

Acquisition Method Info

Method Name Metabolomics_7-8-20_H.m

 Method Path
 D:\MassHunter\methods\Thomas\Metabolomics_7-8-20_H.m

Method Description ESI Positive MRM Reserpine Checkout Method

Device List

Sampler

Binary Pump

Column Oven

QQQ

MS QQQ Mass Spectrometer

Ion Source AJS 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 Scan Type Ion Mode Div Valve Delta EMV (+) Delta EMV (-) Store (min)

1 0 MRM ESI+Agilent To MS 300 300 Yes Jet Stream

Time Segment 1

Scan Segments

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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)	10	40	30	7	Positive
	Malonyl-Coa 13-C	No	877	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Positive
	Succinyl-Coa	No	866	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Positive
	Malonyl-Coa	No	853	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Positive
	Acetyl-Coa 13-C	No	812	Unit/Enh (6490)	303	Unit/Enh (6490)	10	40	30	7	Positive
	FAD 13-C	No	811	Unit/Enh (6490)	454	Unit/Enh (6490)	10	100	42	7	Positive
	Acetyl-Coa	No	810	Unit/Enh (6490)	303	Unit/Enh (6490)	10	40	30	7	Positive
	FAD	No	784	Unit/Enh (6490)	437	Unit/Enh (6490)	10	100	42	7	Positive
	NADPH B	No	775	Unit/Enh (6490)	243	Unit/Enh (6490)	10	30	50	7	Positive
	NADPH	No	775	Unit/Enh (6490)	227	Unit/Enh (6490)	10	30	50	7	Positive
	NADP 13-C	No	765	Unit/Enh (6490)	141	Unit/Enh (6490)	10	135	58	7	Positive
	NADP 13-C	No	763	Unit/Enh (6490)	635	Unit/Enh (6490)	10	135	30	7	Positive
	NADPH	No	744	Unit/Enh (6490)	136	Unit/Enh (6490)	10	135	58	7	Positive
	NADP	No	744	Unit/Enh (6490)	136	Unit/Enh (6490)	10	100	42	7	Positive
	NAD 13-C	No	687	Unit/Enh (6490)	670	Unit/Enh (6490)	10	135	65	7	Positive
	NADH 13-C	No	685	Unit/Enh (6490)	418	Unit/Enh (6490)	10	135	65	7	Positive
	NAD 13-C	No	683	Unit/Enh (6490)	555	Unit/Enh (6490)	10	40	12	7	Positive
	NADH	No	666	Unit/Enh (6490)	649	Unit/Enh (6490)	10	135	65	7	Positive



Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	NAD	No	664	Unit/Enh (6490)	136	Unit/Enh (6490)	10	100	42	7	Positive
	GSSG 13-C	No	631	Unit/Enh (6490)	316	Unit/Enh (6490)	10	40	34	7	Positive
	GSSG	No	613	Unit/Enh (6490)	231	Unit/Enh (6490)	10	40	34	7	Positive
	SAM	No	399	Unit/Enh (6490)	250	Unit/Enh (6490)	10	40	13	7	Positive
	SAH	No	385	Unit/Enh (6490)	136	Unit/Enh (6490)	10	40	19	7	Positive
	GMP	No	364	Unit/Enh (6490)	152	Unit/Enh (6490)	10	40	18	7	Positive
	IMP	No	349	Unit/Enh (6490)	137	Unit/Enh (6490)	10	40	19	7	Positive
	AMP	No	348	Unit/Enh (6490)	136	Unit/Enh (6490)	10	40	21	7	Positive
	UMP	No	325	Unit/Enh (6490)	113	Unit/Enh (6490)	10	40	21	7	Positive
	CMP	No	324	Unit/Enh (6490)	112	Unit/Enh (6490)	10	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)	145.8	Unit/Enh (6490)	10	40	16	7	Positive
	Tyrosine 13- C	No	191	Unit/Enh (6490)	144	Unit/Enh (6490)	10	40	11	7	Positive
	Tyrosine	No	182.2	Unit/Enh (6490)	136	Unit/Enh (6490)	10	40	14	7	Positive
	Tyrosine	No	182.2	Unit/Enh (6490)	91	Unit/Enh (6490)	10	40	19	7	Positive
	Arginine 13- C	No	181	Unit/Enh (6490)	61	Unit/Enh (6490)	10	40	14	7	Positive
	Arginine 13- C	No	177	Unit/Enh (6490)	61	Unit/Enh (6490)	10	40	14	7	Positive
	Arginine 13- C	No	176	Unit/Enh (6490)	61	Unit/Enh (6490)	10	40	14	7	Positive
	Arginine 13- C	No	176	Unit/Enh (6490)	60	Unit/Enh (6490)	10	40	14	7	Positive
	Arginine	No	175.2	Unit/Enh (6490)	60	Unit/Enh (6490)	10	40	14	7	Positive
	Phenylalanin e 13-C	No	175	Unit/Enh (6490)	128	Unit/Enh (6490)	10	40	11	7	Positive
	Phenylalanin e	No	166	Unit/Enh (6490)	120	Unit/Enh (6490)	10	40	25	7	Positive
	Histidine 13- C	No	162	Unit/Enh (6490)	98	Unit/Enh (6490)	10	40	11	7	Positive
	Histidine	No	156	Unit/Enh (6490)	110	Unit/Enh (6490)	10	30	12	7	Positive
	Methionine 13-C	No	155	Unit/Enh (6490)	108	Unit/Enh (6490)	10	40	11	7	Positive
	Glutamine 13 -C	No	153	Unit/Enh (6490)	88	Unit/Enh (6490)	10	40	16	7	Positive
	Methionine	No	150	Unit/Enh (6490)	56	Unit/Enh (6490)	10	40	15	7	Positive
	Lysine 13-C	No	149	Unit/Enh (6490)	86	Unit/Enh (6490)	10	40	11	7	Positive
	Lysine 13-C	No	149	Unit/Enh (6490)	85	Unit/Enh (6490)	10	40	11	7	Positive
	Lysine 13-C	No	148	Unit/Enh (6490)	86	Unit/Enh (6490)	10	40	11	7	Positive
	Lysine 13-C	No	148	Unit/Enh (6490)	85	Unit/Enh (6490)	10	40	11	7	Positive
	Glutamic acid	No	148	Unit/Enh (6490)	84.1	Unit/Enh (6490)	10	40	23	7	Positive
	Lysine	No	147	Unit/Enh (6490)	84.1	Unit/Enh (6490)	10	30	16	7	Positive
	Glutamine	No	147	Unit/Enh (6490)	84	Unit/Enh (6490)	10	40	16	7	Positive



