380	29	2	Positive
DL-Pipecolic acid	No	130.0863	84	3	380	18	2	Positive
Ergothioneine	No	230.0958	60.0573	3	380	12	2	Positive
Erythrono-1,4-lactone	No	119.11	91.1	3	380	10	2	Positive
Ethylmalonate/Methyl Malonate	No	133.0495	115.04	3	380	10	2	Positive
Glucosamine/Galactosamine	No	180.0866	162	3	380	5	2	Positive
Glu-Glu	No	277.103	84.04	3	380	10	2	Positive
Glutamic acid	No	148.0604	84	3	380	17	2	Positive
Glutamine	No	147.0764	130.1	3	380	5	2	Positive
Glutamyl alanine	No	219.0975	84.1	3	380	21	2	Positive
Glu-Tyr	No	311.1238	293.1	3	380	10	2	Positive
Glycerol 3-phosphate	No	173.02	132	3	380	5	2	Positive
Glycine	No	76.0393	30.5	3	380	33	2	Positive
Gly-Gly	No	133.0608	30	3	380	20	2	Positive
Gly-Leu	No	189.1234	130	3	380	10	2	Positive
Guanidine acetic acid	No	118.0611	43.1	3	380	40	2	Positive
Heptanoyl Carnitine	No	260.2	201.2	3	380	9	2	Positive
Histamine	No	112.0869	95.1	3	380	13	2	Positive
Histidine	No	156.0768	110.1	3	380	9	2	Positive
Homoserine	No	120.0655	74.1	3	380	9	2	Positive
Hydroxyglutaric acid	No	132	45	3	380	30	2	Positive
Hypoxanthine	No	137	119	3	380	21	2	Positive
Isobutyryl Carnitine	No	232.1543	85	3	380	21	2	Positive
Isoleucine	No	132.1019	86.1	3	380	9	2	Positive
Isovaleryl Carnitine	No	246.2	85	3	380	17	2	Positive

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Kynurenic acid	No	190.0499	144.1	3	380	16	2	Positive
Kynurenine	No	209.0921	192	3	380	5	2	Positive
Lactic acid	No	91.04	73	3	380	15	2	Positive
L-anthranilic acid	Yes	139	121	3	380	12	2	Positive
L-Arginine	Yes	177.1	159.1	3	380	10	5	Positive
L-Creatinine	Yes	115.1	45.1	3	380	10	2	Positive
L-Jasmonic acid	No	211.1	133.1	3	380	10	2	Positive
L-Tryptophan	Yes	207.1	189	3	380	10	5	Positive
Lysine	No	147.1128	130.2	3	380	5	2	Positive
L-Zeatine	Yes	220	136	3	380	15	5	Positive
Methyl Adenosine	No	282.1	150	3	380	13	2	Positive
Methylglutaric acid	No	147.0652	55.05423	3	380	10	2	Positive
Myo-Inositol	No	181.07	139.9	3	380	5	2	Positive
MYRISTATE (14:0)+Na	No	250	173	3	380	21	2	Positive
Myristoleic acid	No	227.2006	43.1	3	380	25	2	Positive
N, N Dimethyl Glycine	No	104.0706	44	3	380	48	2	Positive
N,N Dimethyl Glycine/Methyl alanine	No	104.0706	58.1	3	380	9	2	Positive
N-acetyl Glucosamine 6 Phos	No	302.0635	284.1	3	380	5	2	Positive
N-Acetyl Lysine	No	189.1234	84.1	3	380	24	2	Positive
N-Acetyl Methionine	No	192	104.1	3	380	9	2	Positive
N-acetylalanine	No	132.0655	44.1	3	380	20	2	Positive
N-acetyl-glutamine	No	189.087	130	3	380	17	2	Positive
N-Acetylneuraminic acid	No	310.1	121	3	380	21	2	Positive
N-Acetylorithine	No	175.1077	70.1	3	380	29	2	Positive
N-Acetylputrescine	No	131.1179	114	3	380	12	2	Positive
Nicotinamide	No	123.0553	80.1	3	380	20	2	Positive
Nonadecanoic acid	No	298.2866	281.4	3	380	10	2	Positive
Octonyl Carnitine	No	288.2	85	3	380	21	2	Positive
Oleic acid	No	283.27	89.2	3	380	13	2	Positive
Phe-Glu	No	295.12889	136.07	3	380	20	2	Positive
Phenyl alanine	No	166.0963	120.1	3	380	13	2	Positive
Proline	No	116.0706	70.1	3	380	17	2	Positive
Propeonyl Carnitine	No	218.1387	85	3	380	17	2	Positive