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Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Isoleucine 13 -C	No	138	Unit/Enh (6490)	91	Unit/Enh (6490)	10	40	11	7	Positive
	Leucine 13-C	No	138	Unit/Enh (6490)	91	Unit/Enh (6490)	10	40	11	7	Positive
	Leucine	No	136	Unit/Enh (6490)	89	Unit/Enh (6490)	10	40	11	7	Positive
	Aspartate 13-	No	136	Unit/Enh (6490)	76	Unit/Enh (6490)	10	40	15	7	Positive
	Asparagine 13-C	No	135	Unit/Enh (6490)	118	Unit/Enh (6490)	10	40	15	7	Positive
	Asparagine 13-C	No	135	Unit/Enh (6490)	75	Unit/Enh (6490)	10	40	15	7	Positive
	Aspartate 13- C	No	134	Unit/Enh (6490)	75	Unit/Enh (6490)	10	40	15	7	Positive
	Aspartate	No	134	Unit/Enh (6490)	74	Unit/Enh (6490)	10	40	15	7	Positive
	Asparagine	No	133.1	Unit/Enh (6490)	74	Unit/Enh (6490)	10	40	15	7	Positive
	d2_ND	No	127	Unit/Enh (6490)	84	Unit/Enh (6490)	10	100	20	7	Positive
	Cysteine 13- C	No	125	Unit/Enh (6490)	78	Unit/Enh (6490)	10	40	27	7	Positive
	Nicotinic acid	No	124	Unit/Enh (6490)	80	Unit/Enh (6490)	10	40	20	7	Positive
	Threonine 13 -C	No	124	Unit/Enh (6490)	77	Unit/Enh (6490)	10	40	11	7	Positive
	Nicotinamide	No	123	Unit/Enh (6490)	80	Unit/Enh (6490)	10	40	20	7	Positive
	Valine 13-C	No	123	Unit/Enh (6490)	76	Unit/Enh (6490)	10	40	11	7	Positive
	Cysteine	No	122	Unit/Enh (6490)	59	Unit/Enh (6490)	10	40	27	7	Positive
	Threonine	No	120	Unit/Enh (6490)	56	Unit/Enh (6490)	10	40	30	7	Positive
	Valine	No	118	Unit/Enh (6490)	72	Unit/Enh (6490)	10	40	15	7	Positive
	Proline 13-C	No	118	Unit/Enh (6490)	70	Unit/Enh (6490)	10	40	11	7	Positive
	Proline	No	116	Unit/Enh (6490)	70	Unit/Enh (6490)	10	40	11	7	Positive
	Serine 13-C	No	109	Unit/Enh (6490)	91	Unit/Enh (6490)	10	40	11	7	Positive
	Serine 13-C	No	108	Unit/Enh (6490)	90	Unit/Enh (6490)	10	40	11	7	Positive
	Serine 13-C	No	107	Unit/Enh (6490)	89	Unit/Enh (6490)	10	40	11	7	Positive
	Serine 13-C	No	106	Unit/Enh (6490)	88	Unit/Enh (6490)	10	40	11	7	Positive
	Serine	No	106	Unit/Enh (6490)	60	Unit/Enh (6490)	10	40	13	7	Positive
	Alanine 13-C	No	92	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	11	7	Positive
	Alanine 13-C	No	91	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	11	7	Positive
	Alanine	No	90	Unit/Enh (6490)	44	Unit/Enh (6490)	10	40	11	7	Positive
	Glycine 13-C	No	78	Unit/Enh (6490)	31	Unit/Enh (6490)	10	40	11	7	Positive
	Glycine	No	76	Unit/Enh (6490)	29	Unit/Enh (6490)	10	40	11	7	Positive
	glyoxylate 13- C	No	75	Unit/Enh (6490)	46	Unit/Enh (6490)	10	40	12	7	Positive
	glyoxylate	No	73	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	12	7	Positive
	GTP 13-C	No	532	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	108	7	Negative
	GTP	No	522	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	108	7	Negative



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Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	ATP 13-C	No	516	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	108	7	Negative
	ATP	No	506	Unit/Enh (6490)	408	Unit/Enh (6490)	10	40	40	7	Negative
	ATP	No	506	Unit/Enh (6490)	159	Unit/Enh (6490)	10	135	108	7	Negative
	GDP 13-C	No	452	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	108	7	Negative
	GDP	No	442	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	108	7	Negative
	ADP 13-C	No	436	Unit/Enh (6490)	139	Unit/Enh (6490)	10	135	108	7	Negative
	ADP 13-C	No	436	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	98	7	Negative
	ADP	No	426	Unit/Enh (6490)	134	Unit/Enh (6490)	10	135	108	7	Negative
	GMP 13-C	No	372	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	60	7	Negative
	GMP	No	362	Unit/Enh (6490)	79	Unit/Enh (6490)	10	100	60	7	Negative
	IMP 13-C	No	357	Unit/Enh (6490)	140	Unit/Enh (6490)	10	40	19	7	Negative
	AMP 13-C	No	356	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	60	7	Negative
	IMP	No	347	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	30	7	Negative
	AMP	No	346	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	21	7	Negative
	Trehalose	No	341.3	Unit/Enh (6490)	179.3	Unit/Enh (6490)	10	40	17	7	Negative
	UMP 13-C	No	332	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Negative
	CMP 13-C	No	331	Unit/Enh (6490)	79	Unit/Enh (6490)	10	135	60	7	Negative
	UMP	No	323	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Negative
	GSH 13-C	No	316	Unit/Enh (6490)	148	Unit/Enh (6490)	5	40	48	7	Negative
	S7P 13-C	No	296	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	20	7	Negative
	S7P	No	289	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	20	7	Negative
	6PG 13-C	No	281	Unit/Enh (6490)	97	Unit/Enh (6490)	10	100	12	7	Negative
	6PG	No	275	Unit/Enh (6490)	97	Unit/Enh (6490)	10	100	12	7	Negative
	G6P 13-C	No	265	Unit/Enh (6490)	203	Unit/Enh (6490)	10	100	12	7	Negative
	F6P 13-C	No	265	Unit/Enh (6490)	97	Unit/Enh (6490)	10	100	10	7	Negative
	G6P 13-C	No	265	Unit/Enh (6490)	97	Unit/Enh (6490)	10	100	12	7	Negative
	Glucosamine 6-phosphate 13-C	No	264	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	63	7	Negative
	G6P	No	259	Unit/Enh (6490)	199	Unit/Enh (6490)	10	40	20	7	Negative
	F6P	No	259	Unit/Enh (6490)	169	Unit/Enh (6490)	10	100	16	7	Negative
	G6P	No	259	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	20	7	Negative
	F6P	No	259	Unit/Enh (6490)	97	Unit/Enh (6490)	10	100	12	7	Negative
	Glucosamine 6-phosphate	No	258	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	63	7	Negative
	R5P 13-C	No	234	Unit/Enh (6490)	97	Unit/Enh (6490)	10	90	6	7	Negative