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purine	No	121.0509	94	3	380	25	2	Positive
Putrescine	No	89.1073	72.1	3	380	8	2	Positive
Pyroglu-Va	No	229.1183	183.11	3	380	10	2	Positive
Quinic acid	No	193.0707	111.04	3	380	10	2	Positive
Sarcosine/Alanine	No	90.055	44.1	3	380	20	2	Positive
Serine	No	106.0499	60.1	3	380	9	2	Positive
Spermidine	No	146.1652	72.1	3	380	17	2	Positive
Tyrosine	No	182.0812	136.1	3	380	9	2	Positive
Uracil	No	113	72	3	380	4	2	Positive
Urea	No	61.0396	44	3	380	10	2	Positive
Valine	No	118.0863	72.2	3	380	9	2	Positive
Xanthine	No	153.04	110	3	380	21	2	Positive

Source Parameters		
Parameter	Value (+)	Value (-)
Gas Temp (°C)	250	250
Gas Flow (l/min)	14	14
Nebulizer (psi)	20	20
SheathGasHeater	350	350
SheathGasFlow	12	12
Capillary (V)	3000	3000
VCharging	1000	1000
Ion Funnel Parameters		
Pos High Pressure RF	150	
Pos Low Pressure RF	60	
Neg High Pressure RF	150	
Neg Low Pressure RF	60	
Auxiliary		
Draw Speed	100.0 µL/min	
Eject Speed	100.0 µL/min	
Draw Position Offset	0.0 mm	
Wait Time After Drawing	2.0 s	
Sample Flush Out Factor	5.0	

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Vial/Well bottom sensing	Yes
Injection	
Injection Mode	Injection with needlewash
Injection Volume	2.00 µL
Needle Wash	
Needle Wash Location	Flush Port
Wash Time	10.0 s
Flow	0.300 mL/min
Use Solvent Types	Yes
Stroke Mode	Synchronized
Low Pressure Limit	0.00 bar
High Pressure Limit	600.00 bar
Max. Flow Ramp Up	100.000 mL/min ²
Max. Flow Ramp Down	100.000 mL/min ²
Expected Mixer	No check
Stop Time	
Stoptime Mode	Time set
Stoptime	23.00 min
Post time mode	Time set
Post time	5.00min

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Timetable

	Time	Function	Parameter			
1	3.00 min	Change Solvent Composition	Solvent Composition A:70.00%B:30.00 %			
2	3.00 min	ChangeFlow	Flow: 0.3 mL/min			
3	12.00 min	Change Solvent Composition	Solvent Composition A:98.00%B:2.00 %			
4	12.00 min	ChangeFlow	Flow: 0.3 mL/min			
5	15.00 min	Change Solvent Composition	Solvent Composition A:98.00%B:2.00 %			
6	15.00 min	ChangeFlow	Flow: 0.3 mL/min			
7	16.00 min	Change Solvent Composition	Solvent Composition A:15.00%B:85.00 %			
8	16.00 min	ChangeFlow	Flow: 0.3 mL/min			
9	23.00 min	Change Solvent Composition	Solvent Composition A:15.00%B:85.00 %			
10	23.00 min	ChangeFlow	Flow: 0.3 mL/min			
Solvent Composition						
	Channel	Ch.1 Solv.	Name 1	Ch2Solv.	Name 2	Percent
1	A	100.0 %Water	0.1FA	100.0 %Water		15.00%
2	B	100.0 %Acetonitrile	100 %CAN	100.0%Ac	0.1FA	85.00%