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Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Xylulose-5- phosphate 13 -C	No	234	Unit/Enh (6490)	97	Unit/Enh (6490)	10	70	4	7	Negative
	R5P	No	229	Unit/Enh (6490)	97	Unit/Enh (6490)	10	90	6	7	Negative
	Xylulose-5- phosphate	No	229	Unit/Enh (6490)	97	Unit/Enh (6490)	10	70	4	7	Negative
	isocitrate 13- C	No	197	Unit/Enh (6490)	179	Unit/Enh (6490)	10	90	6	5	Negative
	Citric acid 13 -C	No	197	Unit/Enh (6490)	116	Unit/Enh (6490)	10	90	10	4	Negative
	Citric acid 13 -C	No	197	Unit/Enh (6490)	90	Unit/Enh (6490)	10	40	27	7	Negative
	Isocitric acid	No	191	Unit/Enh (6490)	155	Unit/Enh (6490)	10	40	10	5	Negative
	Citric acid	No	191	Unit/Enh (6490)	111	Unit/Enh (6490)	10	90	10	5	Negative
	Citric acid	No	191	Unit/Enh (6490)	87	Unit/Enh (6490)	10	40	18	5	Negative
	3PG 13-C	No	188	Unit/Enh (6490)	97	Unit/Enh (6490)	10	80	14	7	Negative
	3PG	No	185	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	20	7	Negative
	Glycerol 3- Phosphate 13-C	No	174	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Negative
	Glyceraldehy de 3- phosphate 13 -C		172	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	25	7	Negative
	DHAP 13-C	No	172	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	15	7	Negative
	Glycerol 3- Phosphate	No	171	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	30	7	Negative
	Glyceraldehy de 3- phosphate	No	169	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	25	7	Negative
	G3P	No	169	Unit/Enh (6490)	97	Unit/Enh (6490)	10	40	20	7	Negative
	DHAP	No	169	Unit/Enh (6490)	79	Unit/Enh (6490)	10	40	15	7	Negative
	Glutamic acid 13-C	No	151	Unit/Enh (6490)	133	Unit/Enh (6490)	10	40	8	4	Negative
	alpha- ketoglutarate 13-C	No	150	Unit/Enh (6490)	105	Unit/Enh (6490)	10	40	17	7	Negative
	alpha- ketoglutarate	No	145	Unit/Enh (6490)	101	Unit/Enh (6490)	10	40	10	5	Negative
	alpha- ketoglutrate	No	145	Unit/Enh (6490)	57	Unit/Enh (6490)	10	40	10	5	Negative
	Malate 13-C	No	137	Unit/Enh (6490)	119	Unit/Enh (6490)	10	40	10	5	Negative
	Oxaloacetate 13-C	No	135	Unit/Enh (6490)	90	Unit/Enh (6490)	10	40	12	7	Negative
	Malic acid	No	133	Unit/Enh (6490)	115	Unit/Enh (6490)	10	40	10	5	Negative
	Malic acid 2	No	133	Unit/Enh (6490)	71	Unit/Enh (6490)	10	40	14	5	Negative
	Oxaloacetic acid	No	131	Unit/Enh (6490)	87	Unit/Enh (6490)	10	40	10	5	Negative
	Oxaloacetic acid 2	No	131	Unit/Enh (6490)	41	Unit/Enh (6490)	10	40	54	5	Negative
	Succinic acid 13-C	No	121	Unit/Enh (6490)	103	Unit/Enh (6490)	10	82	10	5	Negative
	Fumaric acid 13-C	No	119	Unit/Enh (6490)	74	Unit/Enh (6490)	10	70	3	5	Negative
	Succinic acid	No	117	Unit/Enh (6490)	99	Unit/Enh (6490)	10	40	10	5	Negative
	Succinic acid	No	117	Unit/Enh (6490)	73	Unit/Enh (6490)	10	40	10	5	Negative
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Cpd Group	Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
	Fumaric acid	No	115	Unit/Enh (6490)	71	Unit/Enh (6490)	10	40	10	5	Negative
	Fumaric acid	No	115	Unit/Enh (6490)	41	Unit/Enh (6490)	10	40	18	5	Negative
	Serine 13-C	No	107	Unit/Enh (6490)	76	Unit/Enh (6490)	10	40	16	7	Negative
	Serine	No	104	Unit/Enh (6490)	74	Unit/Enh (6490)	10	40	16	7	Negative
	Lactate 13-C	No	92	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	16	7	Negative
	Pyruvate 13- C	No	90	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	12	7	Negative
	Pyruvate 13- C	No	90	Unit/Enh (6490)	45	Unit/Enh (6490)	10	40	12	7	Negative
	Oxaloacetate	No	89	Unit/Enh (6490)	61	Unit/Enh (6490)	10	40	12	7	Negative
	Lactate	No	89	Unit/Enh (6490)	43	Unit/Enh (6490)	10	40	16	7	Negative
	Pyruvate	No	86.8	Unit/Enh (6490)	42.8	Unit/Enh (6490)	10	40	12	7	Negative

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	350	350
Gas Flow (I/min)	9	9
Nebulizer (psi)	45	45
SheathGasHeater	300	300
SheathGasFlow	11	11
Capillary (V)	4000	4000
VCharging	500	500

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

Injection

Injection Mode Injection with needle wash

Injection Volume 5.00 µL

Needle Wash

Needle Wash LocationFlush PortWash Time3 s

High throughput

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

Overlapped Injection

Off



Overlapped Injection Mode

Stop Time

Stoptime Mode As pump/No limit

Post Time

Posttime Mode Off

Name: Binary Pump Module: G7120A

Flow 0.350 mL/min

Use Solvent Types No

Stroke ModeSynchronizedLow Pressure Limit0.00 barHigh Pressure Limit400.00 barMax. Flow Ramp Up100.000 mL/min²Max. Flow Ramp Down100.000 mL/min²

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 ModeTime setStoptime50.00 min

Post Time

Posttime Mode Off

Solvent Composition

	Channel	Name 1	Name 2	Selected	Used	Percent (%)
1	Α	100 Water		Ch. 1	Yes	15.00 %
2	В	100 ACN		Ch. 1	Yes	85.00 %

Timetable

	Time (min)	A (%)	B (%)	Flow (mL/min)
1	5.00 min	70.00 %	30.00 %	0.350 mL/min
2	25.00 min	98.00 %	2.00 %	0.350 mL/min
3	30.00 min	98.00 %	2.00 %	0.350 mL/min
4	50.00 min	15.00 %	85.00 %	0.350 mL/min
5	60.00 min	15.00 %	85.00 %	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 OnYesTemperature Not Ready Limit Value0.8 °CTemperature Equilibration Time0.0 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)
1	400.00 bar
2	400.00 bar
3	400.00 bar
4	400.00 bar
5	400.00 bar